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Watershed Modelling of the Mindanao River Basin in the Philippines Using the SWAT for Water Resource Management

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Abstract

This study aims to simulate the watershed of the Mindanao River Basin (MRB) to enhance water resource management for potential hydropower applications to meet the power demand in Mindanao with an average growth of 3.8% annually. The soil and water assessment tool (SWAT) model was used with inputs for geospatial datasets and weather records at four meteorological stations from DOST-PAGASA. To overcome the lack of precipitation data in the MRB, the precipitation records were investigated by comparing the records with the global gridded precipitation datasets from the NCDC-CPC and the GPCC. Then, the SWAT simulated discharges with the three precipitation data were calibrated with river discharge records at three stations in the Nituan, Libungan and Pulangi rivers. Due to limited records for the river discharges, the model results were then validated using the proxy basin principle along the same rivers in the Nituan, Libungan, and Pulangi areas. The $R^2$ values from the validation are 0.61, 0.50 and 0.33, respectively, with the DOST-PAGASA precipitation; 0.64, 0.46 and 0.40, respectively, with the NCDC-CPC precipitation; and 0.57, 0.48 and 0.21, respectively, with the GPCC precipitation. The relatively low model performances in Libungan and Pulangi rivers are mainly due to the lack of datasets on the dam and water withdrawal in the MRB. Therefore, this study also addresses the issue of data quality for precipitation and data scarcity for river discharge, dam, and water withdrawal for water resource management in the MRB and show how to overcome the data quality and scarcity.

Keywords: SWAT; Mindanao River Basin; Discharge; Watershed Modelling; Precipitation; Proxy Basin.

1. Introduction

Among the developing countries, the Philippines faces a considerable challenge regarding development due to the continuous increase in electricity demands, with an annual average rate of increase of 4.3% [1]. The power demand of the Mindanao island group in the Philippines has increased by 3.8% annually over the past decades [2]. In April 2017, the maximum power peak demand in Mindanao reached approximately 1,696 MW [3]. However, the Mindanao water resources contributed 38%, or 1,947 GWh, of the gross power generation from hydropower in June 2017 [3]. Regardless of the current contribution of water resources to renewable energy, the power demand continues to outpace the supply. Thus, to address this emerging problem, assessment for a potential source of sustainable renewable energy is needed. The purpose of this study is to enhance water resource management for hydropower application in Mindanao to improve the electrification situation and support the implementation of the Renewable Energy Act of the Philippines.

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The renewable energy resources in the Philippines are geothermal, wind, solar, biomass, ocean and hydropower resources [1]. However, among these options, hydropower is more sustainable in this country due to the abundance of water resources in its 18 major basins [4]. Hydropower has the greatest potential, with an estimated contribution of 13.31% of the energy needs of the country [5]. Therefore, to maximize the utilization of water resources for hydropower, assessment of available water resources has to be carried out in the major basins of the country.

On the other hand, water resources are also utilized for irrigation for agricultural productivity; these irrigation systems cover 52.0% and 38.6% of the Philippines and Mindanao, respectively [6]. Hence, the Mindanao irrigation service covers a total of 20,212.71 ha, contributing to the primary income-generating agriculture industry [4]. Moreover, water resources play an important role in the community; for instance, only 82.6% and 86.8% of households have access to safe water supplies in 2011 in the Philippines and Mindanao, respectively. This low rate of access to potable water results in outbreaks of diseases carried by water [6].

The concerns of water resource management in Mindanao are severely affected by geological and hydrogeological hazards due to the physical environment. Mindanao is vulnerable to disasters induced by natural hazards such as storm surges, typhoons, earthquakes, tsunamis, droughts and floods [7, 8].

In 2011, Tropical Storm Washi (known as Tropical Storm Sendong in the Philippines) made landfall in the northern part of Mindanao and caused a heavy rain that led to overflow of the Cagayan Basin, resulting in calamitous flooding in Cagayan de Oro and Iligan City and in 14 provinces, with an estimated damage of 4.17 million USD to agriculture and 0.78 million USD to fisheries [9, 10]. In addition, Typhoon Bopha, caused damage in eastern Mindanao with an overall estimated cost to agriculture of 645 million USD [11]. Furthermore, flooding events occur due to extreme rainfall, tropical cyclones from Monsoon winds and the dynamic climate of tropical cyclones with low pressures [7].

This weather dynamic is very important to consider for the development of water resource management because of its direct influence on the watershed. For instance, high precipitation intensity may cause a flood because of the direct impact of precipitation on river runoff and slow ground absorption. Thus, more precipitation results in a higher possibility of flooding [12]. Therefore, the assessment of the sustainability of the water supply for hydropower application mainly depends on the characteristics of precipitation.

![Figure 1. Study area of the Mindanao island group, Philippines: (a) the 17 regional administrative boundaries of the Philippines; (b) the population at the provincial level; (c) Mindanao, showing the population at the municipality/city level; and (d) the major basins, weather stations and gridded precipitation points in Mindanao used in the SWAT simulations. The dashed lines in Figure 1(d) are the four points used for the estimation of rainfall patterns from the precipitation datasets.](image-url)
Thus, this study carefully investigates the precipitation inputs in watershed modelling by comparing the observational data from the DOST-PAGASA with the global gridded precipitation datasets from the NCDC-CPC and GPCC. In addition, water management can include agricultural water footprint analysis by considering increasingly complex indicators, such as multiple climate variables, soil characteristics, and crop properties, to simulate the water cycle [13]. Therefore, weather-related events must be understood in terms of their possible effects on the watershed since hydropower generation is driven by river discharges. Moreover, SWAT considers other climate variables such as temperature, humidity and solar radiation, while soil characteristics and crop properties are some of the inputs to the hydrologic response unit (HRU) of SWAT [14].

Therefore, the objectives of this study are to evaluate the observed rainfall data with gridded global precipitation datasets to overcome the present data scarcity and to simulate the river discharges of the MRB for water resource management and future hydropower development. The literature review on watershed modelling with SWAT is presented in Section 2. The study area, material and method are presented in Section 3, 4 and 5, respectively. The results and discussion are described in Section 6 and 7, respectively, followed by conclusion in Section 8.

2. Watershed Modeling with SWAT in the Available Literature

The SWAT model was developed in the early 1990s by Jeff Arnold [14], and it has been recognized worldwide as an effective tool in water resource management for assessing the impact of the climate on water supplies and non-point sources of pollution in watersheds [15, 16]. Moreover, SWAT is a scientific tool used to evaluate streamflow, agricultural chemicals and sediment yield in a large basin [17]. For instance, SWAT was applied to a semi-arid climate in India for rainfall-runoff modelling of river basins [18]. SWAT was also applied to short-term climate data for the assessment of potential hydropower in Assam, India [19]. Correspondingly, the climate change impact on hydropower safety in Dak Nong, Vietnam, was carried out using SWAT [20].

Similarly, hydrological modelling of the Hoa Binh reservoir in Vietnam was conducted to optimize the utilization of flood control and hydropower generation. The results revealed a significant reduction in the peak flood downstream during the rainy season and a stable reservoir level during the dry season [21]. However, the hydrological model in the upper Mekong Basin identified a significant variation from the normal seasonal characteristic of river discharges since the hydropower began operation [22]. Moreover, water balance analysis in SWAT was used to quantify agricultural water demand for the sub-arid Mediterranean watershed [23]. SWAT modelling was carried out in a snowy area of Istanbul, in both Asia and Europe, to evaluate the water budgets of water resources in the context of uncertainties due to climate change and population growth in urbanized areas [24]. Land use change was evaluated using SWAT by simulating the streamflow of Murchison Bay in Uganda to further estimate sediment yield and nutrient loss for water resource management [25]. The groundwater analysis of the Taleghan Dam in Iran was also analysed by simulating the runoff river simulation using SWAT [26]. In addition, SWAT was used to demonstrate the importance of precipitation inputs as the main cause of uncertainties during the simulation of the Adige River basin in Italy, using multiple types of precipitation inputs [27]. Researchers found that monthly simulation produced better results than daily simulation in the ungauged Tonle Sap Basin in Cambodia [28]. Furthermore, SWAT was introduced to simulate runoff of the Mekong River to evaluate the hydrological application of tools in large basins [29].

In some parts of the Philippines, SWAT is utilized in different applications, such as for assessment of potential hydropower in the Visayas [30], Misamis Occidental [5], and the Agusan River basin [31], for predicting runoff in an ungauged watershed in Mabacan [32], and for simulating sediment yield in the Layawan watershed in Mindanao, to investigate land use change [33].

However, most of the applications in developing countries face a lack of precipitation and river discharge data, resulting in reliability issues in the validation process [34]. Therefore, we attempted to address how to overcome the data scarcity in the selected study area. Thus, this work used three types of precipitation datasets. Two are gridded datasets with a resolution of 0.5° latitude and 0.5° longitude, the NCDC-CPC dataset, and 1° latitude and 1° longitude, the GPCC dataset, as presented in Table 1. Hence, precipitation datasets were assigned to four stations to proportionally represent large areas of the MRB. Moreover, the calibration was conducted for 3 rivers: the Nituwan, Libungan and Pulangi rivers. Then, validation of the calibrated models was conducted through the proxy basin to facilitate data scarcity. Finally, the SWAT interface was implemented in ArcGIS to carry out a watershed model of the MRB despite the limited hydrological datasets available for validation.

3. Study Area

3.1. The Philippines and Mindanao

The Philippines is situated in Southeast Asia and includes three major zones: Luzon, Visayas and Mindanao, as shown in Figure 1(a). Mindanao is located in the southern Philippines and is the second-largest group of islands, after Luzon [35]. The Philippines had a population of 100,981,437 during the 2015 census [8] and includes a total of 7,107
islands with a land area of 300,000 km² (Figure 1(b)) [36]. Moreover, the Philippines comprises 17 regions, 80 provinces, 143 cities, 1,491 municipalities, and 42,028 barangays (villages) [36]. Mindanao has a land area of 120,812 km² and had a population of 24,135,775 during the 2015 census, as shown in Figure 1(c) [8], and it is subdivided into six administrative regions that further split into 27 provinces, 35 cities, and 422 municipalities [36].

The Philippines has 421 principal river basins and 18 major basins according to the National Water Regulatory Board (NWRB) [30]. Additionally, the Philippines has four types of climate, as defined by the spatial distribution of monthly rainfall, and experiences an average of 20 typhoons annually [7]. From 1990 to 2006, 520 disasters were induced by seven major natural hazards in this country, affecting 19,298,190 families (approximately 95 million people), who were repeatedly hit by natural hazards such as tropical cyclones, floods and landslides within the same period [37]. Considering these characteristics, water resource management is very challenging in the Philippines because of seasonal weather changes. Modelling is an alternative approach to account for the weather factors that influence the watershed.

3.2. Mindanao River Basin (MRB)

The MRB is the second-largest basin in the country [38], with a total area of 21,503 km² [39]. It lies in four regions covering 72 municipalities and 1,732 villages in eight provinces, namely, Maguindanao, Lanao del Sur, Bukidnon, Sultan Kudarat, Davao del Sur, Davao del Norte, North Cotabato, and South Cotabato, as shown in Fig. 2 [39]. Due to the dependency on rain throughout the year, the MRB climate was classified as Types 3 and 4 under the modified Corona Climate Classification System of the PAGASA [4]. Moreover, the MRB includes major rivers, such as the Mindanao River and the Tamontaka River, which enters the sea of the lowest part of Cotabato City in Maguindanao [2]. The Pulangi River originates from Bukidnon Province. The Ambal-Simuay River has its waterhead in Lanao del Sur, and the Ala River navigates the Ala Valley in the south [2].

Moreover, the MRB is located at the coordinates of 12°44′35.71″ longitude and 7°12′17.06″ latitude [4]. MRB has three vast marshes, namely, the Ligawasan, Ebpanan, and Libungan marshes, located within the central and lower parts of the basin. Thus, this large water resource in the MRB will be a potential asset to enhance hydropower development in support of the economic growth of the nearby regions. Therefore, the main reason to choose this study area is to maximize the application of the potential water resources for sustainable hydropower development in Mindanao.

![Figure 2](image-url)
4. Datasets

This study mainly used the available datasets from certain government agencies in the Philippines, as presented in Table 1. These datasets were requested from the corresponding listed agencies, but the available records are limited. The precipitation datasets from global gridded models were obtained online from the corresponding websites.

4.1. Digital Elevation Model

The synthetic aperture radar digital elevation model (SAR-DEM) with a 10-m resolution was obtained from the University of the Philippines Training Center for Applied Geodesy and Photogrammetry (UP-TCAGP) [30, 31]. These datasets were collected from point cloud data at a rate of 300 to 400 km² per day at every sensor by the use of airborne light detection and ranging (LiDAR) technology and appended with SAR in some areas of concern [40]. This DEM was mostly used in the related previous studies because of its high resolution and accessibility [5, 38, 40]. The DEM was projected with the Universal Transverse Mercator (UTM) Zone 51 projection and World Geodetic System (WGS) 1984 as the horizontal datum, as displayed in Figure 2(a).

4.2. Administrative Boundaries

The Philippines administrative boundaries were obtained from a global administrative map and compared with other shapefiles from the Philippines GIS organization. The administrative shapefile was then projected with UTM 51N and WGS 1984, and then the MRB areas were overlaid onto the provincial boundaries, as shown in Figure 2(b), and municipal boundaries, as shown in Figure 2(c). The MRB lies in 72 municipalities of 6 provinces within 4 regions of Mindanao.

| Table 1. Summary of the datasets used in the SWAT simulations of this study |
|---------------------------------------------------------------|
| **Data name** | **Description** | **Year** | **Format** | **Sources** |
| Digital elevation model | RADARSAT SAR (10-m resolution) | 2017 | GeoTIFF | Department of Science and Technology and University of the Philippines Project ([http://www.namria.gov.ph/](http://www.namria.gov.ph/)) |
| Land use and land cover | Landsat 8 (30-m resolution) | 2010-2015 | Shapefile | National Mapping and Resource Information Authority ([http://www.namria.gov.ph/](http://www.namria.gov.ph/)) |
| Soil map | Soil type | 2015 | Shapefile | Philippines GIS Organization ([http://philgis.org/](http://philgis.org/)) |
| Population | Population census | 2015 | Spreadsheet | Philippines Statistical Authority ([https://psa.gov.ph/](https://psa.gov.ph/)) |
| Weather records | Temperature, wind, humidity, and solar radiation | 1995-2017 | Spreadsheet | Philippines Atmospheric, Geophysical and Astronomical Services Administration ([www.pagasa.dost.gov.ph](http://www.pagasa.dost.gov.ph/)) |
| Precipitation | NCDC-CPC, Gridded global daily precipitation (0.5°lat & 0.5°long) | 1979-2017 | NetCDF | National Climatic Data Center ([ftp://ftp.cdc.noaa.gov/Datasets/data/cpc_global_precip/](ftp://ftp.cdc.noaa.gov/Datasets/data/cpc_global_precip/)) |
| | GPCC, Gridded global daily land surface precipitation (1°lat & 1°long) | 1982-2016 | NetCDF | Global Precipitation Climatology Center ([ftp://ftp.cdc.noaa.gov/Datasets/data/cpc_global_precip/](ftp://ftp.cdc.noaa.gov/Datasets/data/cpc_global_precip/)) |
| River discharge | Nituan River | 2005-2010 | Spreadsheet | Department of Public Works and Highways, Bureau of Standards ([http://www.dpwh.gov.ph/dpwh/organization/bureau/BRS](http://www.dpwh.gov.ph/dpwh/organization/bureau/BRS)) |
| | Libungan River | 2006-2008 | Spreadsheet | |
| | Pulangi River | 2009-2010 | Spreadsheet | |

4.3. Land Use and Land Cover

Land use and land cover data from Landsat 8 of 2010 with a 30-m resolution were obtained from the National Mapping and Resource Information Authority (NAMRIA) and validated on the ground in 2015 by the agency. The shapefile of this dataset also used the same projection as the DEM. This dataset is among the main components of the model structure. Thus, the HRU was determined using this dataset, and the reclassification results are presented in Figure 2(d). The HRU results reported the following figures: the total area of the watershed is 2,041,449.74 ha, including the comprising agriculture area (52.65%), bushland (23.78%), open forest (7.84%), closed forest (5.71%), marshland (4.01%), grassland (4.37%), water (1.12%), and built-up area (0.53%). The large agricultural land of the MRB with an area of 1,074,869.37 ha comprises perennial crops and annual crops.

4.4. Soil Type and Slope

The soil map and local soil type classification was obtained from the Bureau of Soil and Water Management (BMWS). Additionally, this soil classification was used in the earlier studies conducted in Mindanao [30, 31]. This
information is provided by a shapefile projected in UTM 51N. The reclassification results for the HRU, as reflected in Figure 2(e), is characterized by mountain soil (39.04%), clay (25.45%), sandy loam (15.87%), clay loam (16.21%), loam (2.39%) and silt loam (1.04%). Mountain soil is a local name, according to the BSWM. Moreover, the reclassified slopes in the study area are divided into five categories: 0-25 (74.07%), 25-50 (19.48%), 50-75 (5.25%), 75-100 (0.99%) and 100-9999 (0.21%), as shown in Figure 2(f).

4.5. Weather Records

The weather records for 22 years, as shown in Figure 3, were obtained from DOST-PAGASA. Three datasets, temperature, humidity and wind speed, are available at four DOST-PAGASA stations in Cotabato, General Santos, Davao and Malaybalay, for the period from 1995 to 2017, but solar radiation is available at only the General Santos station for 2016-2017. The weather dataset is a main input for the SWAT model [14, 17]. Thus, these weather records were applied to simulate the MRB watershed model. The four stations are shown in Figure 1(d) and were used simultaneously during the model simulations.
4.6. Precipitation

The precipitation is a sensitive input in SWAT modelling because of the direct effects on the streamflow output [27, 41]. However, the study area has only 2 weather stations, the Cotabato and Malaybalay stations, located within the domain of the MRB. Two other weather stations, General Santos and Davao, are located outside the MRB. These four stations are not enough to represent the large MRB. Therefore, to address this concern, the datasets from the global gridded precipitation model from NCDC and GPCC were compared with the observational datasets from DOST-PAGASA [12]. Thus, the precipitation records from the abovementioned four DOST-PAGASA stations were then used in a comparison with datasets from the closest points of two global gridded precipitation models to evaluate the quality of the rainfall dataset. The multiple precipitation types were used to address the concern on lack of access to quality inputs in a developing country [34].

The NCDC-CPC precipitation is described as a global daily spatial coverage with a resolution of 0.5° latitude and 0.5° longitude covering 1979 to 2017 [42], while the GPCC precipitation [43], a global daily land surface precipitation with a resolution of 1° latitude and 1° longitude, covers the period from 1982 to 2016. The comparison results of the precipitations are summarized in Table 2.

Moreover, the three precipitation datasets were applied for simulating the watershed of MRB to improve the results of simulated discharges. The MRB was simulated from 2000 to 2017 and assigned 3 years of warm-up. Then, datasets from 2005 to 2010 were used to evaluate the precipitation responses against the simulated discharges during calibration and validation of the models based on the available period of river discharge records, as shown in Figure 4.
Figure 4. Rainfall comparisons between DOST-PAGASA observations and two gridded global precipitation datasets, the NCDC-CPC and GPCC datasets at the a) General Santos, b) Cotabato, c) Davao, and d) Malaybalay stations. Note that the Cotabato and Malaybalay stations are located within the MRB, while the other two stations, General Santos and Davao, are outside the MRB (see Fig. 1(d))

4.7. River Discharge

According to the Bureau of Standards of the Department of Public Works and Highways (DPWH), these records of river discharges were acquired through the information communication centre (ICT) with technical assistance of the United States Agency for International Development (USAID). The data were collected in five regions, which include three stations in the study domain: the Nituan River from 2005 to 2010, the Libungan River from 2006 to 2008, and the Pulangi River from 2009 to 2010. These river discharge records are used in the calibration and validation processes of watershed modelling.
Table 2. Comparison of the precipitation data between the observations (DOST-PAGASA) and global gridded datasets (NCDC-CPC and GPCC) at four stations within and near the MRB in terms of statistical indices such as correlation coefficient \((R)\), index of agreement \((d)\), root mean square error \((RMSE)\)

| Statistical index | Stations | Stations | Stations | Stations |
|-------------------|----------|----------|----------|----------|
| \(R\)             | NCDC-CPC | GPCC     | NCDC-CPC | GPCC     |
|                   | 0.46     | 0.78     | 0.90     | 0.83     |
| \(d\)             | 0.47     | 0.63     | 0.95     | 0.83     |
| RMSE              | 2.63     | 2.27     | 2.06     | 2.76     |

5. Method

As described, SWAT was designed for agricultural, non-point source pollution and runoff river flow research. However, it has many features; for example, it can model stream flow by validating the simulated discharge from measured discharges. The hydrological cycle in SWAT is controlled by the water balance equation presented in Eq. (1). Thus, this water balance equation drives the physics of SWAT, allowing it to model the watershed of a certain basin [24, 44].

\[
SW_t = SW_0 + \sum_{i=1}^t \left( R_{day} - Q_{surf} - E_a - W_{seep} - Q_{gw} \right)
\]

Where \(SW_t\) is the final soil water content \((\text{mm H}_{2}\text{O})\), \(SW_0\) is the initial soil water content \((\text{mm H}_{2}\text{O})\), \(R_{day}\) is the amount of precipitation on day \(i\) \((\text{mm H}_{2}\text{O})\), \(Q_{surf}\) is the amount of surface runoff on day \(i\) \((\text{mm H}_{2}\text{O})\), \(E_a\) is the amount of evapotranspiration on \(i\) \((\text{mm H}_{2}\text{O})\), \(W_{seep}\) is the amount of water entering the vadose zone from the soil profile on day \(i\) \((\text{mm H}_{2}\text{O})\), and \(Q_{gw}\) is the amount of return flow on day \(i\) \((\text{mm H}_{2}\text{O})\).

5.1. Analysis Procedure

This study applied the following procedure to model the MRB watershed with SWAT. Each step of the procedure was clearly stipulated to ensure the process during the model simulation. Moreover, the analysis procedure is summarized in Figure 5 to provide a clear overview of the methods being applied with the SWAT model.

Figure 5. The SWAT modelling and analysis process consists of inputs, model flow and outputs in every step of the procedures in this study
First, input weather datasets were prepared to match required input formats. The geospatial datasets such as the DEM, land use and land cover were processed and unmasked within the basin boundaries. Then, the watershed is delineated by using the processed inputs of the geospatial datasets. The processed land use and land cover were used to generate the HRUs by ArcSWAT. The processed weather dataset was loaded and utilized for the entire modelling process. Then, initial values of model parameters are set up which can be adjusted after calibrating simulation results in SWAT-CUP interface.

Then, calibrations were carried out to improve model performance by adjusting the parameters based on the sensitivity analysis from the SWAT-CUP (SUFI2) outputs. The watershed of the MRB was delineated into 107 sub-basins, as shown in Figure 6. Then, the calibration period was carried out from 2005 to 2010, as reflected in Figure 4. Due to a limited number of river gauges in the study area, the only rivers with a record were the Nituan River, from 2005 to 2010 the Libungan River, from 2006 to 2008, and the downstream Pulangi River, from 2009 to 2010. Therefore, these rivers were utilized for calibration: sub-basin 28 was assigned to the Nituan River (Figure 7), sub-basin 40 was assigned to the Libungan River (Figure 8), and sub-basin 45 was assigned to the downstream of the Pulangi River (Figure 9). Then, validations were carried out using the proxy basin principle [45] due to the relatively short records of river discharges. For instance, the calibrated/fitted parameters of River A (the Nituan River) were applied to River B (the Libungan River and Pulangi River) to validate the simulated discharges against the observed discharges. Since the record data of stream flow is not enough to split into two equal parts therefore the same datasets of the Nituan, Libungan, and Pulangi were also used in the proxy basin validation.

Table 3. Summary of the fitted parameters during calibration of the model by SUFI2 of SWAT-CUP. The sub-basins 28, 40, and 45 indicate the Nituan, Libungan, and Pulangi basins, respectively. r_parameter means modifying the parameters by multiplying the existing value to 1+ the given value, and v_parameter means using the given value to replace the parameter (see K.C. Abbaspour, 2015)

| Parameters            | Description                                      | DOS-PAGASA | NCDC-CPC | GPCC |
|-----------------------|--------------------------------------------------|------------|----------|------|
|                       |                                                  | Sub-basin  | Sub-basin| Sub-basin |
|                       |                                                  | 28  | 40   | 45   | 28  | 40   | 45   | 28  | 40   | 45   |
| r_CN2.mgt             | SCS runoff curve number for moisture condition II| -0.14       | -0.20  | 0.12  | -0.20| -0.19 | 0.07  | 0.14 | 0.24 | 0.19 |
| v_ALPHA_BF.gw         | Base flow alpha factor (days)                    | 0.87        | 0.90   | 0.67  | 0.91 | 0.68  | 0.62  | 0.36 | 0.84 | 0.09 |
| v_GW_DELAY.gw         | Threshold depth of water in shallow aquifer for return flow (mm) | 43.44       | 96.71  | 489.25| 29.29| 78.18 | 472.49| 37.91| 410.93|      |
| v_GW_QMN.gw           | Groundwater delay (days)                         | 0.86        | 0.80   | 0.67  | 0.95 | 0.61  | 0.69  | 0.34 | 0.08 | 0.82 |
| v_GW_REVAP.gw         | Groundwater revap coefficient                    | 0.02        | 0.04   | 0.04  | 0.13 | 0.64  | 0.04  | 0.26 | 0.08 | 0.20 |
| v_REVAPMNR.gw         | Threshold depth of water in the shallow aquifer for revap to occur | 475.69      | 245.18 | 234.86| 82.60| 170.47| 146.05| 482.59| 479.50| 105.42|
| v_HRU_SLP.hru          | Average slope steepness (m/m)                    | 0.94        | 0.96   | 0.01  | 0.98 | 0.64  | 0.15  | 0.10 | 1.00 |      |
| v_SLSUBBSN            | Average slope length (m)                         | 120.93      | 109.65 | 99.97 | 149.54| 170.47| 115.01| 73.56| 109.24| 153.59|
| v_OV_N.hru            | Manning’s n value for overland flow              | 8.57        | 19.22  | 28.78 | 11.95| 15.68 | 29.82 | 13.78| 29.22 | 9.42 |
| v_ESCO.hru            | Soil evaporation compensation factor             | 0.17        | 0.36   | 0.38  | 0.74 | 0.09  | 0.45  | 0.49 | 0.32 | 0.99 |
| v_SOL_AWC().sol       | Soil available water storage capacity (mm H2O/mm soil) | 0.81        | 0.74   | 0.03  | 0.96 | 0.55  | 0.11  | 0.08 | 0.32 | 0.09 |

Table 4. General criteria for performance evaluation in a statistical test for watershed scale

| Performance Rating   | R² | RSR | PBIAS | NSE |
|----------------------|----|-----|-------|-----|
| Not satisfactory     | ≤ 0.50 | ≥ 0.7 | ≥ ±25 | ≤ 0.50 |
| Satisfactory         | 0.50 - 0.60 | 0.6 - 0.7 | ±15 - ±25 | 0.50 - 0.70 |
| Good                 | 0.60 - 0.70 | 0.5 - 0.6 | ±10 - ±15 | 0.70 - 0.80 |
| Very Good            | ≥ 0.80 | 0.5 - 0.0 | < ±10 | ≥ 0.8 |

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5.2. SWAT Calibration

The SWAT-CUP program was established to support the SWAT tool to minimize concerns about uncertainties [46][47]. Moreover, a sensitivity analysis was included inside the SWAT-CUP to tune the parameters according to the recommended results from a number of iterations [48]. Hence, the range of parameters was also enumerated in the absolute values section of SWAT-CUP [47]. Furthermore, SWAT-CUP also incorporates the statistical formulas for the Nash-Sutcliffe coefficient (NSE), coefficient of determination (R²) and percent bias (PBIAS), as presented in Appendix A, to evaluate the model performance. Thus, this study used the sequential uncertainty fitting version 2 (SUFI2) in the SWAT-CUP program for the calibration of the model performances for the Nituan, Libungan and Pulangi rivers.

The calibration was executed with 500 simulations in every iteration, and we conducted 5 iterations per recommendation in the previous studies [46, 47, 49]. Model calibration does not guarantee the improvement in the performance of the DOST model; 0.33 and 0.50 were estimated by p-factor and r-factor at the Nituan river, 0.27 and 0.50 at the Libungan river, 0.50 at the Libungan River and 0.42 at the Pulangi River. The PBIAS at the Nituan River, 0.50 at the Libungan River and 0.42 at the Pulangi River for the DOST model; 0.17 and 1.04, respectively, for the NCDP-CPC model; 0.06 and 0.85, respectively, for the GPCC model. The p-factor and r-factor at the Libungan River are 0.08 and 0.34, respectively, for the NCDP-CPC model; and 0.37 and 0.09, respectively, for the GPCC model. These results are obtained in the 95% percentage of uncertainty (PPU) in the simulated discharge model.

6. Results

6.1. Calibration

The calibration results were measured through the statistical indices shown in Table 5, depicting an R² of 0.61 at the Nituan River, 0.50 at the Libungan River and 0.42 at the Pulangi River for the DOST-PAGASA model. The NCDP-CPC model has R² values of 0.66 at the Nituan River, 0.49 at the Libungan River and 0.55 at the Pulangi River. Additionally, the R² values of the GPCC model are 0.62 at the Nituan River, 0.51 at the Libungan River and 0.27 at the Pulangi River. The PBIAS at the Nituan River of the DOST-PAGASA model is better compared with that of the NCDP-CPC model, with 13.70, and the GPCC, with 16.30. Then, the percentage of uncertainty in the models were estimated by p-factor and r-factor at the Nituan River with 0.42 and 0.50, respectively, for the DOST-PAGASA model; 0.33 and 0.50, respectively, for the NCDP-CPC model; and 0.54 and 0.74, respectively, for the GPCC model. The p-factor and r-factor at the Libungan River are 0.08 and 0.71, respectively, for the DOST-PAGASA model; 0.17 and 1.04, respectively, for the NCDP-CPC model; and 0.06 and 0.85, respectively, for the GPCC model. The p-factor and r-factor at the Pulangi River are 0.25 and 0.20, respectively, for the DOST-PAGASA model; 0.04 and 0.10, respectively, for the NCDP-CPC model; and 0.08 and 0.34, respectively, for the GPCC model. These results are underestimated due to a lack of information on the reservoir management of dams and the water withdrawal from agricultural irrigation in the study basins.

Table 5. Summary of the statistical results for the calibration of the river discharges of the models at sub-basins 28, 40, and 45, which indicate the Nituan, Libungan, and Pulangi basins, respectively

| Statistical index | DOST-PAGASA | NCDC-CPC | GPCC |
|-------------------|-------------|----------|------|
|                   | Sub-basin   | Sub-basin| Sub-basin |
| R²                | 0.61        | 0.50     | 0.42  |
|                   | 0.66        | 0.49     | 0.55  |
|                   | 0.62        | 0.51     | 0.27  |
| PBIAS             | 4.00        | 58.0     | 51.4  |
|                   | 13.70       | 65.9     | 63.3  |
|                   | 16.30       | 30.2     | 64.7  |
| KGE               | 0.48        | 0.15     | 0.24  |
|                   | 0.37        | 0.20     | 0.09  |
|                   | 0.60        | 0.34     | 0.02  |
| NSE               | 0.13        | -7.33    | -1.54 |
|                   | 0.01        | -9.12    | -2.63 |
|                   | 0.22        | -2.06    | -2.42 |
| RSR               | 0.93        | 2.89     | 1.49  |
|                   | 1.01        | 3.18     | 1.75  |
|                   | 0.88        | 1.75     | 1.83  |
| p-factor          | 0.42        | 0.08     | 0.25  |
|                   | 0.33        | 0.17     | 0.04  |
|                   | 0.54        | 0.06     | 0.08  |
| r-factor          | 0.50        | 0.71     | 0.20  |
|                   | 0.50        | 1.04     | 0.10  |
|                   | 0.74        | 0.85     | 0.34  |

A negative NSE means that the model performance is unsatisfactory and is characterized by extreme values [50]. A negative statistical performance indicates that the observed average streamflow is better than the simulated streamflow. The simulated discharges at the Libungan and Pulangi rivers are underestimated due to a lack of information on the reservoir management of dams and the water withdrawal from agricultural irrigation in the study.
area. The system of water storage, release and distribution has a very significant effect on the behaviour of river discharge in a watershed [51]. Then, this has an excessive impact on model performance, as shown in Figures 8 and 9. In addition, sub-basins 40 and 45 have a wetland (marshland) component, and the elevation difference between upstream and downstream is high. Therefore, the terrain of the MRB has a large heterogeneous component that may not be able to be accounted for during the modelling process. The SWAT application is very challenging in a large-scale model and in wetlands. The wetlands normally absorb the surface and subsurface water between the inlet and outlet at several points, even if the inlet is well-defined [52]. Although SWAT already employs the basic concept of wetlands (marshlands), its ability to emulate the riparian wetland-river interaction is still under-studied [53]. Furthermore, most of the statistical model results do not show a significant difference between them.

Figure 6. The delineated watershed of the MRB; the watershed was divided into 107 sub-basins. The monitoring points are the links between the rivers/stream networks or junctions. Sub-basins 28, 40, and 45 indicate the Nituan, Libungan, and Pulangi rivers, respectively.
Figure 7. Calibration results of river discharge at the Nituan River with three different precipitation inputs: (a) the observation dataset from the DOST-PAGASA, (b) the gridded precipitation from the NCDC-CPC dataset and (c) from the GPCC dataset.
Figure 8. Calibration results of river discharge at the Libungan River with three different precipitation inputs: (a) the observation from the DOST-PAGASA, the gridded precipitation (b) from the NCDC-CPC dataset and (c) from the GPCC dataset.

Figure 9. Calibration results of river discharge at the Pulangi River with three different precipitation inputs: (a) the observation from the DOST-PAGASA, the gridded precipitation (b) from the NCDC-CPC dataset and (c) from the GPCC dataset.
Results of this study are similar to the previous studies conducted in the Philippines due to lack of accessibility of datasets [34]. For instance, the SWAT modelling results in Pagsanjan-Lumban Basin in the Philippines show an $R^2$ and NSE of 0.42 and 0.22, respectively, because of the lack of information on dams and paddy areas (Marshland) [51]. The SWAT water balance simulates the seasonal average discharges of 6.53 m$^3$/s for DOST-PAGASA, 5.26 m$^3$/s for NCDC-CPC, and 4.73 m$^3$/s for GPCC in Nituan River. The seasonal average simulated discharge in Libungan River are 5.08 m$^3$/s for DOST-PAGASA, 3.97 m$^3$/s for NCDC-CPC, and 4.37 m$^3$/s for GPCC. The seasonal average simulated discharges in Pulangi River are 261.69 m$^3$/s for DOST-PAGASA, 215.63 m$^3$/s for NCDC-CPC, and 250.45 m$^3$/s for GPCC. The observed seasonal average discharges are 6.20 m$^3$/s in Nituan, 11.37 m$^3$/s in Libungan, and 470.64 m$^3$/s in Pulangi. Among the simulated discharge models, the DOST-PAGASA model has closer values with the observed river discharges. Therefore, the DOST-PAGASA simulated discharges in the river mouth of the Mindanao river basin which is located in sub-basin 42 has an average simulated discharge of 502.03 m$^3$/s, with the peak and lowest discharges of 1,239 m$^3$/s and 2.29 m$^3$/s, respectively.

Figure 10. Summary of the calibrated results of river discharge models at the (a) Nituan River from 2005 to 2010, (b) Libungan River from 2006 to 2008, and (c) Pulangi River from 2009 to 2010
6.2. Validation: Proxy Basin

Access to enough data is a common problem in a developing country, and the Philippines is into exception [34]. Due to the challenges of limited access to river discharge records and a limited number of river gauges located in the study area, model validation was used to create a proxy basin. This principle is not new; it was introduced under the hierarchical scheme for systematic testing of hydrological simulation [45]. It was explained that streamflow at Basin C is to be selected as ungaged, and two basins within the region will be selected as gauged rivers, for example, Basins A and B. Then, the models will be calibrated in one of these basins and validated in another basin within the region. For instance, the model is calibrated in Basin A and validated in Basin B, or vice versa. In addition, the proxy basin is useful if the available streamflow record in a basin is not insufficient for equal split-sample and only if two validation results are acceptable and identical [45]. Moreover, the proxy basin was also used for model development of ungagged basins and at regional scales of watershed models [54]. The validation of the calibrated model was also carried out with SUFI2 of SWAT-CUP at the same rivers and in the same period as mentioned in the calibration section. However, the conventional way to split the available dataset is not applicable due to the insufficient length of the data record for river discharge and inconsistency of the duration, as shown in Figure 10. Therefore, from the proxy basin, the resulting parameters from the Nituan River were applied to the Libungan and Pulangi rivers, and vice versa, in this study to conduct the validation of the calibrated model and address the issues on data scarcity.

The validation results for the DOST-PAGASA model are similar to the $R^2$ results of 0.61 and 0.61 at the Nituan River and 0.50 and 0.50 at the Libungan River during calibration and validation. In contrast, the model performance at the Pulangi River decreased from 0.42 to 0.33 for the DOST-PAGASA model, 0.55 to 0.40 for the NCDC-CPC model, and 0.27 and 0.21 for the GPCC model. Moreover, the PBIAS at the Nituan River did not change much, remaining at the good and satisfactory level according to the general ratings for the watershed provided in Table 4. In contrast, the NSE values for all the sub-basins remain unsatisfactory with negative values, as depicted in Table 6. The simulated discharges at Libungan and Pulangi remain underestimated. In addition, the p-factor and r-factor of all the models did not change significantly from calibration to validation, even though proxy basins were applied. With these results, the calibration and validation satisfied only the Nituan River model. The Libungan and Pulangi rivers are the subject of more in-depth studies. Thus, the model performance will improve only if the dam management and irrigation water withdrawal will be accounted for in the model. Although datasets for dams and irrigation are not available; however, these results may be useful for understanding the role of dams and irrigation systems, especially downstream of rivers. In addition, the purpose of validation is to evaluate the fitness of the model after tuning the parameters during the calibration process. The proxy basin validation was carried out to evaluate the application of the SWAT model in a large basin with limited hydrological datasets. Therefore, regional modelling of large-scale basins with limited datasets does not accurately account for all the heterogeneous characteristics of the watershed.

### Table 6. Summary of the statistical results for the validation of the river discharges of the models by proxy basin using the fitted parameters from the calibration results at sub-basins 28, 40, and 45, which indicate the Nituan, Libungan, and Pulangi basins, respectively

| Statistics | DOST-PAGASA | NCDC-CPC | GPCC |
|------------|-------------|----------|------|
|            | Sub-basin   | Sub-basin| Sub-basin|
| $R^2$      |             |          |       |
|            | 0.61| 0.50 | 0.33 | 0.64| 0.46| 0.40 | 0.57 | 0.48 | 0.21 |
| PBIAS      | 5.6  | 57.8  | 70.4  | 25.4 | 60.2 | 71.4 | 30.9 | 39.7 | 58.9 |
| KGE        | 0.33 | 0.14  | 0.09  | 0.45 | 0.17 | 0.05 | 0.60 | 0.29 | 0.05 |
| NSE        | -0.14| -7.33 | -2.76 | -0.10| -7.85| -2.80| -0.03| -3.51| -1.90|
| RSR        | 1.07| 2.88  | 1.94  | 1.05| 2.98 | 1.95 | 1.01 | 2.12 | 1.70 |
| p-factor   | 0.51| 0.06  | 0.08  | 0.60| 0.11 | 0.00 | 0.60 | 0.11 | 0.08 |
| r-factor   | 1.50| 0.58  | 0.20  | 1.70| 0.33 | 0.10 | 0.83 | 0.85 | 0.34 |

7. Discussions

7.1. Effects of Precipitation on Simulated Discharge

Since river discharge is basically characterized by precipitation patterns, the observed precipitation inputs were carefully examined by evaluating the global gridded datasets and ground-truth dataset discussed in the previous precipitation section. The results of the correlation between the global gridded datasets and the observational dataset are 0.46 for the NCDC-CPC data and 0.78 for the GPCC data at General Santos, 0.90 for the NCDC-CPC data and 0.83 for the GPCC at Cotabato, 0.95 for the NCDC-CPC data and 0.63 for the GPCC data at Davao, and 0.92 for the NCDC-CPC for the GPCC and 0.52 for the GPCC for the GPCC at the Malaybalay station.
These strong correlations of the precipitation at the 3 stations indicate that the precipitation datasets have similar intensity and seasonal precipitation patterns in Mindanao. Thus, both global gridded precipitation models, either NCDC-CPC or GPCC, and DOST-PAGASA produce a trend of simulated discharges. However, among them, the precipitation model from DOST-PAGASA produced higher simulated discharges, as observed in the peak and base flow in Figure 10. In addition, the characteristics of simulated discharges physically influence the precipitation behaviours, as presented in Figures 7 to 9, respectively.

The three precipitation models proved that a high intensity of rainfall usually occurs in the months of June, October, and November, as reflected in the peak flow of the discharges in Figure 10. Moreover, the simulated peak discharge is slightly higher than the observed peak discharge in June for the Nituan and Libungan rivers, unlike that at the Pulangi River, which has a lower simulated peak discharge in June and November. Therefore, this situation might be affected by the dam system upstream of the Pulangi River. Thus, precipitation patterns for the Nituan River are valuable information for the nearest basin and for the upstream sub-basin to create a scenario for monthly seasonal discharge. However, for the Libungan and Pulangi rivers, the precipitation pattern is not beneficial for hydropower analysis because the simulated model is underestimated, and the area of interest is in wetlands with low elevations. Then, this terrain is not suitable for hydropower development; the ground is soft, and the elevation difference is not enough to generate power. Therefore, for the purpose of this study, utilization of the Nituan River will be suggested for the planning and development of hydropower in the study area.

7.2. Quality of Observation

As stated in the previous sections, the number of river gauges and river discharge records are very limited in MRB, and there are only 3 gauges with inconsistent records. Hence, the methods and types of instruments used for data collection were not mentioned in the source. This also affects the model performances; for instance, a shorter period of recorded data is most likely to produce low statistical index results, as observed for the Libungan and Pulangi rivers. Moreover, the ideal calibration and validation require enough river gauges data to split a dataset into two equal periods.

The quality of the river discharge has substantial effects on model calibration and validation. Aside from the length of records and the number of gauges available in the study domain, the method of collecting and processing the data are very serious factors to be considered. As explained previously, these datasets are part of a pilot project to support the technical capability of responsible agencies in certain regions. In short, a transitional process for transferring technology know-how from the service provider to the agency might lead to transitional development. Thus, the datasets duration is inconsistent among the stations, and the number of gauges is very limited despite the large size of this basin, with hundreds of streams and rivers. Therefore, as an alternative, using the regional watershed model and proxy basin process is an efficient way to implement model validation in the MRB.

8. Conclusion

The main purpose of this study was to contribute to the improvement in water resource management for hydropower applications. Watershed modelling in the MRB in Philippines was carried out using SWAT. Since precipitation is a critical input that has a direct influence on river discharges, measured precipitation dataset within the MRB is desirable as many as possible. However, only 2 DOST-PAGASA weather stations are available in MRB while another 2 stations are located close to MRB, despite the large area. Therefore, global precipitation gridded datasets from NCDC and GPCC were utilized to investigate the quality of precipitation in the MRB. Each precipitation dataset was individually used in SWAT simulations. Then, the simulated discharge was calibrated at 3 river gauges in the Nituan, Pulangi, and Libungan rivers using SWAT-CUP (SUF1). Moreover, due to limited short records from the 3 river gauges, the proxy basin process was applied for the validation of calibrated models of the same rivers. The models of the Nituan River provide better results compared with those of the Libungan and Pulangi rivers, even though a calibration was executed, and a proxy basin was also applied.

Lack of enough and qualified data is a common problem in a developing country. Due to the challenges of limited access to river discharge records and a limited number of river gauges located in the study area, model validation based on a proxy basin principle was applied in this study; for instance, the model was calibrated in Basin A and validated in nearby Basin B, or vice versa, to overcome the data scarcity in the study area. The proxy basin was also used for model development of ungaged basins at regional scales of watershed models. Therefore, this approach of calibration and validation of watershed modelling based on the proxy basin principal with various precipitation inputs demonstrates a method of watershed modelling for regions with insufficient precipitation and discharge data in developing countries.

The underestimated results of the Libungan and Pulangi rivers are mainly due to a lack of information on dams and irrigation water withdrawal. The study area has a vast wetland (marshland) and is characterized by a high elevation difference between the upstream and downstream, contributing to the uncertainty in the models and weak performance
of the models in wetlands with limited datasets. Thus, these findings will be applicable to only the upstream side of the MRB for identifying potential sites for hydropower development.

In addition, comparison results for the precipitation inputs may be useful references to improve the meteorological measurements by adding additional weather stations in the regions. The trend of simulated discharges against precipitation inputs at 3 stations demonstrates the monthly seasonal characteristics of a watershed. Thus, this information can be used to determine which month might have a high potential for hydropower generation. Finally, this study specifically discussed the importance of meteorological agencies improving data collection and the application of the collected data in large areas; additionally, this study discussed the very significant role of river discharge, dam management and agriculture water withdrawal data for watershed analysis.

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10. Conflicts of Interest

The authors declare no conflict of interest.

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Appendix A: Equations of the Statistical Indices Used to Evaluate the Model Performance

The index of agreement between two variables is computed by the following formula [55, 56]:

\[
d = 1 - \frac{\sum_{i=1}^{n} (P_i - O_i)^2}{\sum_{i=1}^{n} (|P_i - \bar{O}| + |O_i - \bar{O}|)^2}
\]  

(1)

Where

- \(d\) is the index of agreement of two variables predicted and observed
- \(P_i\) is the predicted value in a sample
- \(O_i\) is the observed values in a sample
- \(\bar{O}\) is the mean value of the observed samples
- \(n\) is the number of observations

The correlation coefficient shows the strength of the relations between two variables by:

\[
R_{xy} = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^{n}(X_i - \bar{X})^2 \sum_{i=1}^{n}(Y_i - \bar{Y})^2}}
\]  

(2)

Where

- \(R_{xy}\) is the correlation coefficient of the linear relationship between two variables, such as \(x\) and \(y\):
- \(X_i\) is the value of the \(x\)-variable of a sample
- \(\bar{X}\) is the mean value of the \(x\)-variables
- \(Y_i\) is the value of the \(y\)-variable of a sample
- \(\bar{Y}\) is the mean value of the \(y\)-variables

The coefficient of determination between two model simulations and measured values is [47, 57]:

\[
R^2 = \frac{\sum_{i=1}^{n}[(Q_{m,i} - \bar{Q}_m)(Q_{s,i} - \bar{Q}_s)]^2}{\sum_{i=1}^{n}(Q_{m,i} - \bar{Q}_m)^2 \sum_{i=1}^{n}(Q_{s,i} - \bar{Q}_s)^2}
\]  

(3)

Where

- \(R^2\) is the coefficient of determinants
- \(Q_{m}\) is the measured discharge
- \(\bar{Q}_m\) is the mean of the measured discharge
- \(Q_{s}\) is the simulated discharge
- \(\bar{Q}_s\) is the average of the simulated discharge

The root mean square error (RMSE) is used to measure the absolute fitness between the observed and the modelled results:

\[
RMSE = \sqrt{\frac{\sum_{i=1}^{n} (P_i - O_i)^2}{n}}
\]  

(4)

Where

- \(RMSE\) is the root mean square error of the samples
- \(P_i\) is the predicted values in a sample
- \(O_i\) is the observed values in a sample
- \(n\) is the number of observations
The Nash-Sutcliffe coefficient is calculated as follows [57, 58]:

\[
NSE = 1 - \frac{\sum_{i=1}^{n}(Q_m - Q_s)^2}{\sum_{i=1}^{n}(Q_m - \bar{Q_m})^2}
\]  

Where

- \(NSE\) is the Nash-Sutcliffe coefficient
- \(Q_m\) is the measured discharge
- \(\bar{Q}_m\) is the mean of the measured discharge
- \(Q_s\) is the simulated discharge

\(PBIAS\) measures the model fitness in terms of average tendency, and a small value of \(PBIAS\) indicates a better model fitness. \(PBIAS\) is calculated by [47, 57]:

\[
PBIAS = 100 \times \frac{\sum_{i=1}^{n}(Q_m - Q_s)}{\sum_{i=1}^{n} Q_{m,i}}
\]  

Where

- \(Q_m\) is the measured discharge
- \(Q_s\) is the simulated discharge
- \(n\) is the number of observations

\(RSR\) is a standardization of the RMSE to measure how well the model results fit with the observed values, and a lower value of \(RSR\) indicates a better model fitness. \(RSR\) is calculated by the following equation [47, 57]:

\[
RSR = \sqrt{\frac{\sum_{i=1}^{n}(Q_m - Q_s)^2}{\sum_{i=1}^{n}(Q_m - \bar{Q}_m)^2}}
\]  

Where

- \(Q_m\) is the measured discharge
- \(\bar{Q}_m\) is the mean of measured discharge
- \(Q_s\) is the simulated discharge
- \(n\) is the number of observations

The Kling-Gupta efficiency \((KGE)\) is used to examine the decomposition of the Nash-Sutcliffe efficiency, with a value close to 1 indicating a better performance. \(KGE\) is calculated by the following equation [47, 59]:

\[
KGE = 1 - \sqrt{(r - 1)^2 + (\alpha - 1)^2 + (\beta - 1)^2}
\]  

Where

- \(r\) is a linear regression coefficient between the simulated and the observed data
- \(\alpha\) is a ratio of standard deviation between the simulated and measured data (\(\alpha = \frac{\sigma_s}{\sigma_m}\))
- \(\beta\) is a ratio of the means between simulated and measured data (\(\beta = \frac{\mu_s}{\mu_m}\)).

The \(r\)-factor is the thickness of the 95% predicted uncertainties \((95PPU)\) [60]:

\[
r - factor = \frac{1}{n} \sum_{i=1}^{n} (y_{i,97.5\%}^M - y_{i,2.5\%}^M) / \sigma_{obs}
\]  

Where

- \(y_{i,97.5\%}^M\) is the upper boundary of the 95PPU \((95\% \text{ predicted uncertainties})\)
- \(y_{i,2.5\%}^M\) is the lower boundary of the 95PPU \((95\% \text{ predicted uncertainties})\)
- \(\sigma_{obs}\) is the observed standard deviation.
Rational Hybrid Analytical Model for Steel Pipe Rack Quantification in Oil & Gas Industries

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Abstract

The objective of this work is to develop an analytical model to overcome the shortfalls in current engineering practices that are being used to estimate the pipe rack steel quantities during the pre-bid engineering phase in Oil & Gas industries. The research methodology consists of performing data analysis of past projects and devising a new system by developing suitable structure formulation techniques, loading system creation, structural stability analysis and LRFD design calculations, along with steel quantification procedures, which are completed in a single run. Then this rational hybrid analytical model is applied to examine a real-time project pipe rack structure module. As research findings, the results of the analytical model are compared with the outcome of both the conventional methods as well as the benchmark detailed engineering calculations. It is found that the quantity obtained using the new method is extremely close to the detailed engineering quantity with the least time consuming. Hence, this novel analytical model has proved to be a boon to structural engineers working in Oil and Gas industries since the crux of pre-bid engineering is to process voluminous data and calculate the quantities more precisely within a shorter time frame to be a successful bidder.

Keywords: Steel Pipe Racks; Steel Quantity Estimation; Oil and Gas Industries.

1. Introduction

The energy sector is the key factor in the economic growth of any country. The production process is highly based on the growth of energy sectors in a country, and due to this fact, the economic development of all countries has a strong correlation with high energy consumption levels. The per capita Gross National Product (GNP) is naturally having a relationship with the energy consumption activity. Countries with higher per capita GNP obviously consume a lot of energy per person. As an illustration, the per capita energy consumption in the United States is around 16 times that of India. Similarly, Japan’s energy consumption is almost 8 times that of India.

The energy industry represents all the forms of industries in total, which are occupied in the production and sale of energy, covering drilling and extraction of crude fuel, processing, refining and distribution to the retail market. Civilized mankind uses huge quantities of fuel, and the energy sector plays a crucial part in the development of infrastructure and maintenance of the societal needs in almost all nations. Oil and gas are vital to many factories and are very important for the creation and development of industrial civilization, and thereby are a real concern for all countries.

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The total energy consumed in a year is measured for the entire human civilization and is known as the world energy consumption. This indicates the overall energy obtained from all energy resources. This accounts for all the humanity’s efforts across every single technological and industrial domain of all the nations in the world. Coal was the main source of energy from 2000 to 2012. The energy consumption by the entire world population has a straightforward impact on the socioeconomic political field. The development of oil and natural gas has had tremendous growth, followed by hydropower and renewable energy. The development of nuclear energy has slowed down due to the nuclear disaster incidents such as Three Mile Island 1979, Chernobyl 1986, and Fukushima 2011.

Total global energy (9,694 Mtoe) consumption from various energy sources is depicted in the form of pie chart in Figure 1 as per the International Energy Agency (IEA) Publication [1].

![Figure 1. World energy consumption from various energy sources](image)

From Figure 1, it is evident that more than 50% of the world’s primary energy needs are fulfilled by the Oil and Gas industries, where Mtoe stands for Million Tonnes of Oil Equivalent.

The various phases in any Oil and Gas Engineering, Procurement, Construction and Commissioning (EPCC) project are listed below:

- Conceptual/Feasibility Studies
- Pre-Bid Engineering
- Front End Engineering Design (FEED)
- Basic Engineering and
- Detailed Engineering.

Among the various phases of Oil and Gas EPCC projects, the Pre-Bid engineering phase plays the most crucial part on Contractor’s side to bid and win the project. The crux of pre-bid engineering is to process volumes of data and calculate the quantities more precisely within a shorter time frame to be the successful bidder. In Oil and Gas plants, steel pipe racks generally quantify more than 50% of the total steel quantities. Pipe rack structural steel quantification poses many challenges to the structural engineers working in this domain.

Parameters affecting the design and thereby the quantities of Pipe racks are:

- Structural Configuration
- Design Loads
- Load Combinations
- Material Grades
- Client Standards
- Design Specifications
- Country Code
- Column Base Connection Types

Generally, the time span available for pre-bid engineering is between two and three months, whereas detailed engineering activities can last twelve to eighteen months. Hence, in just one-sixth of the time, structural engineers have to carry out all the necessary structure formation activities, loading calculations, analysis, design and
quantification so as to ascertain as accurately as possible the steel quantities that will be obtained after the detailed engineering calculations. Moreover, the availability of input data, such as structure configuration and loading data, would also be very much incomplete during the pre-bid engineering phase. Conventional methods which are being currently used have many drawbacks, such as a lack of inability to deal with incomplete input data, the lack of proper analysis and stability design calculations, a lower degree of accuracy of quantified data, and a more time consuming process. Therefore, a new rational hybrid analytical model is developed in this study to overcome the shortfalls and difficulties present in the existing conventional methods.

2. Materials and Methods

2.1. Conventional Procedures

Presently there are two methods being adapted for the steel quantification during pre-bid engineering in the Oil and Gas industries, which are:

- Statistical data method
- Rigorous software method

The first method is less accurate and the second is more time consuming. Statistical data analysis may not be applicable for all cases under consideration, and in conventional rigorous structural steel design, apart from structural configuration, modeling and load calculations and the preliminary selection of the optimum member size itself is a highly complicated and tedious process. It is also to be noted that during the pre-bidding process, quantification is done with some bias due to the many assumptions that need to be made because of the limited, incomplete data and time constraints.

This study aims to devise a novel method to overcome the difficulties of the existing methods. To accomplish this, a customized analytical tool is required to carry out the load calculation, configuration modeling, analysis, design and quantity estimation in a single run. Therefore, through a grounded theory study, a theoretical framework will be introduced to enhance the steel pipe rack quantity estimation process in pre-bid engineering in the Oil and Gas industries by analyzing the important factors that influence the steel estimation process and to provide a hybrid rational design strategy to enhance the quantification process by taking into account the best parts of the two existing methods. This area has still not been significantly explored, and not much research has been carried out to cater to this need. A systematic research study and possible solution methodology for this problem is needed, and it would be of immense use to verify the steel incidences obtained from statistical data, or to deduce them in the absence of such statistical data. Based on literature review, it is determined that no universally accepted design procedures, standards, or codes of practices are available currently for the design of steel pipe racks [2, 3].

The challenge is to overcome the difficulties posed due to incomplete input data, a lack of proper analytical and design methods, and the much shorter periods of time available.

2.2. Research Method

The goal of this study is to develop a hybrid rational analytical model to enhance the steel pipe rack quantity estimation process in pre-bid engineering in the Oil and Gas industries by analyzing the important factors that influence steel estimation. This model will take into account the best conceptual parts of the two existing methods and incorporate new analytical procedures for load calculations and define a new set of primary load cases, load factors and load combinations, suitable analysis method (DAM), stability design calculations, and rational estimation with the capability of dealing with incomplete input data. The new hybrid rational analytical model will function in an integrated platform so that all activities such as model creation, analysis and material quantification are performed in a single run. Due to this, there is a considerable reduction in overall time consumption. Thus, the new method can overcome all challenges that are faced in the pre-bid engineering phase.

In the new hybrid model, proper loading data is estimated by means of qualitative data analysis by calculating the minimum and maximum pipe diameter with a permuted arrangement, along with blanket loading and various primary load cases, as per the detailed engineering design format, which enhances the level of optimization of the quantities of primary and secondary steel. Primary frame members would be designed as a 2D frame with proper loading effect from secondary members with rigorous analysis.

Steel design is performed using the LRFD (Load and Resistance Factor Design) method, incorporating the rational stability method of analysis (Direct analysis method – DAM surpassing the currently used effective length method) as stipulated in AISC specification 360 – 2010.

Secondary members, such as longitudinal beams and secondary beams along the length of the pipe rack, are also designed with the LRFD approach with proper load combinations. Then, tertiary members are quantified using statistical data, which will be applied on the primary and secondary steel, which are quantified by the hybridized rational analytical model.
Thus, the new model developed applies the new design approach by employing DAM with rational quantification parameters. Because of the fact that it employs the basic concepts of both conventional methods, this is a hybrid as well.

The new Hybrid model is designed to overcome the drawbacks existing in the conventional methods, and has been found to be more effective, as detailed in Table 2. This new rational hybrid model is capable of working with limited input information by assuming suitable data derived from a statistical database and relevant calculations. It is intended for use in low seismic zones where wind loads are governing. The analytical model’s automated calculations are developed in the MS-Excel platform and by using Visual Basic Application. This model is developed such that it satisfies all design requirements of steel members as per the following standards / codes and Saudi Aramco best practices. It also satisfies other major international codes of practices along with Process industry practices (PIP) standard PIP STC 01015:

- AISC LRFD Manual
- ASCE-07-2005- Minimum Design Loads for Buildings and Other structures
- ASCE Task Committee report – Wind Loads for Petrochemical and Other Industrial Facilities
- SABP-M-006 - Wind Loads on Pipe racks and Open Frame Structures and
- SABP-M-007- Steel Pipe rack Design

Table 1. Comparison of the existing methods with the new rational hybrid analytical model

| Sl. no. | Parameter                               | Statistical data method          | Rigorous software method                          | Rational hybrid analytical model                                      |
|--------|-----------------------------------------|----------------------------------|--------------------------------------------------|-----------------------------------------------------------------------|
| 1      | Load calculation                        | Not done                         | Approximate load is calculated                    | Detailed load calculations are carried out based on qualitative inputs with necessary permutations |
| 2      | Analysis                                | Not done                         | Analysis is done using sophisticated software package | Analysis is done using stiffness matrix method                         |
| 3      | Structural design                       | Not done                         | Design using sophisticated software package       | Rational stability design method adapted                               |
| 4      | Steel quantification calculations       | Using statistical percentages for all primary, secondary and tertiary steel quantities | From software output for primary steel and allied percentages for secondary and tertiary steel quantities | Based on calculations for primary and secondary steel members and using statistical percentages for tertiary members. The statistical percentages are applied on calculated primary and secondary steel quantities |
| 5      | Procedure to deal with incomplete input data | Not available                   | Not available                                    | Available                                                             |
| 6      | Time consumption                        | Less                             | More                                             | Least                                                                 |
| 7      | Steel quantities optimization level     | Low                              | Medium                                           | High                                                                  |

Figure 2. Flowchart for the Research Method
2.3. Problem Statement

In this work, a real time project structure was considered for the analysis, design and steel quantity estimation, and the results are compared against two parameters, namely accuracy and time consumption. Generally, after considering a real time problem for the study, the problem parameters are to be normalized to suit the working philosophy of the analytical method.

The problem presented here is normalized accordingly. In this problem, a single bay three-storied pipe rack is considered with a bay width of 9 m. The spacing of pipe rack frames is 6 m. There are eight frames in the pipe rack module considered. Vertical bracings are provided in the central bay along the longitudinal direction at both alignments. Plan bracings are considered as shown in the 3D view.

Shear connections would be considered along the longitudinal direction, where vertical bracings (Non-sway frame) are provided. Moment connections would be considered along the transverse direction of the pipe rack, where vertical bracings are provided only in the bottom storey (Sway frames).

Longitudinal girt beams are considered to reduce the effective length of the columns about the minor axis in the bottom tier. Secondary beam projections in the form of cantilever-type beams are considered at both ends of the pipe rack module for a length of 1.5 m to facilitate the piping connections to the adjacent modules. All the main steel structural connections shall be of bolted type only. The three-dimensional view of the pipe rack module is shown in Figure 3. The bottom connections of base plates to the concrete pedestals are pinned type, which do not transmit any moments to the foundations.

![Figure 3. Three-dimensional view of pipe rack module](image)

The bottom tier has a height of 7 m, and the other two tiers each have a height of 2.5 m. Hence, the total height of the pipe rack is 12 m. A photograph of the pipe rack module structure for the present study is shown in Figure 4.

![Figure 4. Photograph of the pipe rack module under consideration](image)
General Input Data:

The input parameters required for the analysis are:

1. Steel grade
2. Steel prefabrication requirement
3. Number of bays
4. Number of storeys
5. Number of frames
6. Bay width
7. Bottom storey height
8. Overall height of the pipe rack
9. Spacing of frames
10. Initial indicative sizes for all members
11. Column support conditions
12. Tier load
13. Wind speed
14. Wind exposure category
15. Seismic building category
16. Seismic zone
17. Air coolers availability

Pipe Loading Data:

In all projects, the loading data on the pipe racks from the piping discipline are not available or are incomplete during the pre-bid engineering phase. To handle this, proper loading data is estimated by means of qualitative data analysis by calculating minimum and maximum pipe diameter with a permuted arrangement along with blanket loading. There are three qualitative pipe diameters identified, which are designated as Low, Medium and High, which correspond to 12", 18" and 30" pipe diameters, respectively. Based on pipe diameter, insulation thickness and minimum gap requirements between pipes, the permutations are carried out to find the worst load case scenario.

The pipe loading data generation based on the pipe rack span and spacing is developed to determine the appropriate pipe diameter which would cause the worst load case scenario as shown Figure 5.

| Piperack span | Length of pipe (Spacing) | Pipe Dia | Pipe Dia | Pipe Dia | Pipe thickness | Pipe thickness | Pipe weight | Insulation thickness | Overall diameter of pipe | Min. Safe gap | C/c dist | Insulation weight | Total dead load for one pipe | No of pipes | Intermediate Spacing | End spacing | Beam self weight | Total dead load per m run of beam | Total live load per m run of beam | Total load per m run of beam | Load per unit area |
|---------------|--------------------------|----------|----------|----------|----------------|----------------|-------------|---------------------|------------------------|---------------|-----------|-----------------|--------------------------------|-------------|-------------------|------------|------------------|-------------------------------|-----------------------------|-----------------------------|-------------------|
| m            | m                        | m        | m        | m        | m              | m              | m           | m                   | m                      | m             | m         | m               | m                                             | m           | m                 | m          | m                | m                                                          | m                          | m                                          | m                 |
| 9            | 6                        | 12       | 0.3048   | 1        | 0.0504        | 1.72            | 2            | 0.4064              | 0.1                    | 0.5064        | 0.148      | 1.864           | 8                             | 0.72         | 0.36              | 2           | 11.9            | 2.65                        | 14.59                      | 2.43                                 |
| 9            | 6                        | 14       | 0.3566   | 1        | 0.0504        | 2.03            | 2            | 0.4572              | 0.1                    | 0.6573        | 0.169      | 2.198           | 7                             | 0.83         | 0.41              | 2           | 12.3            | 3.34                        | 15.60                      | 2.60                                 |
| 9            | 6                        | 18       | 0.4504   | 1        | 0.0504        | 2.34            | 2            | 0.5080              | 0.1                    | 0.8080        | 0.190      | 2.531           | 7                             | 0.78         | 0.39              | 2           | 15.8            | 4.56                        | 19.36                      | 3.06                                 |
| 9            | 6                        | 18       | 0.4572   | 1        | 0.0504        | 2.65            | 2            | 0.5888              | 0.1                    | 0.8588        | 0.211      | 2.664           | 6                             | 0.94         | 0.47              | 2           | 15.5            | 5.09                        | 16.55                      | 3.09                                 |
| 9            | 6                        | 22       | 0.5588   | 1        | 0.0504        | 3.08            | 2            | 0.6604              | 0.1                    | 1.7604        | 0.253      | 3.531           | 5                             | 1.14         | 0.57              | 2           | 13.8            | 6.63                        | 20.40                      | 3.40                                 |
| 9            | 6                        | 24       | 0.6599   | 1        | 0.0504        | 3.59            | 2            | 0.7112              | 0.1                    | 1.8112        | 0.274      | 3.864           | 5                             | 1.09         | 0.54              | 2           | 14.9            | 8.02                        | 22.90                      | 3.82                                 |
| 9            | 6                        | 28       | 0.8044   | 1        | 0.0504        | 3.90            | 2            | 0.7620              | 0.1                    | 1.8620        | 0.295      | 4.197           | 5                             | 1.04         | 0.52              | 2           | 16.0            | 9.54                        | 23.53                      | 4.26                                 |
| 9            | 6                        | 28       | 0.7112   | 1        | 0.0504        | 4.21            | 2            | 0.8128              | 0.1                    | 1.9128        | 0.316      | 4.530           | 4                             | 1.44         | 0.72              | 2           | 14.1            | 8.96                        | 23.04                      | 3.84                                 |
| 9            | 6                        | 32       | 0.8728   | 1        | 0.0504        | 4.52            | 2            | 0.8636              | 0.1                    | 2.0636        | 0.337      | 4.864           | 4                             | 1.39         | 0.69              | 2           | 15.9            | 10.39                       | 26.36                      | 4.23                                 |
| 9            | 6                        | 32       | 0.8128   | 1        | 0.0504        | 4.84            | 2            | 0.9144              | 0.1                    | 1.8144        | 0.358      | 5.197           | 4                             | 1.34         | 0.67              | 2           | 15.9            | 11.93                       | 27.79                      | 4.63                                 |
| 9            | 6                        | 34       | 0.8828   | 1        | 0.0504        | 5.15            | 2            | 0.9652              | 0.1                    | 1.8652        | 0.379      | 5.550           | 4                             | 1.78         | 0.64              | 2           | 16.8            | 11.57                       | 28.33                      | 5.05                                 |
| 9            | 6                        | 36       | 0.9144   | 1        | 0.0504        | 5.46            | 2            | 1.0560              | 0.1                    | 1.1160        | 0.421      | 5.863           | 3                             | 1.98         | 0.99              | 2           | 13.7            | 11.49                       | 25.22                      | 4.20                                 |

Dia of pipe which would give worst loads (in): 34

Figure 5. Pipe load data generation

Wind Load Calculations:

A wind load calculation template is developed to calculate the forces on members as per ASCE 07 (Minimum design loads for buildings and other structures). Basic wind speed is taken from the relevant project design data. The Directionality factor, Topographic factor and Importance factor are considered as per the guidelines provided in the ASCE 07.

Earthquake loads are generally not considered in the pre-bidding analysis, and following primary loads, load combinations and load conditions are considered in the analysis.

Loads and Load combinations:

- Dead Load (D)
- Live Load (L)
- Temperature Load (T)
- Wind Load (W)
- Member Local Check Load (LC)
Sample wind pressure intensity calculation is presented below.

Wind Pressure Calculations as per ASCE 7-05

\[
q_z = 0.613 \ K_z \ K_{zt} \ K_d \ V^2 \ I
\]

| Height (m) | \(K_z\) | Height (m) | \(q_z\) (kN/m²) |
|------------|--------|------------|----------------|
| 0-4.6      | 1.03   | 0-4.6      | 1.22           |
| 4.6-6.1    | 1.08   | 4.6-6.1    | 1.28           |
| 6.1-7.6    | 1.12   | 6.1-7.6    | 1.33           |
| 7.6-9.1    | 1.16   | 7.6-9.1    | 1.37           |
| 9.1-12.2   | 1.22   | 9.1-12.2   | 1.44           |
| 12.2-15.2  | 1.27   | 12.2-15.2  | 1.50           |

Design Load Cases/Conditions:
- Erection / Shutdown
- Operation
- Hydro - Testing

Various load combinations are adapted in the design of structural steel pipe racks under the following heads when they are considered for each of the three Load cases:

1) Load Combinations for Global Steel Design
2) Load Combinations for Local Member Steel Design

**Analysis, Design and Steel Quantification:**

Using the first method, the inputs are very minimal and the final steel quantities can be found and tabulated.

For the second method, which involves the use of sophisticated software, the analysis and design would be carried out and an estimate would be created, then the steel quantification results would be tabulated.

The stiffness method of analysis is carried out in the Hybrid rational analytical model using the direct analysis method as per AISC 360 – 2010. Structural steel design follows the LRFD approach. Then, the steel quantification results are tabulated for comparison.

**3. Results and Discussion**

The final steel structural design is mainly checked for strength and serviceability load combinations. For serviceability, the vertical deflections of beams and horizontal drifts of columns are checked against the permissible limits as per steel design code. The unity ratio is checked for strength load combinations for all structural members.

For steel quantification purposes the overall steel incidence in kg/m³ is the key factor. The steel incidences obtained from various methods and the detailed engineering process are tabulated in Table 2. From this table it is clearly seen that the rational hybrid model produces closest result to the detailed engineering (DE) value, and comes out higher, so as to remain conservative. These details are depicted by the chart in Figure 6.

| Steel incidences | Statistical | Rigorous | Hybrid model | Detailed Engg. |
|------------------|-------------|----------|--------------|----------------|
| Incidence (kg/m³)| 23          | 20       | 17           | 16             |

**Table 2. Steel incidences**
The overall steel quantities from each method are further split into four categories such as light steel, medium steel, heavy steel and extra heavy steel based on their weight per meter run. The weight ranges are less than 25 kg/m, 25 kg/m to less than 70 kg/m, 70 kg/m to less than 125 kg/m, and above 125 kg/m, respectively, to ease the procurement planning. Tertiary members are quantified as percentages of main frame members based on improved statistical data analysis. The Medium steel and Heavy steel classification of steel quantities do not have many practical implications, and many contracting firms have three classifications only, namely Light steel, Medium steel and Heavy steel.

Finally, after the detailed engineering calculations are done, the quantities are checked and compared to find the difference and which method is closest to the detailed engineering outcome. Keeping the detailed engineering quantity as the benchmark with 100% accuracy, the incidences arrived from the two conventional methods and rational hybrid analytical model are calculated in percentages. Thus, the degree of accuracy of the steel quantity calculations in percentage terms are tabulated in Table 3 for comparison. A chart depicting the values provided in the quantification accuracy percentage comparison table is shown in Figure 7.

The time taken for the quantity calculations using each method is also compared and is provided in Table 4. A bar chart showing the time taken using each method is illustrated in Figure 8.

### Table 3. Quantification accuracy percentages

| Steel Incidence | Statistical | Rigorous | Hybrid model | Detailed Engg. |
|-----------------|-------------|----------|--------------|----------------|
| Light steel     | 35          | 20       | 30           | 20             |
| Medium steel    | 40          | 15       | 17           | 55             |
| Heavy steel     | 15          | 7        | 53           | 20             |
| Extra heavy steel | 10      | 58       | 0            | 5              |
| Steel incidence | 56.25       | 75       | 93.75        | 100            |

### Table 4. Time consumption

| Time (hours) | Statistical | Rigorous | Hybrid model | Detailed Engg. |
|--------------|-------------|----------|--------------|----------------|
|              | 4           | 48       | 2            | 200            |

Detailed engineering man hours generally range from 200 to 300 hours; however, the lower value has been considered in the above comparison. Even though the statistical method consumes less time, its steel incidence results are too far from the detailed engineering calculations, as shown in Table 2, resulting in highly uneconomical values, and leads to over estimation of the steel quantities, which is highly undesirable in the pre-bid engineering calculations.

![Figure 6. Incidence chart](image-url)
4. Conclusion

Based on the results provided in the steel incidences table (Table 2), it is evident that the results obtained through the rational hybrid analytical model are much closer to the actual detailed engineering results in terms of the steel incidence ratio, which is the basis for the quantification and pre-bidding calculations. It is also clear that the hybrid model comes out slightly on the conservative side, which is necessary for the pre-bid engineering phase. It also takes much less time than the rigorous software method.

This work provides a comprehensive solution for the quantification of steel pipe rack structures in Oil and Gas plants, which is necessary as many onshore plants are cropping up around the world to cope with the increased demand for Oil and Gas consumables, as discussed in the Introduction section. Therefore, it is clear that the newly developed hybrid rational model will be a boon to contracting firms involved in the bidding for Oil and Gas EPCC projects worldwide by giving them the ability to quantify the materials needed with more accuracy and within least possible timeframe. It has been discovered that the rational hybrid analytical model will be of much use to structural engineers in calculating steel quantities more accurately and in less time.
The limitations of this method can be viewed as the inability to deal with pipe racks of more than one bay and more than seven stories, which is very rare and seldom occurs in any Oil and Gas onshore plant. In future research, the same analytical model could be further developed to design the structural steel members using the Allowable stress method (ASD), and to check and compare the quantities arrived at using that methodology.

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6. Conflicts of Interest

The authors declare no conflict of interest.

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Effect of Interaction between Bridge Piers on Local Scouring in Cohesive Soils

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Abstract

Local scour at the piers is one of the main reasons of bridge foundation undermining. Earlier research studies focused mainly on the scour at a single bridge pier; nevertheless, modern designs of the bridges comprise wide-span and thus group of piers rather than a single pier are usually used to support the superstructure. The flow and scour pattern around group of piers is different from the case of a single pier due to the interaction effect. Reviewing the literature of local scour around bridge piers group revealed that the local scour around bridge piers group founded in cohesive soil bed was not investigated, and most of the scour studies were related to scour in cohesionless soils. The objective of the present study is to investigate the effect of the interaction between two in-line (tandem) circular bridge piers of variable spacings founded in cohesive soil on the local scour. A set of laboratory flume experiments were conducted under the clear-water scour condition to investigate this effect. This study is the first that investigates experimentally the scour around group of bridge piers in cohesive bed. It was found that the maximum scour depth at the upstream pier of the two in-line piers occurred at a spacing of two times the diameter of the pier, scour at the downstream pier was reduced due to a sheltering effect, the interference effect will be reduced for pier spacings larger than three times of the pier diameter. A recent pier scour equation was used to estimate the scour depths at the two in-line piers in cohesive soil and compare the estimated value with the measured scour depths in the laboratory. The comparison indicated that the proposed scour equation overestimates the scour depths at both the upstream and the downstream pier.

Keywords: Tandem Piers; In-Line Piers; Bridge Pier Interaction; Cohesive Soils; Sand-clay Bed.

1. Introduction

Local scour around the piers and abutments of bridges is a primary risk of structural instability and collapse. Local scour occurs due to the erosive action of the flowing water that excavates and carries away the soil from around the bridge piers and abutments when they are constructed in erodible beds. Therefore, the understanding of the scour mechanisms at the foundations of a bridge must be considered for design purposes. Studies of bridge pier scour have been conducting since the 1950s, and numerous design methods and predictive equations were developed for the assessment of the local scour depth around bridge piers from various points of view and under different conditions. There are a considerable number of research studies about the scour and flow structures around a single bridge pier, on the other hand fewer researches were done about the scour and flow field around group of piers.

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In recent practice the designed bridges are typically of wide-spans and thus group of piers rather than a single pier are used to support the superstructure. The scour processes at pier groups are more complicated because of the interaction of the flow structures and consequently, the scour pattern differs from that of a single pier. Local scouring around bridge pier groups in cohesionless soil beds was investigated in researches of [1-13, 15]. Laursen and Toch [1] presented the scour patterns at the foundation of two bridge piers arranged in-line and parallel to the flow direction, they observed that the scope of scour cultivates as the two piers orientation diverges from the approach flow direction. Hannah [2] observed that the maximum scour depth is influenced by the dimension of the piers group from the upstream direction, he found that the worst case in clear water scour around group of two piers happens at a spacing of 2.5 of the pier widths. Elliott and Baker [3] examined experimentally the impact of bridge pier group spacing on the local scour. From the results of the experimental runs, the effect of pier spacing on scour depth was quantified using empirical formulae. However, those formulae were developed considering clear water scour, one pier arrangement, one case of flow shallowness and one bed material type. Nazariha [4] also investigated local scouring at groups of bridge piers with the aim of developing design relationships for the prediction of local scour under clear water steady uniform current. The developed equations involved two important parameters describing the group effect, these are pier spacing to pier diameter ratio and the flow attack angle.

Zarrati et al. [5] examined in their study the efficiency of pier collars and riprap layer in reducing the local scour depth around bridge pier groups. They conducted an experimental study and compared their findings with those of earlier studies on single piers with collars and pier groups without collars. The results showed that in the case of two in-line piers with continuous collars and a riprap layer produced the most significant reduction in the scour depth, equal to 50 and 60% for the front and rear piers, respectively. In the other cases, individual collars around each one of the two in-line piers showed better efficiency than a continuous collar around both piers. The results indicated that collars are not so effective in reducing the scour around two side by side piers. Heidarpour et al. [6] extended the experimental investigation of the effect of collars on the reduction of scour around group of two piers to include three piers, they used circular collars around the front and the rear piers. They concluded that collars are effective in reducing the scour around two and three in-line piers, the scour reduction was more when the collars covered the space between the piers completely, the efficiency of the collars in reducing the scour depth in the rear pier was more than that at the front pier due to a weaker down flow at the rear pier and the collars presence slowed the scour development at the piers.

Ataie-Ashtiani and Aslani-Kordkandi [7] studied experimentally the flow field around two circular piers placed side-by-side for two bed configurations, with and without a scour hole. They used a synthetic glue to freeze the bed and investigate the flow field only. They presented the features of the flow field in details and stated that it is different from that of a single pier and the interference between the horseshoe vortices is responsible for the greater scour depth observed between the two piers. Saghravani and Azhari [8] investigated the local scour around a single and three in-line circular piers by laboratory flume tests and numerical simulations. They used a 2-phase Eulerian model to simulate the local scour in bed of uniform sand under clear-water scour condition. They got number of findings from their research as follows. (1) The laboratory tests and the numerical simulations showed the same scour pattern, which means that the 2-phase Eulerian model was able to simulate the local scour around the bridge piers, (2) in the all tests the resulting scour depth was larger at the front pier, less at the middle one and the smallest at the rear pier and (3) an 8% increase in the scour depth at the front pier in the group of 3 in-line piers as compared to the single pier because of the effect of the reinforcement of the turbulence flow structures. Ataie-Ashtiani and Aslani-Kordkandi [9] conducted another research to study the flow field around two in-line bridge piers founded in a relatively rough flat bed. They compared the features of the flow field at a single pier to that at the group of piers. The results indicated that the interaction between the piers changes the flow structure to a great extent, particularly in the near-wake region. The velocity of the flow near the rear pier decreases to 0.2–0.3 times of the approach flow velocity which indicates the sheltering effect of the front pier. It was found that the formation of flow with different Reynolds number along the flow depth because of bed roughness and pier spacing influences the type of flow regime around two in-line piers.

Beg [10] studied the characteristics of the local scour hole around two unequal sized bridge piers installed in-line with flow direction. They investigated experimentally the influence of mutual interference of two piers of various spacing subjected to steady flow and under clear-water scour. Kim et al. [11] presented a numerical study for the flow and local scour around two circular piers positioned in staggered line with different spacing ratios (S/D) and alignment angles (θ). The spacing ratio of center-to-center distance between the piers (S) to the pier diameter (D) varied from 1.25 to 5.0 and the alignment angles ranged from 0° to 90°. The simulation was done by using a large eddy simulation (LES), a Lagrangian sediment transport model and a morphodynamical model. The results of the study showed that the scour depth is more influenced by the spacing ratio and alignment angles at the rear pier. For small alignment angles, the scour rate at the rear pier increased with the increase in the spacing ratio. For larger alignment angles (45°-60°) the scour depth at the rear pier increased subsequently.

Keshavarzi et al. [12] derived a formula for the prediction of the maximum scour depths around two inline bridge piers aligned with the flow, their formula involved the influence of bridge piers spacing and they evaluated the
predicted scour depths with that of the most common scour equations and arrived at accepted results. Das et al. [13] investigated the local scour around a group of three piers, where two in-line piers are placed parallel to the flow and a third pier is placed eccentrically in middle of the tandem piers. They conducted a set of laboratory experiments to explore the pattern and location of scour formed around the piers group and the dune formed downstream of this arrangement. They used various spacing between the tandem piers to identify the spacing that produces the maximum scour depth. The investigation showed that for such three piers arrangement, the scour at the staggered piers was maximum and the scour around tandem downstream pier was minimum. They also proposed empirical equations to estimate the scour depth around each pier of the piers group individually.

Most of the implemented research work on local bridge pier scour was concerning non-cohesive soils riverbed. Scour around piers in a cohesive soil is more complicated than the scouring in cohesionless soil, in addition to the complex flow structures, the chemical and physical bonding of the cohesive soil particles are involved in the scour influencers. In cohesionless soils of gravel/sand the gravity forces and the submerged density of the soil particles are the main resistance forces to scouring; while in cohesive soils the inter-particle bonding forces resist scouring and control the scouring rate. Few researchers studied the scour around bridge piers in cohesive soils. Debnath and Chaudhuri [14] conducted an extensive experimental study on local scour around single bridge piers in clay–sand mixed bed. They stated that “it is the combined effect of shearing resistance of soil bed and the applied shear stress generated by flow that determines the location of maximum scour depth at the pier, and that the scour initiates at the sides of the pier and then propagates to downstream”. Li [15] conducted a research that involves an experimental program to study the scour at bridge pier of complex geometry using Porcelain clay as a channel bed material. The effect of pier groups was studied, and correction factors were proposed to enable a more accurate estimate of scour depths at side by side bridge piers. The study by Li [15] was the only reported research in the literature that considered scour around group of piers founded in cohesive soils. They presented a method of scour depth estimation at side-by-side piers with different spacings but there was no description for the pattern of scour hole nor the effect of pier interaction on scour depth development.

This paper is dedicated to explaining the effect of the interaction between two in-line (tandem) circular bridge piers on the local scour hole around bridge piers founded in cohesive soil by using physical modeling and laboratory experiments. For this purpose, in the next sections the materials and experimental setup used in the study were explained, the results of local scour hole geometry and maximum scour measurements were also presented, finally, a comparison of the measured maximum scour depths versus values computed using a pier scour equation was presented.

2. Materials and Methods

To investigate the effect of bridge pier interaction on the local scour, several experiments were conducted in a rectangular-section flume 14 m long, 1 m wide and 1 m deep located at the Porous Media Laboratory, Amirkabir University of Technology, Tehran, Iran. The bed and sides of the flume were made of glass supported by a metal frame. The flume is equipped with a vertical sluice gate which regulates the approach flow depth and velocity. The discharge into the flume was by an inlet valve and the flow rate was measured by a sharp crested rectangular weir located at the flume outlet. The tests were conducted in the sediment recess 5.0 m downstream of the flume inlet, which is 2.5 m long and 0.30 m deep (Figure 1).

A circular plexiglass pier models of 5 cm diameter (D) were used. Experiments were conducted using a single pier and two in-line (tandem) piers placed parallel to the flow direction. The piers were placed at the longitudinal centerline of the flume in the sediment recess. For the two in-line piers experimental runs, the center-to-center spacing between piers (S_p) were selected to vary as S_p = 2D, 2.5D, 3D, 4D, 6D and 8D. Figure 2 displays a graphical representation of the two in-line circular pier models placed in the test section of the flume.

A cohesive soil mixture made up of kaolinite clay mixed with uniform fine sand having d_50=0.15 mm was used as the bed material in the scour experiments. The cohesive soil comprises 30% clay mixed with 70% fine sand by dry weight. The sand-clay mixture was placed in the sediment recess in the flume and the flume filled with water to saturate the soil for a duration of 3 hours. This step allows the clay-sand mixture to form cohesive bonds similar to the natural cohesive soils. The bed material preparation procedure was based on the observations and recommendations of previous researchers who studied scouring in the cohesive soils [14-18]. Soil tests were performed for the sand-clay mixture after saturation and before the inanition of the scour experiments, soil-testing procedures were according to the ASTM. A summary of the cohesive soil properties is given in Table 1.

A set of experimental runs were conducted using a single pier and two in-line piers having various spacings. Each experimental run lasted for a 24-hr duration. This time interval was enough to arrive at the state of no observed sediment movement around the piers. All the experiments were carried out under clear water scour conditions. The approach flow velocity was selected to be near the critical velocity, V_c, for the sand fraction in bed material and was predicted using the Shield’s method. The flow intensity (V/V_c) was set to 0.94. The applied flow rate to achieve these
conditions was 37.5 l/s. The approach flow depth (y) was constant and equal to 15 cm. At the end of each experiment, the flume was drained slowly and carefully. Then, the bed level around the piers was measured using a laser-meter. The scour depth and scour hole geometry around both piers were measured. It is worth to mention that the size of the flume, pier models and other dimensions were selected to satisfy the universal criteria for scouring experiments and avoid scale effects.

![Figure 1. A schematic representation of the flume used in the experiments](image1)

![Figure 2. A graphical representation of the two in-line circular pier models arrangement](image2)

| Soil property                  | Value  |
|-------------------------------|--------|
| Liquid limit (%)              | 19     |
| Plastic limit (%)             | 12     |
| Plasticity index (%)          | 7      |
| Water content (%)             | 21.5   |
| Specific gravity              | 2.64   |
| Median size, d₅₀ (mm)         | 0.085  |
| Undrained shear strength (KPa)| 13.5   |
3. Results and Discussion

3.1. Scour Hole Patterns at Single and Two In-line Piers in Cohesive Soil

Table 2 presents the results of 7 experimental runs that were conducted to investigate the effect of bridge piers interaction. It was reported in the literature that the local scour hole around a single bridge pier founded in sand starts at the front of the pier and propagates to the downstream and the maximum scour depth is observed at the pier sides. For the case of scour in cohesive soils, the scour mostly starts from the pier sides and the scour depths at the two sides of the pier may not be identical. These observations were reported by Ansari et al. [18], Debnath and Chaudhuri [14]. In this study, the first experimental run was for a single circular bridge pier of D = 5 cm founded in sand-clay soil and subjected to a steady flow of 37.5 l/s. After duration of 24 hr, the final scour hole was recorded and the maximum scour depths at four scales 0°, 90°, 180° and 270° were measured. The result of this test agreed with the previous observations of researchers.

The flow field around a group of bridge piers is different from that of a single pier and it is more complex. In the study published by Ataie-Ashiani and Aslani-Kordkandi [9] the flow field around two tandem piers and around a single pier was compared based on laboratory flume experiments. The results illustrated that the existence of the downstream pier alters the flow structures principally at the rear region of the upstream pier. A sheltering effect due to the upstream pier reduces the flow velocity near the downstream pier to 0.2–0.3 of the velocity at wake of a single pier. In tandem arrangement, higher values of turbulence characteristics were observed at the downstream pier. The results also indicated a weakness in the vortices at the rear of the tandem piers as compared to single one.

In this study, the resulted scour hole patterns at single and two in-line piers with variable spacings in cohesive soil are displayed in Figure 3. For a pier that is a part of two in-line piers parallel with the flow direction, reinforcement and sheltering affect the local scour depth. A reinforcement is observed when a downstream pier is placed at a distance from the upstream pier that their scour holes intersect. This effect increases the removal of the bed soil from around the upstream pier and thus increasing its local scour depth. It was found that the scour at the downstream pier was reduced due to the sheltering effect resulting from the upstream pier that reduced the effective flow velocity for the downstream pier and consequently reduced the scour depth at the downstream pier.

For large ratios of pier spacing to pier diameter (S/p/D), it was observed that the sheltering effect is pronounced on the scour depth at downstream pier (Figure 3). Based on the piers spacings range, S/p that were investigated, the following observations were made. Smaller pier spacing results in a larger interference of flow structures between the piers. When the spacing ratio (S/p/D ≤2.5) the piers group will behave as one pier. The interaction effect will be reduced for pier spacing of (S/p/D >3) with the consideration of the pier-group arrangement. These findings were in general agreement with those of previous research on local scour around two in-line piers in cohesionless soil [1-13].

It was observed that the sediment that was eroded from the scour hole at the piers was transported and deposited at the downstream of the piers. The sediment deposit at the downstream was variable for the piers’ arrangement. It was simple and little in the case of single pier, while it extended wider in the case of two in-line piers. The formation of the downstream hill deposit had different shape for two in-line piers varied with the space between the piers as it is shown in Figure 4.

| Run | S/p/D | d1 (mm) | d2 (mm) | d3/d1 | d4/d1 |
|-----|-------|---------|---------|-------|-------|
| 1   | Single | 61      |         | -     | -     |
| 2   | 2     | 67      | 59      | 1.10  | 0.97  |
| 3   | 2.5   | 55      | 52      | 0.90  | 0.85  |
| 4   | 3     | 51      | 48      | 0.84  | 0.79  |
| 5   | 4     | 61      | 51      | 1.00  | 0.84  |
| 6   | 6     | 60      | 45      | 0.98  | 0.74  |
| 7   | 8     | 64      | 38      | 1.05  | 0.62  |

Table 2. Experimental measurements for the effect of piers interaction
Figure 3. Scour hole patterns at circular single pier and two in-line piers with variable $S_p$ in cohesive soil. (a) Single (b) $S_p=2D$ (c) $S_p=2.5D$ (d) $S_p=3D$ (e) $S_p=4D$ (f) $S_p=6D$ (g) $S_p=8D$
3.2. Maximum Scour Depths at Two In-line Piers in Cohesive Soil

Referring to Table 2, the experimental data of measured scour depths at the upstream pier and the downstream pier shows that at spacing equals 2D the scour depth of the upstream pier was maximum. Igarashi [19] found that “the maximum drag force around a two in-line piers occurs when the spacing between them is less than 2.5D”. Gao et al. [20] pointed out that “two recirculation regions surrounded by the shear layers can be observed at the rear of two in-line piers of $S_p/D = 2.4$”. Therefore, the reported result in this study matches the observations by Igarashi [19] and Gao et al. [20] where they studied the local scour around group of piers in cohesionless soils. In addition, in this study it was observed that the maximum scour depth was 10% greater than that of the single pier which is in consistent with the observation by Keshavarzi et al. [12]. Keshavarzi et al. [12] also stated that “the maximum scour depth might occur at a spacing ratio between 2 D and 3 D. For the case of the spacing between piers is 1D, the observed scour depth was like the scour depth for the single pier case” [12]. The scour depth at the upstream pier increased when the spacing between the piers increased to 2.5 D and decreased when the spacing increased above 3D. At the spacing ratio $S_p/D > 4$ the local scour depth converges to that of the single pier. This observation may be attributed to the found by Igarashi [19]. In the present study, the piers spacing was the effective parameter that was investigated and was tested in a range of 2D to 8D (D = pier diameter). The range of pier spacing were selected according to the most common conditions in the field and the recorded scour depths at the piers were equal to the scour depth at the single pier.

Figures 3 and 4 and Table 2 show the effect of interaction between two in-line circular piers on the maximum scour depth at the upstream and downstream pier. From the results, it is obvious that the scour depth at the downstream pier is always smaller than the single pier case. The reason for that is the destruction of the horseshoe vortex in front of the downstream pier as was illustrated by Hannah [2] and Keshavarzi et al. [12]. The scour depth at the upstream pier is always larger than that of the downstream pier. It was reported in the literature that “not only under steady state flow the maximum scour depth at the upstream pier is greater than that of the downstream pier, results of an experimental study conducted by Tafarojnoruz et al. [21] showed that this performance was observation also under hydrograph test when the flow varies with time. Possibly it is due to the sheltering effect that created by the upstream pier. The sheltering effect is observed when the piers spacing ration $S_p/D$ is less than 10, which causes a decrease in the approach flow velocity at the downstream pier and consequently decreasing the scour depth” [12].

3.3. Comparison of the Predicted Maximum Scour Depths with the Measured Data

The measured scour depths at the upstream pier and the downstream pier are compared with scour depths predicted by the TAMU-scour method developed by Briaud [22]. This method was developed for the prediction of the scour hole depth at bridge supports taking into consideration the soil erosion characteristics. It is one of the recent methods that were presented in the literature to predict the local scour around bridge piers in cohesive soils. The equation for the maximum local scour depth at a bridge pier in cohesive soil is given by:

$$\frac{d_s(\text{pier})}{b} = 2.2K_{pw}K_{psh}K_{pa}K_{ps}(2.6 \cdot Fr(\text{pier}) - Fr_c(\text{pier}))^{0.7}$$

(1)

Where $d_s(\text{pier}) = \text{maximum pier scour depth}; b = \text{effective width of the pier}; K_{pw} = \text{flow shallowness factor for pier scour depth}; K_{psh} = \text{pier nose shape influence factor}; K_{pa} = \text{aspect ratio influence factor (the aspect ratio L/B is the}
ratio of pier length $L$ over pier width $B$ for non-circular piers; $K_{pwp}$ = pier spacing influence factor for pier groups arranged side by side; $F_{r(pier)} = \text{pier Froude number based on the approach flow velocity}$ $V$; and $Fr_{c(pier)} = \text{critical pier Froude number based on critical velocity for soil particles motion.}$ This critical velocity is estimated for the cohesionless soils from the Shields method or tested in an erosion apparatus (such as the erosion function apparatus EFA that developed by Briaud et al. [23]) for cohesive soils. The effective width $\hat{b}$ is found as:

$$\hat{b} = b\left(\cos \theta + \frac{c}{b} \sin \theta\right)$$

(2)

Where $\theta$ = attack angle, which is the angle between the flow direction and the pier main axis. The correction factors involved in the TAMU-scour method can be calculated as below. The shape correction factor $K_{psh}$ is presented in Table 3. The correction factor for the aspect ratio is considered by using the effective width $\hat{b}$, $K_{psh}$ value is always 1.

Table 3. Pier nose shape correction Factors (Kpsh)

| Shape          | Kpsh |
|----------------|------|
| Square nose    | 1.1  |
| Round nose     | 1.0  |
| Circular cylinder | 1.0  |
| Sharp nose     | 0.9  |

$$K_{pwp} = \begin{cases} 
0.89 \left(\frac{c}{b}\right)^{0.33} & \text{for } \frac{y}{b} < 1.43 \\
1.0 & \text{else}
\end{cases}$$

(3)

$$K_{pwp} = \begin{cases} 
2.9 \left(\frac{c}{b}\right)^{-0.91} & \text{for } \frac{y}{b} < 3.22 \\
1.0 & \text{else}
\end{cases}, S \text{ is pier spacing}$$

(4)

$$F_{r(pier)} = \frac{V}{\sqrt{g \hat{b}}}$$

(5)

$$F_{rc(pier)} = \frac{V_c}{\sqrt{g \hat{b}}}$$

(6)

Briaud [22] evaluated the TAMU-method by using 10 data sets. The data sets included laboratory flume test results and field measurements for the scour depth. The evaluation process indicated that multiplying the estimated scour depth of TAMU-method by a factor of 1.5 gave safe estimations for the design purposes.

For the present study, the local scour depth at a circular pier in cohesive bed is predicted by the TAMU-scour method developed by Briaud [22] and the computed results were compared to the measured scour depths at the upstream and downstream pier in the laboratory. The results of the prediction are showed in Figures 5 and 6 for upstream and downstream piers, respectively. From the comparison it is apparent that the TAMU-scour method consistently overestimates the measured scour depths. The TAMU-scour method considers the effect of piers spacing in a direction perpendicular to the flow direction and considers its effect on the scour depth up to a spacing ratio of $(S_p/D < 3.22)$. The overestimation in the downstream pier scour depth was more than that of the upstream pier. The TAMU-scour method involves a parameter to describe the bed soil erodibility which gives different scour depth prediction in different soils. This parameter is presented in the critical pier Froude number in equation (1), which can be estimated for the case of sand or cohesionless soils as the critical velocity for particles motion from Shields methodology. Or for the case of cohesive soils from the erosion function test (using the EFA). For the prediction of the scour depth at the two in-line piers in this study, the critical velocity for initiation of motion of the sand fraction in the clay-sand bed soil was used to predict the critical pier Froude number. The overestimation in the scour depths at the two in-line piers that is observed when using the TAMU-scour method by Briaud [22] may be attributed to this reason. Moreover, equation (1) predicts the local pier scour depth assuming a constant flow velocity that lasts long enough to reach the maximum equilibrium scour depth. In the present study, the experiments were conducted for a duration of 24 hr until a stable scour hole depth was reached. These scour depths might be considered as final scour depths after a specific time interval.
Local scour around bridge piers is one of the main reasons of bridge failures. It occurs due to the erosive action of the flowing water that excavates and carries away the soil from around the bridge piers, that may result in the exposure of the bridge foundation to the water flow and consequently causes structure’s undermining. Extensive research studies about the scour and flow structures around a single bridge pier were conducted, while on the other hand fewer researches were done about the scour and flow field around group of piers. The modern bridges of wide spans consist of group of piers that used to support the superstructure. The scour processes at pier groups differs from that for the case of a single pier. Many of the researchers who investigated the local pier scour related the scour depth to the flow...
parameters and pier geometry without considering the erosional characteristics of the bed. A few researchers considered the effect of the cohesive soil characteristics on the scour depths. However, most of the studies on local scour in cohesive soils were restricted to single bridge pier. A new research is proposed to study the local scour around group of bridge piers founded in cohesive soil bed. It is based on a set of laboratory flume experiments that were conducted to investigate the effect of the interaction between two circular bridge piers placed in-line parallel to the flow direction on the local scouring.

The size of the used flume, pier models and other dimensions for flow parameters and bed sediment were selected to satisfy the universal criteria for scouring experiments and to avoid scale effects. The following observations were noted based on the experimental measurements. The scour depth measured at the upstream pier was greater than that measured at the downstream pier in all experiments. The maximum recorded scour depth for the two in-line piers observed at a space ratio of $S_p/D < 2.5$ and this scour depth was 10% higher than the scour depth at the single pier. For large space ratios ($S_p/D > 3$), the upstream pier scour depth approximates to the single pier scour depth. An important conclusion that can be drawn from this research is that the scour patterns and sediment transportation characteristics both change in case of group of bridge piers. From this investigation, the scour hole geometry and downstream sediment deposition characteristics are configured for the effect of piers interaction. However, the observed effects of the interference of piers of a bridge could be seen for many pier spacing and pier arrangement of any bridge. A recent pier scour equation, namely TAMU scour method, was used to predict the scour depths at the upstream and downstream piers in sand-clay bed. The results of the proposed equation were compared with the measured scour depths in the laboratory. The comparison showed that the proposed equation overestimates the scour depths at both the upstream and the downstream pier.

5. Conflicts of Interest

The authors declare no conflict of interest.

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Dynamic Identification of an Early 20\textsuperscript{th} Century Civil Architectural Building

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Abstract

Historical structures are important in terms of both original construction techniques and cultural heritage. Therefore, material properties, construction techniques and dynamic behaviours of these structures must be identified in order to preserve them in the future by restoration studies. This study is aimed to serve as an example for similar buildings in the region whose walls were constructed using filled brick with lime mortar and constructed using both timber and reinforced concrete slabs. In this study, the plan layout, construction techniques and the material usage of the building were investigated in detail. The mechanical and dynamic properties such as compressive stress, elastic moduli, shear stress, natural frequencies and mode shapes of the building were determined in-situ by flat-jack, shear and vibration tests. The finite element model of the structure was prepared, and the modal analysis of the structure was performed. The calibration of the model was ensured according to the vibration test results. The results obtained from this study show us that in-situ tests are extremely important for the accuracy of finite element models. It has been determined that the mechanical test data can be used with over 80\% success in finite element models.

Keywords: Timber; Masonry; Construction Technique; Operational Modal Analysis; Mechanical Tests.

1. Introduction

The studied building is situated in the centre of the Edremit district. It was constructed in the first quarter of the 20\textsuperscript{th} century. The building is a modern architectural heritage in terms of its architectural features. The building has lots of values such as value of originality, value of rarity, economic value, social value, functional value and political value, as discussed by B. M. Feilden and J. Jokiletho [1]. The house, which gained its importance with the hosting of Mustafa Kemal Atatürk in 1934, is known as the Atatürk House in the collective memory of the district.

In terms of historical features, today's codes and standards are not sufficient for the restoration of the masonry structures. The complexity of the structure, the diversity in the use of materials, the different construction techniques, the absence of knowledge about the changes in time and causes of damage throughout its existence are the important problems. The mechanical properties and dynamic characteristics of the building should be identified by in-situ tests. The most effective methods for identifying the mechanical properties of masonry structures are flat-jack and shear tests. In these tests, a flatjack is inserted in a cut slot in the mortar and displacements are continuously read while hydraulic oil pressure is inflated into the metal plate. These test methods have been used over a long time by researchers [2-4]. The most common experimental study for identifying the dynamic properties of masonry structures is the Operational Modal Analysis (OMA) test method. In this test method, the dynamic parameters such as natural frequencies, mode shapes and damping ratios are estimated from output-only responses. There are many studies using

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the OMA technique to identify the dynamic parameters of masonry constructions [5-13].

After performing the in-situ tests, the finite element model of the structure should be prepared in order to find out the structural behavior of the building. However, in many research studies, the finite element models did not accurately represent the real behavior of the structure. This was due to the estimation of the material properties without performing any in-situ tests. In some research studies, the material properties performed by test methods but vibration tests did not performed. For this reason, identifying the material properties and dynamic characteristics of the building gains importance before the finite element analysis of the building. The finite element model should be controlled and calibrated by comparing the modal analysis results and the in-situ vibration test results. After the calibration, the finite element model can represent the real behavior of the building. The mass participation factors, the mode shapes and the other structural analyses such as earthquake analysis, pushover analysis, etc. can be performed by using this model. In addition, the success of the flat-jack and shear test results is also investigated by the researchers.

In the first part of the paper, the methodology of the research is explained with a flowchart. This is followed by the expression of the plan, construction techniques and material usage of the building. After this, the mechanical properties and dynamic characteristic of the building are investigated by using in-situ tests. The modal analysis is performed using a finite element analysis program. After the calibration of the finite element model, the mode shapes, natural frequencies and mass participation factors are presented in tables and the results are discussed in the conclusion part.

2. Research Methodology

In this study, the plan layout, construction techniques and material usage of the building were investigated on-site and the mechanical properties such as compressive stress, elastic moduli and shear stress of the masonry walls were investigated by using in-situ flat-jack and shear tests. The dynamic characteristics such as mode shapes and natural frequencies of the structure were analyzed by using in-situ vibration tests. The OMA test method was used for determining the dynamic characteristics of the structure. The finite element model of the structure was prepared, and the modal analysis of the structure was performed by using the ALGOR finite element program. The finite element model calibrations were done by comparing the frequencies obtained from the vibration tests and the finite element modal analysis. The process was repeated until the difference was under 10% and the finite element model was formed at the end. The flowchart of the study is presented in Figure 1.

![Flowchart](image.png)

Figure 1. The flowchart of the study

3. Plan, Construction Techniques and Material Usage

The studied building, Edremit Atatürk House, is situated at the centre of the district. Edremit is a district of Balıkesir Province which is located in the north-west of Turkey and on the coast of the Aegean Sea. The building is situated on Çayıçi Street which is one of the most frequented streets in Edremit. The location of Edremit district and the studied house is presented in Figure 2.
Figure 2. Edremit district and the studied building (Google Earth)

The house gained its importance with the hosting of Mustafa Kemal Atatürk in 1934. The construction of the house began in the first quarter of the 20th century according to the architectural features. After it was exposed to a fire in 1991, the house was unavailable for use (Figure 3). Timber beams, timber slabs and the roof of the building collapsed after the fire.

Figure 3. The studied building a) Outside view of the building b) Inside view of the building

The house has three storeys; basement, ground floor and first floor. The house has a courtyard. The basement height is 2.10 m, while the ground and first floor heights are both 3.50 m. The basement floor plan can be seen in Figure 4.

Figure 4. The basement floor plan of the building
The walls of the building were constructed using brick material. Lime mortar was used as a binding material. Brick was used in the interior and exterior walls. The wall thicknesses are different for the exterior and interior walls. The exterior wall thicknesses are 50cm in the basement, and 40cm in the other storeys. The interior wall thicknesses are 45cm in the basement, 30cm in the ground floor and 25cm in the first floor. Two different techniques were used in the slab constructions. Timber slab was used in the living areas, while reinforced concrete slab was used in the wet areas and the entrance of the building. It is believed that these two types of slabs were constructed at the same time because there were no construction joints in the intersection of the walls, and the slab elevations are equal. Despite the fire, the reinforced concrete slabs are intact today (Figure 5).

Figure 5. The reinforced concrete slab in the entrance part of the building

The reinforced concrete slab and timber slab usage in the construction of the building is shown in Figure 6.

Figure 6. The reinforced concrete and timber slabs of the building

4. The Mechanical Properties of the Brick Walls

The mechanical properties such as compressive stress, shear stress and elastic moduli of the walls were investigated by using in-situ flat-jack and shear tests. The single flat-jack method was used for determining the compressive stress and elastic moduli of the walls. In this method, a flatjack is inserted in a cut slot in the mortar and displacements are continuously read while hydraulic oil pressure is inflated into the flatjack (Figure 7). The tests were conducted according to ASTM C1197 and ASTM C1314 [14, 15].
The method C was used in the shear test according to ASTM C1531-09 [16]. In this method, the flatjack is horizontally inserted at one end of the test unit (Figure 8). The oil pressure is applied until the slip of the mortar occurs.

The average compressive stress, shear stress and elastic moduli of the walls are presented in Table 1.

Table 1. Mechanical properties of brick walls

| Property          | Value   |
|-------------------|---------|
| Compressive stress| 2.10 N/mm² |
| Shear stress      | 0.50 N/mm² |
| Elastic moduli    | 2750 N/mm² |

5. Vibration Tests

Vibration tests were conducted in-situ by placing sensitive accelerometers on the walls of the building. The Operational Modal Analysis test method was used to obtain the dynamic parameters of structure. Natural vibration frequencies and mode shapes were obtained by using this non-destructive test method.

The dynamic parameters of the structure from output-only experimental data were found by this technique. The loads were environmental forces and the modal identification was based on responses only. The Dynamic Data
Acquisition/Structural Health Monitoring Device Testbox 2010 series data acquisition system was used in the study [17]. Six uniaxial accelerometers were used and for the accuracy of the tests, 20–30 minute test periods were applied. In the sensor placements, the perpendicular orientations were carefully checked for all walls. The sensors were placed on top of the first and second floor corners. Three sensors were placed on each floor. The orientations of the sensors on the plan view are shown in Figure 9.

![Figure 9. The sensor orientations on plan views a) Second floor b) First floor](image)

The placements of sensor number 5 and sensor number 6 on the second floor and the test equipment can be seen in Figure 10.

![Figure 10. The sensor placements and the test equipment](image)

Frequency Domain Decomposition (FDD) was used in determination of the dynamic characteristics. The singular values of the spectral densities of the test setups are shown in Figure 11. The first mode frequencies can be seen in the figure.
6. Finite Element Analysis

The three-dimensional finite element model of the studied building was prepared using the Algor finite element analysis program [18]. The building is modeled using brick elements having three degrees-of-freedom at every node. The material properties of the walls were obtained from the experimental studies. After the finite element models were prepared, the modal analysis of the building was performed. The mode shapes, natural frequencies and mass participation factors were obtained from numerical analyses. The material properties and the boundary conditions were updated in order to represent the real behavior of the building which was obtained from the experimental vibration tests.

The elastic moduli of the walls were taken with an average of 2250 N/mm^2 after the calibrations. There is only an 18% difference between the flat-jack test results. The first four mode shapes and the frequencies are presented in figure 12. The first mode is the displacement in the y direction, the second mode is the torsion, the third mode is the displacement in the x direction and the fourth mode is the torsion.
The comparisons of the first four mode frequencies of the studied building between the vibration test results and the finite element analysis results after calibrations are presented in Table 2. It was determined that there was a maximum 5% difference between the frequency values. It can be stated that the finite element model of the structure now represents the real behavior of the structure correctly. Earthquake analysis, pushover analysis, and etc. can be done by using this model.

Table 2. First four mode frequencies (experimental vibration test versus finite element analysis)

| Mode Number | Vibration test | Finite element | Error |
|-------------|----------------|----------------|-------|
| 1           | 4.32           | 4.33           | % 0.23|
| 2           | 4.93           | 4.73           | % 4   |
| 3           | 5.51           | 5.59           | % 1.43|
| 4           | 6.20           | 5.86           | % 5.48|

The mass participation factors of the first four modes in the x and y directions are presented in Table 3. Due to the lack of horizontal connections between the walls, the whole structure could not be completely included in the mass ratios. Therefore, the total mass participation ratios are low in the first four modes.

Table 3. The mass participation factors of the first four modes in the x and y directions

| First mode | Second mode | Third mode | Fourth mode |
|------------|-------------|------------|-------------|
| x          | y           | x          | y           | x          | y          |
| 0.12       | 31.11       | 0.20       | 1.32        | 14.50      | 0.75       | 0.46       | 0.09       |

7. Conclusions

Understanding the current status of historical buildings will enable them to be restored in a healthy way. The construction techniques, the material usage, the mechanical properties of the walls and the dynamic characteristics of the structure must be determined precisely. The finite element models must represent the real behavior of the structure. Finally, the structural behavior of the building in all load cases should be performed by computer analysis.

Due to the unique construction techniques and material usages of each historical structure, the material properties obtained from the codes and standards are not sufficient for analysing a masonry structure. In some studies, the material properties of the structures were estimated by the researchers without any in-situ tests. Sometimes, the material properties were performed by test methods, but vibration tests were not performed. In all cases, the finite element models could not be sufficient for representing the real behavior of the structure. Only comprehensive on-site investigations and effective in-situ test methods can ensure the correct finite element models of the structure.

In this study, the dynamic identification of an early 20th century civil architectural building was investigated by using on-site investigations, in-situ experimental tests and finite element analysis.

The general conclusions of this study are outlined below.

- To understand the construction techniques and the material usage of the structure is important to ensure the correct finite element model.
- The flat-jack, shear and vibration tests were necessary to identify the mechanical and dynamic properties of the structure.
- The finite element model must be calibrated by comparing the vibration test results with the modal analysis results.
- There is only an 18% difference in elastic moduli values between the tests results and the calibrated finite element models. It can be stated that even if vibration tests are not performed, a close finite element model can be formed only with flat-jack and shear test data.
- After calibration of the material properties, the errors between the vibration test results and the modal analysis ranged from a minimum of 0.23% to a maximum of 5.48%. These results show us that there was very good harmony between the frequencies and the finite element models.
- Due to the lack of horizontal timber beams between the walls, about 20–30% of the whole structure could only be included in the mass ratios after the total of the first four mode frequencies.
- A full understanding from on-site investigations, in-situ tests and the finite element analysis has great importance for the success of the restoration works.
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9. Conflicts of Interest

The authors declare no conflict of interest.

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Healing of Generated Cracks in Cement Mortar Using MICP

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Abstract
This research is carried out to investigate pre-existing repair cracks in cement mortar using the microbiologically induced calcium carbonate precipitation (MICP) technology. In the study, 20-cylinder mortar samples (45 mm in diameter and 40 mm in length) were split to have cracked width of various sizes. Out of twenty cracked samples, sixteen samples of average crack width ranging from 0.12 to 1.3 mm were repaired using the MICP method, while four cracked samples, with an average crack width ranging from 0.16 to 1.55 mm were soaked under distilled water. The water permeability and split tensile strength (STS) of these repaired mortars were tested. The amount of CaCO₃ precipitated on the cracked mortar surfaces was evaluated. The results indicated that the MICP repair technique clearly reduced the water permeability of the cracked samples within the range of 73 to 84 %; while water-treated samples were too weak to undergo test. MICP-repaired samples had STS ranging from 29 to 380 kPa after 24 rounds of treatment. A relationship between the STS and percentage amount of CaCO₃ precipitated was observed for samples with an average crack width between 0.29 and 1.1 mm, which indicated that STS increased with percentage increase in CaCO₃ precipitated on the crack surfaces.

Keywords: MICP; Split Tensile Strength; Cement Mortar; Permeability.

1. Introduction
The generation of cracks in concrete is a natural phenomenon due to earthquakes, weathering or manmade activities which will adversely affect the life and durability of the structures. The measure cause of the crack is due to lower tensile strength and brittle nature of concrete. The harmful pollutants, chemicals, and water penetrate through the cracks which lead to deterioration of concrete. The present methods existing to repair such cracks are the use of chemicals, grout, or surface treatment which could be harmful to the end-users as well as to the environment. Eco-friendly, sustainable and new technique MICP as the new area of interest is a substitute to repair cracks [1]. MICP process depends on ureolytic non-pathogenic bacteria (Bacillus pasteurii) to hydrolyze urea in the presence of calcium ion which leads to calcite precipitation. Purified bacterial cells, containing the enzyme in high concentrations, were used to catalyse the hydrolysis of urea and produce ammonium and carbonate ions. Urease enzyme decomposes urea into ammonium (NH₄⁺) and carbonate ions (CO₃²⁻). The combination of this negative carbonate ions and positive Calcium ions (Ca²⁺) available from cementing solution, result in the formation of Calcium Carbonate. The reactions involved are as follows:

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This bio generated CaCO$_3$ binds loose particles of matter together, plugs fine pores and cracks. The ultimate effect of this is to increase the engineering properties of concrete and fill the existing cracks, if any. MICP process can be applied for repairing cracks in two ways. First, as pre-treatment where bacteria and cementation solution are mixed with fresh concrete to prevent crack development. This is referred to as autogenous repair or self-healing and another is post-treatment where bacteria and cementation solution are applied in the crack influenced areas of concrete. The use of the MICP method to repair cracks in concrete was studied by several earlier researchers. Substantial and noticeable work was carried by researchers [2-5]. The method of crack healing induced by MICP can be employed in two ways. Alkali-resistant spore-forming bacteria get activated by water and oxygen which infiltrated through cracks and further feed on an available substrate. Subsequently decomposition of a substrate to produce calcium carbonates result in the healing of cracks [4]. Researchers commonly use spore-forming Bacillus species micro-organism. Bacillus pesudoformus, Bacillus sphaericus, Bacillus alkalinitrilicus with calcium lactate were used for investigation. Quantification of crack-healing shows that up to 0.46 mm wide cracks are repaired by bacteria and control specimens after 100 days submersion in water [5].

Another method of self-healing is by mixing of ureolytic microbes which can survive in high alkaline conditions and urease-calcium as nutrients during concrete production. The successful healing of 0.81 mm cracks width after 28 days treatment was reported by using Bacillus subtilis with graphite nano-platelets (GNP) and light-weight aggregate (LWA) as carrier compounds [6]. The progress of self-healing by mixing bacteria in fresh concrete is satisfactory. This method is not suitable for the remediation of existing cracks in concrete. Minimum research is available on the repair of existing cracks in concrete. Manual generation of 3.175 mm width of crack at two different depths by saw cut in mortar beam of size 25x25x150 mm was applied during investigation [7]. Remediation was carried by sand and Bacillus pasteurii. The compressive strength test on the remediated mortar beams after 28 days of curing in the urea-CaCl$_2$ solution was conducted. Test results show that cracks were healed and an increase in compressive strength as compared with virgin was noted. An increase in compressive strength by 50% was noticed after MICP treatment given to cement mortar having a crack of 0.3 mm width, 20 mm depth and 50 mm in length. Author Ramachandra concluded that the remediation of shallow cracks in comparison with deeper cracks can be achieved effectively with MICP. The experimentation on repairing crack of dimension 0.3 mm wide × 20 mm deep × 50 mm length in 50 mm cubic mortar by injecting a mixture of Sporocinapasteurii, urea-CaCl$_2$, and sand showed 50% increase in compressive strength as compared to untreated samples [8]. A similar experiment conducted by (Achal et al., 2013), have used Bacillus sp., to investigate durability properties and remediation of simulated cracks (3 mm in width and 13-27 mm in depth) in 70 mm cubic mortar samples [9]. They found that, more than 50% reduction in porosity, 40% increase in compressive strength and successful healing of the simulated cracks of various depths. Cement mortar specimen of 1:3 cement-sand ratios with different porosity achieved by varying w/c ratio as 0.5, 0.6, and 0.7 and was used to verify the performance of Bacillus sphaericus carbonate precipitation. The result shows that the based-on porosity, reduction of water absorption of specimens was in the range of 65 to 90% [10]. The enhancement in durability and water tightness due to precipitation of calcite in the cracks was used to achieve self-healing of concrete [11].

The detailed study for the repair of cracks in concrete using various methods was mentioned [12]. Most of the above-referred study mentions regain in compressive strength and reduction of permeability as an indicator for crack repair effectiveness using MICP. Also limited research on remediation of realistic cracks and widely varied procedures adopted by researchers. Application of MICP in the field of building material, preservation of monuments and soil bio clogging was highlighted by Joshi et al., (2017) [13]. He concludes that the application of MICP is effective for self-healing of cracks in concrete and mortar. Use of Bacillus sphaericus with sodium alginate was employed during concrete mixing and hardening by adopting three techniques such as freeze-drying, extrusion, and spray drying [14]. Enhancement of mechanical properties of concrete such as split tensile, compressive and flexural strength and reduction in permeability, water absorption, sulphate ion concentration and volume of voids, by using MICP techniques [15, 16]. Use of ureolytic and non-ureolytic bacteria in recycled aggregate and recycled aggregate concrete to reduce the water absorption and increase in specific gravity of the material [17]. The development of cracks in concrete is a symptom of weakness in the tensile strength of concrete. Evaluation of the effectiveness of cracks repairs through split tensile strength (STS) and the amount of CaCO$_3$ precipitation as an indicator has focused the objective of this research.

This paper hereby aims to determine the filling of generated crack width by using MICP and its efficacy of repair. The study encompasses a reduction in permeability, a percentage amount of CaCO$_3$ precipitation the cracks and recoups of the tensile strength of cracked mortar after implementation of proposed MICP treatment.
2. Materials and Sample Preparation

Figure 1 represent the basic flowchart which gives detail information about the selection of bacteria and its cultivation of culture. Preparation of desired molarity cementation solution of CaCl$_2$ using standard OPC cement, locally available sand with desired water cement ratio. Cement mortar was prepared by using this mixture. Artificial cracks were generated as mentioned in section 2.2. and followed by MICP treatment. The repaired sample were tested for permeability and split tensile test using standard methods.

![Flowchart](image)

**Figure 1.** Represent flow diagram of the overall process followed

2.1. Bacterial Culture and Cultivation

Due to the high urease activity of *Bacillus pasteurii* or *Sporosarcinapasteurii*, these microbes are extensively preferred to produce a high amount of precipitates within a short period of time [18]. Bacterial culture of *Bacillus Pasteurii NCIM* 2477 shown in Figure 2(a) was collected from the National Collection of Industrial Microorganism, Pune, Maharashtra (India). *Bacillus Pasteurii* is cultivated in the laboratory using nutrient agar media with protocol and instruction mentioned on the container of culture medium. 20 grams of agar and four grams of nutrient agar powder were mixed well in 250 ml distilled water and the pH was adjusted between 7 to 7.5. The Nutrient agar solution was then heated up to boiling point 100°C using the heater. The autoclave was used for sterilization of nutrient solution and other glassware. Figure 2(b) shows the Cultivation of culture.

![Images](image)

**Figure 2.** (a) Bacterial culture; (b) Cultivation of culture (microorganism)
2.2. Preparation of Cementation Solution

Ureolytic driven calcite precipitation was achieved by using urea calcium cementation media. From the AR grade of urea and calcium chloride (CaCl₂) were used. For complete production of calcite, molecular weights of urea (CO(NH₂)₂) and anhydrous calcium chloride (CaCl₂) is approximately 60.06 g/mole and 111 g/mole, respectively. The cementation solution of 0.25 M of concentration was made by dissolving 15.1 g of urea (solid) and 27.75 g of anhydrous CaCl₂ (solid) into 1 liter of water. To facilitate precipitation of small size and strong calcium carbonate which can penetrate in small cracks, a low chemical concentration was used as suggested by Al Qabyan et al. (2013) [19].

2.3. Preparation of Mortar Specimens

Type I ordinary Portland cement (OPC) of 53 grade, river sand, and distilled water were used to prepare mortar. Figure 3a illustrates the grading curve of sand used. The cement had a specific gravity of 3.12, normal consistency 29%, bulk density 1400 Kg/m³ and Blaine fineness 330 m²/kg. The sand had a specific gravity of 2.68 and a fineness modulus of 2.62 and density 1600 Kg/m³. The water-to-cement (w/c) ratio was 0.4 and the sand-to-cement (s/c) ratio was 3.0. To prepare a homogeneous mix of the mortar, the cement was first added into water and mixed by hand for 2 min followed by sand mixing for another 2 min. Thin plastic pipes (45 mm in diameter and 90 mm in height) were used for casting. Two half rods of 10 mm diameter and 90 mm length were placed in molds to ensure single and straight crack in the sample. The freshly mixed mortar was poured into these molds as shown in Figure 3b, in two layers, and each layer of all samples was compacted to the equal desired density. After casting, the mortar samples were sealed and placed in a lab environment (24 to 26°C) for 28 days for curing. At the age of 28 days, three virgin samples (ST1, ST2, ST3) were tested for split tensile strength according to IS-5816-1999 and the rest cylinder samples were cut to develop/gain different crack sizes and then to perform crack repair.

2.4. Generation of Cracks in Mortar Specimens

In the process of generation of artificial cracks of different sizes in all 10 mortar samples, end portions were trimmed by 10 mm and the middle 80 mm was cut in equal two half with their plastic molds on, each of 45 mm diameter and 40 mm in length. These, 20 short discs samples were split to have different crack widths using a jaw clamp as shown in Figure 4. A sample crack generated is shown in Figure 5. A small clamping arrangement was made to keep crack open, and photographs of both end cross-section were taken. At the end of 28 days, small clamps were removed, and crack repair work was initiated.
Figure 4. Crack generation

Figure 5. Camera picture

Figure 6. Image through CAD
Figures 5 and 6 show a photograph and the features received through CAD respectively for a few samples. A photography examination was done to understand the size and pattern of cracks generated. The photo images were then inputted to (CAD) to characterize the crack features and compute crack areas and widths. For a correct representation of crack width and to account for irregularity of cracks at two ends of the disc, the average crack size of the two ends was used and further calculation was made using the Equations 3 and 4.

Crack area (%) = \( \frac{\text{crack area}}{\text{sample cross section area}} \times 100\% \)  

Crack width (mm) = \( \frac{\text{average crack area}}{\text{average crack length}} \)

The four samples (UTC1 to UTC4) out of 20, with the average crack width in the range 0.16 mm to 1.55 mm, were placed in distilled water for 24 days to understand autogenously crack healing of mortar. These samples are referred to henceforth as untreated samples. The balances of sixteen samples (TC1 to TC16), with the average crack width ranging from 0.12 to 1.30 mm, were used for the MICP repair tests which were treated with MICP.

2.5. Crack Repair

MICP treatment for sixteen samples was performed in bacterium solution and urea-CaCl₂ solution at room temperature 30 ± 2°C. Each cracked sample was soaked in bacterium solution for 2 hours as shown in Figure 7(a) and allowed the samples to saturate. After taking out from the bacterium solution, samples were made to drain off. Then all these samples were put in a container having urea-CaCl₂ cementation solution as shown in Figure 7(b) for the MICP process to happen. These 24 hours is counted as one round of treatment. The whole assembly of the sample with cementation solution was kept circulating with the help of a plate and stirrer bar. Repeat all these steps for the next 8, 16, 24 rounds of the treatment.

3. Test and Methods

3.1. Water Permeability

Permeability test on all sixteen samples was conducted using the constant head method as per IS-2720 (Part17)1986 to find the efficacy of repair using MICP treatment and curing period concerning crack width. All samples were soaked in water for 24 hours for saturation before conducting the permeability test. A sample of 45 mm diameter and 40 mm length was trimmed at the end to just fit at bottom of transparent graduated glass pipe of 45 mm diameter, 150 mm height. The proper arrangement was made to seal the joints of the pipe and specimen. This assembly of permeability mould as shown in Figure 8(a) and experimental set up shown in Figure 8(b). Tap water was continuously filled in a glass pipe to maintain a constant head with a proper outlet for overflow. The volume of water flowing out from the container and corresponding time was recorded to calculate the coefficient of permeability k using the formula mentioned in Equation 5.

\[ k = \frac{qL}{Ah} \]

Where \( k \) = Coefficient of permeability in mm/sec; \( q \) = discharge in mm³/sec; \( L \) = Length of specimen in mm; \( A \) = Cross-sectional area of specimen in mm² and \( h \) = Constant head in mm.
3.2. Splitting Tensile Strength (STS)

At the end of 28 days, three virgin samples (ST1, ST2, ST3) of 45 mm diameter and 90 mm in height which were not subjected to MICP treatment, were tested for STS according to IS 5816-1999. Sixteen samples (TC1 to TC16) were split to gain different sizes of crack and then used for crack repair using MICP treatment and four samples (UTC1 to UTC4) as control samples without MICP treatment. These sixteen (TC1 to TC16) were dried under an ambient environment for two days and tested for STS as per IS 5816-1999. The amount of CaCO$_3$ deposited on both end fractured surfaces were measured and expressed as percent of the total fractured surface area.

4. Results and Discussion

Permeability test on all sixteen samples was conducted using the constant head method as per IS2720-1986 (Part17) to find the efficacy of repair using MICP treatment and curing period concerning crack width. All samples were soaked in water for 24 hours; the results obtained for sixteen MICP treated samples through permeability, STS and percent of precipitated CaCO$_3$ are summarized in Table 1. Table 2 depicts the results of permeability on four untreated samples. Figure 9 illustrate the linear relation of crack width generated and percent of fractured area. Figure 9 satisfies strong linear association among the crack width and fractured area.

| MICP Treated Sample | Original fracture | Permeability (mm/sec) | STS (kPa) at 24th round | % of CaCO$_3$ at 24th round |
|---------------------|-------------------|-----------------------|------------------------|---------------------------|
| TC1                 | 0.32              | 0.008335              | 0.002812               | 0.002104                  | 77.76845 | 43.26   | 4.95   |
| TC2                 | 0.37              | 0.01652               | 0.005967               | 0.004717                  | 0.004175 | 74.7285 | 29.85  | 5.13   |
| TC3                 | 0.41              | 0.1157                | 0.03697                | 0.029283                  | 0.02589  | 77.62316 | 33.85  | 4.12   |
| TC4                 | 0.52              | 0.1312                | 0.04889                | 0.03857                   | 0.03521  | 73.16311 | 45.2   | 4.68   |
| TC5                 | 0.54              | 0.1473                | 0.04825                | 0.03693                   | 0.032271 | 78.09165 | 51.91  | 6.73   |
| TC6                 | 0.58              | 0.1587                | 0.05812                | 0.04812                   | 0.04136  | 73.93825 | 95.32  | 7.19   |
| TC7                 | 0.65              | 0.1868                | 0.06867                | 0.05054                   | 0.04869  | 73.93469 | 122.34 | 15.68  |
| TC8                 | 0.78              | 0.28689               | 0.08912                | 0.07012                   | 0.06839  | 76.1616 | 128.38 | 17.32  |
| TC9                 | 0.84              | 0.3768                | 0.151869               | 0.11104                   | 0.08945  | 76.26062 | 148.48 | 21.14  |
| TC10                | 0.87              | 0.6107                | 0.265946               | 0.208238                  | 0.13674  | 77.6093 | 178.32 | 19.46  |
| TC11                | 0.98              | 0.7532                | 0.29678                | 0.22985                   | 0.147851 | 80.37029 | 195.67 | 20.08  |
| TC12                | 1.45              | 0.9476                | 0.41935                | 0.28745                   | 0.2003   | 78.86239 | 242.58 | 52.32  |
| TC13                | 1.92              | 1.1254                | 0.37384                | 0.27758                   | 0.1712   | 84.78763 | 275.82 | 65.84  |
| TC14                | 2.13              | 1.2147                | 0.43748                | 0.30367                   | 0.19894  | 83.62229 | 292.38 | 79.25  |
| TC15                | 2.38              | 1.3254                | 0.53858                | 0.32756                   | 0.25131  | 81.03893 | 380.5  | 82.34  |
| TC16                | 2.45              | 1.4721                | 0.81367                | 0.62576                   | 0.51576  | 64.96434 | 311.58 | 69.27  |
Table 2. Test result of Untreated (controlled) samples for autogenous healing

| Untreated sample (Soaked in water only) | % Fraction Area | Ave. crack width (mm) | Permeability (mm/sec) |
|----------------------------------------|----------------|-----------------------|-----------------------|
|                                        |                |                       | 0 Round | 8th Round | 16th Round | 24th Round |
| UTC1                                   | 0.43           | 0.16                  | 0.08053   | 0.067258  | 0.06136    | 0.06013    |
| UTC2                                   | 0.82           | 0.3                   | 0.19751   | 0.17145   | 0.1648     | 0.1596     |
| UTC3                                   | 1.37           | 0.76                  | 1.01637   | 0.8983    | 0.86771    | 0.85472    |
| UTC4                                   | 2.47           | 1.55                  | 1.98531   | 1.84654   | 1.780194   | 1.75483    |

Figure 9. Generated crack width Vs % fracture area of mortar sample

4.1. Crack Healing

Progress of crack healing at different rounds for the representative sample is shown in Figure 10. It is observed from Figure 10, that due to MICP treatment, cracks are gradually healed over the number of treatment round. Healing of cracks varies with the percent of precipitation of CaCO₃. Smaller cracks get healed at earlier round. It is to note that internal cracks could not get repaired 100% in spite of precipitation of a sufficient quantity of CaCO₃. Table 1 depicts that, for the sample TC15, the maximum percent of deposition of CaCO₃ on the cracked surface was 82.34 rather than 100%. Also, negligible healing of crack is observed in samples (UTC1 to UTC4) which are untreated (soaked in water only). Similar report has been mentioned by author Chen et al. (2019) [20] that MICP can effectively use for healing of crack due to deposition of calcium carbonate deposition.

Figure 10. Cracks repairs at different rounds of MICP treatments. (a) At 8th round; (b) At 16th round; (c) At 24th round
4.2. Permeability

Figure 11(a) and 11(b) and Tables 1 and 2 represent crack repairing performance of MICP treated and untreated mortar samples on permeability respectively. Increase in permeability with an increase in average crack width, as seen in Figure 11(a). As crack width increases from 0.12 mm to 1.3 mm, permeability has increased from 0.008335 mm/sec to 1.4721 mm/sec. The authors are of opinion that results obtained are in line with Tittelboom et al. (2010) [1] in which the average crack width of the split cylinder increased from 0.15 to 0.30 has resulted in an increase in permeability from 0.05 mm/sec to 0.5 mm/sec. In the present study crack width ranges from 0.12 to 1.3 mm. The slope of (permeability vs crack width, Figure 11(a) curve is steeper for 0th round in comparison with the 24th round of MICP. Also, Figure 11(b) depicts an average 60% reduction in permeability of all cracked samples at end of 8th round after MICP treatment. The however smaller rate of reduction in permeability was observed at the end of 16th (25%) and 24th (14%) round respectively. This point out the percent of healing of cracks is faster up to 8th round and it slows down thereafter. This could happen because of the amount and dissemination of CaCO₃ in the cracks which have reduced permeability. At the end of the 24th round, the maximum reduction was in the range 73 to 85% as that of 0th round, indicating, 100% reduction in permeability could not be achieved because of the non-healing of all cracks.

From the above discussion, it is cleared that, number of MICP treatment rounds influences the reduction of permeability. Also, a higher rate of decrease in permeability at an early stage (8th cycle) as compared to the lower rate of decrease with an increase in the number of the round. Sample with wider cracks will have a higher rate of decrease in permeability as compared with fine cracks. This could happen because of more MICP solution can easily penetrate through wider cracks and deposits CaCO₃. On the contrary small cracks get plugged at the early stage of treatment. A decrease in R-squared values of curves in Figure 11(a) from 0.93 (0th round) to 0.75 (24th round) might be due to the amount and size of precipitated CaCO₃ in the cracks.
Figure 11 represents crack repairing performance of untreated (soaked in water only) mortar samples on permeability. The decrease in permeability up to 25% for the sample (UTC1) with fine 0.16 mm average crack width, from 0.08053 mm/sec at 0th round to 0.06013 mm/sec at 24th round could be the result of autogenous healing due to hydration of cement [18]. As anticipated for sample (UTC4) with a major crack of 1.55 mm, reduction in permeability on account of autogenous healing due to hydration of cement was negligible (11%).

4.3. Split Tensile Strength

The results of STS conducted on three virgin samples (ST1, ST2, ST3) at the age of 28 days, was 3674±126 kPa. This test was also conducted on MICP treated samples (TC1 to TC16) at the end of the 24th round. However, the test could not be possible on the untreated sample (UTC1 to UTC4) as it fails immediately on the application of negligible load. This could be because of insufficient binding developed due to the autogenous healing of cracks. The results obtained from the split tensile test on TC1 to TC16 samples are shown in Figure 12. Based on these following findings are noted.

- There is no co-relation of crack width on STS. The maximum values of STS were in the range of 29.85kPa to 380.5 kPa, almost 10% of the virgin sample (3674 kPa).
- The majority of the MICP treated sample has shown linear stress-strain behaviour with brittle failure at various axial strains.

It is presumed that the lower value of STS could be because of insufficient healing of cracks imperfect bonding developed among the cracked sample. Relationships between the STS, crack width, and percent of precipitation of CaCO₃ on the fractured crack surface and effectiveness of crack healing by MICP were studied. A similar result has been found by the potential application of bacteria for improvement of the split tensile test of concrete over the conventional concrete by the researcher Gavimath et al. (2012) [21].
Figure 12. (a) Crack width from 0.12-0.26 mm; (b) Crack width from 0.27-0.6 mm; (c) Crack width from 0.72-1.1 mm

Figures 12(a) to 12(c) STS vs strain curves for repaired specimens with different crack widths. Figure 13 (a), depicts the graphical presentation of the amount of CaCO₃ precipitated Vs. crack width. A peanut swing from 4.12 to 7.19% in calcium carbonate deposition is seen in a region I, where crack width is less than 0.27 mm. This could be due to minimal entry of bacteria or cementation solution in small cracks followed by 15 to 20% increase in CaCO₃ in region II of crack width 0.29 to 0.6 mm. Substantial increases in region III (52 to 82%) imply that the favorable crack width for repair through MICP is 0.72 to 1.1 mm. For region IV for 1.3 mm crack, an unexpected slight decrease in CaCO₃ may due to unidentified reasons.
The relationship between STS and crack width as shown in Figure 13(b) indicates that in the region I for crack width less than 0.29 mm, there is no clear co-relation. This could be because of quick sealing of small cracks might have stopped the entry of bacteria and cementation solution resulting in lower values of STS. Exactly reverse of this is observed in the region III, despite large crack width (1.3 mm), STS has decreased (311 kPa) over prior values (380 kPa). One of the causes could be insufficient sticking/formation of the bond between cracks and smaller size and microstructure of distribution of CaCO₃. This indicates from region II that, 0.31 to 1.1 mm crack width sizes in mortar can be effectively repaired by MICP.

5. Conclusions

The present study investigates the following

- Generated cracks in cement mortar can be repaired/healed by MICP. The performance of healing increases with an increase in treatment rounds. Almost all cracks rapidly get repaired in the first 8th round and thereafter process of healing becomes slower.

- The smallest and largest crack width was 0.12 and 1.3 mm respectively. The percent of reduction in permeability for the cracks ranging from 0.12 to 1.3 mm was in the range from 65 to 85%. The initial permeability of the smallest crack width was 0.008335 mm/sec which has reduced to 0.002812 mm/sec in 8th round, 0.002104 mm/sec in 16th and 0.001853 mm/sec in 24th round. While for the largest crack of width, reduction in permeability was from 1.4721 to 0.81367 mm/sec in 8th round, 0.62576 mm/sec in 16th round followed by 0.51576 mm/sec in 24th round. A maximum percent of reduction in permeability was observed for crack width of 0.8 mm which is from 1.1254 mm/sec to 0.37384 at 8th round, and 0.27758 to 0.1712 mm/sec at 16th and 24th round respectively.

- For untreated specimen having small crack width (0.16 mm), a considerable reduction in permeability took place in the first 8th round as compared to a large crack width of 1.55mm. This implies autogenously crack healing due to hydration of cement is more prominent in a small crack in comparison to larger crack width. The percent of reduction in permeability through autogenously crack healing was 25 to 11% for 0.16 and 1.55 mm crack width respectively.

- The results of STS conducted on three virgin samples (ST1, ST2, ST3) were 3674±126 kPa while on MICP treated samples (TC1 to TC16) it varies in the range 43 to 380 kPa i.e.1 to 10% of virgin samples. Conventional failure of concrete mortar is at 3% axial strain with stress-strain behaviour as linear. In our case, most of MICP repaired specimens of small crack (0.12 to 0.26 mm) have failed at axial strain less than 1% and specimens with larger crack (0.5 to 1.3 mm) at axial strain more than 2%, indicating a good improvement in repair after MICP treatment.

- Based on the test results obtained for percent of deposition of CaCO₃, STS, axial strain at failure, it implies, repairs through MICP is most effective for the size of cracks width within the range of 0.29 to 1.1 mm crack width.

6. Conflicts of Interest

The authors declare no conflict of interest.
7. References

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Effect of Fly Ash and Un-crushed Coarse Aggregates on Characteristics of SCC

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Abstract

This research paper discusses the change in the workability and strength characteristics of Self Compacting Concrete (SCC) due to addition of fly-ash and use of un-crushed Coarse Aggregate (CA). Laboratory based experimental work was carried out by preparing 12 SCC mixtures among which six mixtures contained crushed aggregate and other six mixtures contained un-crushed coarse aggregate. A total of 550 kg/m³ binder content and fixed Water-Binder (W/B) ratio as 0.35 were used. Two mixtures were controlled by using Portland Cement (PC) and other ten mixtures contained PC and Fly Ash (FA). Slump flow time, slump flow diameter and J-Ring height tests were conducted to study the fresh properties of SCC. Furthermore, compressive strength was calculated at 7, 14 and 28 days of curing. The outcomes indicated that the slump flow time, slump flow diameter and J-Ring height for all the mixes are within the limits specified by EFNARC guidelines. The compressive strength of SCCs depends upon dosage of fly ash. Compressive strength for SCCs with crushed CA was better than obtained in case of un-crushed CA. The maximum compressive strengths were observed as 64.58 MPa and 58.05 MPa for SCC with crushed and un-crushed CA respectively.

Keywords: Self-Compacting Concrete; SCC; Fly Ash; Un-crushed Coarse Aggregates; Fresh Properties; Compressive Strength.

1. Introduction

Compaction at narrow places is one of the major problems observed in reinforced concrete construction. However, the SCC is the best option in such situations. SCC is the one that flows through its own weight and hence is very effective in pouring at heavily-reinforced, narrow and deep sections without any vibrational efforts required [1-3]. SCC is the mixture of cement, aggregates, water, admixtures and some mineral additives analogous to the normal concrete. Unlike normal concrete, SCC requires more amount of fillers materials and Super Plasticizers (SP) to give better strength and workability. SCC results in reduction of labour work and also economizes the cost of concreting [4-8]. High quantity of fine-materials such as fly-ash is utilized for acquiring required workability to SCC. This also reduces the issue of segregation and bleeding while transportation and placement of concrete. Many researchers concerned with environmental conservation have criticized the use of cement as a binding material.

Since the demand of cement in concrete production is amplified, it has caused resource depletion, environmental damages and huge amount of carbon-dioxide (CO₂) emission during cement manufacturing process [9]. This has made serious concern of the practitioners and researchers to bring alternative materials of cement such as fly ash. These types of materials are considered safer for emitting. Thus, investigating symbolic properties of these waste materials open new possibilities for concrete development [10]. Use of such waste material in concrete is also very useful in enhancing the properties of concrete and also enhancing durability values [11-14]. Hence, this study has focused to...
conduct symbolic work for studying behaviour of fly ash in SCC. Fly ash generated from burnt coal is waste material and available at huge amount worldwide which creates more chances to use it as an alternate for cement concrete works. When the fly ash is inserted in concrete, it forms Calcium Hydrated Silicate Gel due to its reaction with calcium hydroxide during process of hydration at ambient temperature. Research works has highlighted that availability of Fly ash can provide the opportunity of replacing OPC up to 60% of its mass [9].

Several researchers have proposed and tested fly ash as mineral admixture for improving the properties at fresh and hardened state as well as the durability of the SCCs. Phathak and Siddique (2012) investigated of SCC with class F Fly ash by replacing cement with (0%, 30%, 40% and 50%) of fly-ash while temperature variation was considered as 20°C, 100°C, 200°C and 300°C. Test results revealed that compressive strength was in between 21.43 MPa and 40.68 MPa while tensile strength was recorded in between 1.35 MPa (min) and 3.60 MPa (max). The authors concluded that 28 days curing caused increment in compressive as well as tensile strength. Further, it was noted that compressive strength had improvement at the temperature of 200°C to 300°C while tensile strength was slightly reduced when temperature was raised above 20°C [15]. Fernando et al. (2018) developed SCC with reduced amount of cement. They added metakaolin and fly-ash as cementitious materials in SCC for evaluating flow ability and strength characteristics of concrete. From research work, it can be argued that metakaolin and fly ash addition is very usable in manufacturing low strength SCC with required workability and lower use of binder [16].

A research work conducted by Dinesh et al. (2017) showed comparison of effect of silica-fume and fly-ash as cementitious materials. The study revealed that silica fume exhibited positive results in increasing the concrete properties as compared to fly ash [17]. Jalal et al. (2015) studied the rheological characteristics of SCC when cement was partially replaced by silica nano, SF and fly ash. Experiments showed that fly ash is helpful in improving the rheological properties when compared with the other materials. However, when SF and silica nano particle are mixed together as cementitious material, they revealed considerable effect on both the mechanical and rheological characteristics [18]. Considering the need of sustainability, it is more advisable to utilize waste materials as new construction materials. This will exert positive impact on environment as well social values. Hence, this study is aimed to use fly ash as cementitious material to reduce the quantum of OPC. Also un-crushed coarse aggregates obtained from sieving of hill sand are used as coarse aggregate. For this purpose, total 12 concrete mixes were designed. Out of them six mixes for crushed and six for un-crushed CA with respect to the inclusion of fly ash. Fly ash has partially replaced (by weight), the cement at the levels of 0% to 20% with 4% increment. This article is structured systematically to study the behavior of fly ash in SCC. It is stated with introduction following the material and methodology used for conducted the research work. Finding of the current work are presented and the article is ended up with conclusion of the research work.

2. Materials and Methods

Methodology is systematic process for carrying out any research work. Stepwise approach used for this research is presented in following figure.

Figure 1. Flowchart to produce optimum SCC mix design
Figure 1 above depicts that the first step for conducting this study is selection of the material. The SCC mixtures used in this study were prepared with PC; lucky brand; conforming to the requirements specified in ASTM C150/C150M-18, class F fly ash (FA) according to ASTM C 618, the coarse aggregate used was both crushed and uncrushed in nature with a maximum size of 13 mm, while crushed hill sand passing from number 4 sieve was used in this study. The gradation curves for used material are presented in Figures 2 to 6.
A polycarboxylic-ether based super plasticizer having relative density of 1.08 and pH value equals to 6.2 was used in all mixtures. For comparing the effect of fly ash, 10 mixes were prepared as binary mixes i.e. blending OPC and FLA where fly ash replace equal amount of cement by weight while remaining 2 mixes were control mixes i.e. OPC was used as binder. W/B ratio for these mixes was taken as 0.35. Initially, mix proportions were considered in accordance with EFNARC guidelines [19] which were finalized through several laboratory trials. Description of various mix proportions are shown in Table 1.

Table 1. A detail of SCC mixes with quantities of ingredients for 1 m³

| S. No. | Mix ID  | Cement kg/m³ | Fly ash kg/m³ | Binder kg/m³ | W/B (%) | SP (%) | Sand kg/m³ | CA kg/m³ | SP kg/m³ | Water kg/m³ |
|--------|---------|---------------|----------------|--------------|---------|--------|------------|----------|----------|-------------|
| 1      | CM      | 550           | 0              | 550          | 0.35    | 2      | 850        | 890      | 11       | 192.5       |
| 2      | 4% Fly ash | 528       | 22             | 550          | 0.35    | 2      | 850        | 890      | 11       | 192.5       |
| 3      | 8% Fly ash | 506       | 44             | 550          | 0.35    | 2      | 850        | 890      | 11       | 192.5       |
| 4      | 12% Fly ash | 484       | 66             | 550          | 0.35    | 2      | 850        | 890      | 11       | 192.5       |
| 5      | 16% Fly ash | 462       | 88             | 550          | 0.35    | 2      | 850        | 890      | 11       | 192.5       |
| 6      | 20% Fly ash | 440       | 110            | 550          | 0.35    | 2      | 850        | 890      | 11       | 192.5       |
In assessing fresh properties of the mix compositions, flow ability was measured through slump flow time and flow diameter test while passing ability test was performed through J-ring test. Furthermore, compressive strength was checked at 7, 14 and 28 days curing to appraise the hardened properties of the concrete. Flow ability of all the mixes was controlled by slump flow diameter to maintain the required range i.e. 70 to 80 cm as advised by EFNARC (2002) [19]. For each mix proportions, several trial batches were prepared by varying the amount of super plasticizer to obtain the preferred value of slump flow diameter. Cubes having dimensions as 100 × 100 × 100 mm were casted and tested under compression to assess the hardened properties of the SCCs. Five cube specimens of each mix were casted from each batch. Ultimate compressive strength was computed based on average of five values as shown in Tables 3 and 4.

3. Results and Discussions

3.1. Fresh Properties

The Slump Flow time, Slump flow diameter and J-Ring Tests were performed in lab as EFNARC guidelines [19]. The results of the slump flow tests of concrete with fly ash are presented in Table 2. The spread diameter of slump flow ranges between 69.5-76.3 cm. From the Table 2 it can clearly be interpreted that spread diameter raised with enhancement in fly ash percentage, indicating that fly ash reduces the viscosity of the SCC mixes and thus encourages segregation. The same findings have also been reported by Bouzoubaa and Lachemi (2001) [20]. An identical trend is observed in slump flow time and J-Ring height for all the mixes within the limits specified by [19]. Un-crushed coarse aggregates have a flat surface. The flatness of the coarse aggregates enhances workability parameters. Table 2 depicted that workability of SCC mixes is more pronounced while using un-crushed CA.

| S. No. | Mix ID | Slump flow time \( T_{50} \) (sec) limits 2-5 sec | Slump flow diameter (cm) limits 65-80 cm | J-ring height (mm) limits 0-10 mm |
|--------|--------|--------------------------------|--------------------------------|-----------------|
|        |        | Crushed | Un-Crushed | Crushed | Un-Crushed | Crushed | Un-Crushed |
| 1      | CM     | 4.6     | 4.3        | 69.5    | 70.4        | 9.6     | 9.4        |
| 2      | 4% Fly ash | 4.4     | 4.2        | 70.25   | 71.2        | 9.53    | 9.2        |
| 3      | 8% Fly ash | 4       | 3.84       | 71.45   | 72.9        | 9.46    | 9          |
| 4      | 12% Fly ash | 3.92    | 3.79       | 72.15   | 74          | 9.2     | 8.6        |
| 5      | 16% Fly ash | 3.72    | 3.6        | 73.6    | 75.6        | 9.13    | 8.3        |
| 6      | 20% Fly ash | 3.54    | 3.2        | 74.8    | 76.3        | 8.9     | 8          |

Figure 7. Pictorial views of slump flow and J-ring tests

3.2. Compressive Strength

The results of average compressive strength with crushed and un-crushed (CA) at various testing curing ages are drawn in tabular form as in Tables 3 and 4.
Table 3. Average Compressive strength (Crushed Aggregates)

| S. No. | Mixes | Compressive Strength (MPa) |
|--------|-------|-----------------------------|
|        |       | 7 days | 14 days | 28 days   |
| 1      | 0% FA | 53.46  | 56.03   | 60.50     |
| 2      | 4% FA | 56.07  | 60.84   | 61.82     |
| 3      | 8% FA | 62.97  | 63.45   | 64.58     |
| 4      | 12% FA| 53.42  | 56.54   | 57.92     |
| 5      | 16% FA| 44.99  | 48.74   | 52.00     |
| 6      | 20% FA| 42.66  | 45.65   | 47.47     |

Table 4. Average Compressive strength (Un-crushed Aggregates)

| S. No. | Mixes | Compressive Strength (MPa) |
|--------|-------|-----------------------------|
|        |       | 7 days | 14 days | 28 days   |
| 1      | 0% FA | 45.90  | 51.39   | 55.85     |
| 2      | 4% FA | 48.83  | 54.17   | 57.38     |
| 3      | 8% FA | 51.44  | 55.18   | 58.05     |
| 4      | 12% FA| 39.81  | 45.02   | 47.23     |
| 5      | 16% FA| 38.95  | 44.20   | 45.94     |
| 6      | 20% FA| 32.92  | 37.02   | 38.72     |

Figure 8. Compressive strength at 7 days curing with crushed and un-crushed coarse aggregates

Figure 9. Compressive strength at 14 days curing with crushed and un-crushed coarse aggregates
Tables 3 and 4 presents the results of the average compressive strength profile of SCCs using crushed and un-crushed coarse aggregates at different curing ages respectively. It is observed that the compressive strength is improved by raising the dosage of fly ash up to 8%. The average increase was observed 6.7% and 4% at 28 days curing for SCC manufactured by using crushed and un-crushed aggregates respectively. While for more replacement levels of fly ash, the compressive strength is slightly decreased for both the concretes at all curing ages. Similar study was conducted by Jalal et al. (2015) by adding 10% fly ash where compressive strength measured at 28 day was recorded as 37.3 MPa [18]. Comparing the results of current study as in Table 2 with the work of Jalal et al. (2015), it can concluded that the compressive strength with 8% fly ash at 28 days obtained is approximately 18% higher than that achieved by Jalal et al. (2015). Figures 8, 9 and 10 shows the graphical comparison of compressive strength of...
proposed concrete by using crushed and un-crushed coarse aggregates for 7, 14 and 28 days curing respectively. Figures 11 and 12 gives graphical view of compressive strength at all curing ages for crushed and un-crushed aggregates concretes respectively. From these figures it may be observed that SCCs manufactured with crushed CA exhibited the higher compressive strength than concretes with un-crushed CA in the respective group of mixes having the same replacement levels of fly ash and curing ages.

4. Conclusions

From the obtained results subsequent conclusion are drawn:

- Fresh properties of SCC depend upon mix proportions and these can be adjusted with the appropriate dosage of SP;
- The optimum dosage of SP used to maintain the required specified values of slump flow diameter between 70 to 80 cm is 2% ;
- An identical trend was observed in slump flow time and J-Ring height for all the mixes were found to be within the limits specified for EFNARC;
- It was observed that the values of fresh properties are remarkably increased while using un-crushed CA;
- Compressive strength of SCCs depends upon the dosage of cement replacement levels of fly ash;
- The 28 days compressive strength of SCC with crushed and un-crushed CA increases by raising the percentage of fly ash to 8% instead of 6.7% and 4% of their respective controlled mix;
- The strength properties were improved when SCC was manufactured with crushed CA. The maximum compressive strength at 28 days was recorded 64.58 MPa at 8% replacement level of fly ash.

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6. Conflicts of Interest

The authors declare no conflict of interest.

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Model Development for the Prediction of the Resilient Modulus of Warm Mix Asphalt

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Abstract

Increasing material prices coupled with the emission of hazardous gases through the production and construction of Hot Mix Asphalt (HMA) has driven a strong movement toward the adoption of sustainable construction technology. Warm Mix Asphalt (WMA) is considered relatively a new technology, which enables the production and compaction of asphalt concrete mixtures at temperatures 15-40 °C lower than that of traditional hot mix asphalt. The Resilient modulus (Mr) which can be defined as the ratio of axial pulsating stress to the corresponding recoverable strain, is used to evaluate the relative quality of materials as well as to generate input for pavement design or pavement evaluation and analysis. Based on the aforementioned preface, it is possible to conclude that there is a real need to develop a predictive model for the resilient modulus of the pavement layer constructed using WMA. Within the experimental part of this study, 162 cylindrical specimens of WMA were prepared with dimensions of 101.6 mm in diameter and 63.5 mm in thickness. The specimens were subjected to the indirect tension test by pneumatic repeated loading system (PRLS) to characterize the resilient modulus. The test conditions (temperature and load duration) as well as mix parameters (asphalt content, filler content and type, and air voids) are considered as variables during the specimen's preparation. Following experimental part, the statistical part of the study includes a model development to predict the Mr using Minitab vs 17 software. The coefficient of determination (R²) is 0.964 for the predicted model which is referred to a very good relation obtained. The Mr value for the WMA is highly affected by the temperature and moderately by the load duration, whereas the mix parameters have a lower influence on the Mr.

Keywords: Warm Mix Asphalt (WMA); Hot Mix Asphalt (HMA); Resilient Modulus (Mr).

1. Introduction

Warm-Mix Asphalt (WMA) is an asphalt mixture that is commonly used in technologies that allow the manufacturing of asphalt mixtures at lower temperatures than those used for the preparation of Hot-Mix Asphalt (HMA). WMA is used as a technique to reduce the emissions of pollutant, energy consumption, and viscosity of the asphalt binder. The benefits of reducing the viscosity are that sufficient aggregate coating is obtained during the mixing, which enhances its workability and allows mix compaction at reduced temperatures [1].

WMA is offers different advantages from the conventional HMA. Firstly, it allows reduction of the production temperature of asphalt mixtures, which in turn help save more energy as compared to that by HMA, which depends mainly on the type of fuel used and the production temperature. Secondly, it offer the possibility of reducing greenhouse gas emissions through the reduced temperature of WMA production [2]. WMA achieve all the properties

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similar to HMA meanwhile reducing flaws of HMA by adding different types of additives like emulsions, wax-based, chemical and foam technologies [3]. All these steps reduce the bitumen viscosity, which improves the workability of the mixture to produce lower emissions and improve its working conditions [4]. Goh et al. (2007) briefly summarized the benefits of this technique as reduced fuel cost, reduced mixing and compaction temperature, slower aging of the binder, lower plant wear, reduced fumes and emissions, more ease of opening the work site early, improved workability, and extended paving window [5]. In this study, zeolite has used as an additive to achieve the desired asphalt warm mixture and added the same to the mixture at about 0.3% of its weight, which resulted in a reduction of the production temperature by about 30°C as compared to the control mixture [6]. The resilient modulus is the elastic modulus which is related to the theory of elasticity. It is well known that most of the paving materials are not elastic, but after load repetition and due to traffic load some permanent deformation occurs [7].

The Resilient modulus (Mr) is the modulus of elasticity of material under the influence of repeated loads. This value is used to measure the load’s distribution through the pavement layers. Generally, under the uniaxial dynamic loading, the proportion of the maximum applied stress to the maximum unit deformation is known as the Mr. Typically, pavement materials can be described as un-elastic, and, each time the load is repeated, it produces a small amount of plastic (permanent) deformation. However, if the strength of the material is greater than a load of traffic and, after a certain number of load repetitions, the deformation in each load is almost completely recoverable and proportional to the load and hence can be considered as elastic [8]. After approximately 100–200 load repetitions, the strain is practically all recoverable, as indicated by (ε). In confining the triaxial test, the ratio of deviator stress (σ = σ1 - σ3) to recoverable strain (εε) is termed as the Mr [8, 9]. The indirect tension test is the most common test under repeated load because of its simplicity for the measurement of the Mr of asphalt. In this test, a compressive load is applied with sine waveform in the vertical diametral plane of cylindrical specimens and then the resulting horizontal recoverable deformation is measured [10]. Owing to the difficulty of testing the Mr and the unavailability of the required equipment, it becomes necessary to predict the modulus of resilience from several variables, including temperature, loading waveform, and loading time [11]. Wibisono and Nikraz (2019) showed an increase in air voids, short load duration, a coarse aggregate gradation, and a small diameter of specimens gives the highest resilient modulus value [12].

You et al (2011) illustrated the effect of test and compaction temperature on the Mr by indirect tensile test. Two types of mixtures (HMA and WMA) were tested at 4 different temperatures (4, 21.1, 37.8, and 54.4 °C) for the 2 different percentages of Aspha-min (WMA additive) (0.3 and 0.5%). At the high temperature, the Mr increased slightly for both the Aspha-min® additive percentages in comparison to HMA. The test results at the high temperatures reveal that the Mr of WMA when compacted at 120°C was slightly higher when compared to those for WMA compacted at 100°C. Finally, when the compaction temperature increased, the Mr increased and made the high-temperature asphalt extremely soft and flowy [13]. Hurley et al. (2005) concluded that the addition of Aspha-min did not affect the Mr; however, the Mr decreased with a decrease in the compaction temperature [14]. Hamzah et al. (2008) noted that the Mr decreased by >90% when the temperature increased from 10°C to 40°C, which suggests that asphalt mix is sensitive to temperature change [15].

WMA with Aspha-min additive showed similar Mr at different temperatures as that of HMA [16]. Hilal (2018) reported that the average Mr decreased by 65.73% when the temperature increased from 10 to 25°C, while the average Mr decreased by 97.71% when the temperature increased from 25 to 40°C [17]. The average resilient modulus for WMA is lower than that of HMA by 23.8% at highest temperature of 40 °C as shown by Albayati (2018) [18]. Abdulmajeed et al. (2017) studied the effect of temperature on the Mr by using 3 types of asphalt binder and found that the Mr reduced by 39, 37, and 30% with asphalt binders 80-100, 60-70, and PG76, respectively, when the temperature increased from 30 to 40 °C. In addition, when the temperature increased from 40 to 50 °C, the three samples, respectively, showed lowering of the Mr by 77, 67, and 59% [19]. Little et al. (1992) reported that the most significant factors affecting the modulus of the asphalt-treated materials was the duration of the applied dynamic load. The increase in the duration of applied dynamic load decreased the modulus of the mixture [20].

Khan et al. (2015) proposed that the decrease of Mr from 30 to 18% increased the loading time of the vehicle; this increase indicates that the pavement deformed rapidly [21]. Shafabakhsh et al. (2016) explained the results of indirect tensile tests on Marshall specimens at different temperatures and loading times for haversine and square pulses, with different pulse widths for simulating the diverse vehicle speeds, while the square and haversine pulse forms represented stress pulse in the surface and binder layers successively. The Mr ratios at the low temperatures of 5 and 25°C slightly depended on the loading duration. At the high test temperature of 40°C, the differences between Mr of the binder and surface layers were time-dependent and decreased with an increase in the loading duration. The test results revealed that the difference between resilient behavior of the binder and surface layers was more apparent at high temperatures and under fast traffic loadings, as also reported elsewhere [22]. Under different traffic loading the WMA less elasticity than that of HMA mixture as illustrated by Sarsam and Nihad (2019) [23]. Neham (2015) illustrated the effect of asphalt content on the resilient modulus, it was showed that the resilient modulus increased by 18.35 % when asphalt content increased just 1% by weight of mix design [24]. Puzi (2010) showed that increasing of
asphalt content lead to rapidly reduced the values of MR, this increase reduce the strength of the specimen [25]. Hilal (2018) noted the values of Mr changed with filler type, when it was used Portland cement as a mineral filler is almost 4.422% increases the value for resilient modulus corresponding to limestone as a mineral filler [17]. Huan et al. (2011) illustrated the effect of three types of fillers (cement, hydrated lime, and quicklime) on resilient modulus, it is noted that cement gives the highest resilient modulus because cement displayed a much stronger and more active reaction capacity rather than hydrated lime, and quicklime [26].

The main objective of this research was to predict the Mr model of WMA from several variables that are otherwise used in mix design condition, such as asphalt content, filler content, filler types, and passing sieve no. 4, along with other variables that are used in test conditions such as temperature and load duration.

2. Materials and Methods

Local raw materials were used in this research, which were used for the pavement construction in Iraq: asphalt binder, aggregate, and mineral filler. Laboratory physical properties tests were implemented to the materials, and the results are given in the following paragraphs. The flowchart of the experimental design is presented in Figure 1.

![Flowchart of the experimental design](image)

Figure 1. Flow chart of the experimental design
2.1. Asphalt Binder

A type of asphalt binder used (40-50) was of penetration grade provided from the Dora refinery. Different tests were conducted (Table 1) for the determination of the physical properties of asphalt binder.

Table 1. Physical properties of asphalt cement

| Physical Properties | ASTM Designation | Asphalt Cement 40-50 |
|---------------------|------------------|----------------------|
| Penetration (100 gm; 250 C, 5 sec., 0.1 mm) | D5 | 46 | 40-50 |
| Ductility (250 C, 5 cm/min) | D113 | 132 | >100 |
| Softening point (4±1) 0 C/min. | D36 | 49 | - |

Properties After Thin - Film Oven Test ASTM D 1754

| Physical Properties | Test Result | SCRB Specification |
|---------------------|-------------|--------------------|
| Penetration(100 gm; 250 C; 5 sec., 0.1 mm) | D5 | 29 | - |
| Retained Penetration (250 C) | - | 65 | 55 (Min.) |
| Ductility (250 C, 5 cm/min) | D113 | 80 | >25 |
| Softening point (4±1) 0 C/min. | D36 | 50.6 | - |

2.2. Aggregate

In this study, the source of aggregate for sample preparation was crushed quartz provided from the Al-Nibaie quarry. The physical properties of coarse and fine aggregates are presented in Table 2. The aggregate gradations was selected according to the SCRB R/9 2003 [27] of wearing courses (Table 3), with the maximum aggregate size of 19 mm (¾ inch), filler contents (4%, 6%, 8%) using passing sieve no. 4 (59 ± 6) (See Figures 1 to 4).

Table 2. Coarse and fine aggregate physical properties

| Physical Properties | Test Results | SCRB Specification limit |
|---------------------|--------------|-------------------------|
|                      | Coarse aggregate |                |
| Apparent Specific Gravity | 2.675 | - |
| Bulk Specific Gravity | 2.64 | - |
| Water Absorption,% | 0.15 | - |
| Percent Wear (Los Angeles Abrasion),% | 19.55 | 30 Max |
| Soundness Loss by Magnesium Sulphate Solution, % | 3.62 | 18 Max |
|                      | Fine aggregate |                |
| Apparent Specific Gravity | 2.685 | - |
| Bulk Specific Gravity | 2.624 | - |
| Water Absorption,% | 0.46 | - |
| Sand Equivalent,% | 60.45 | 45 Min |
| Clay Lumps and Friable Particles,% | 2.75 | 3 Max |

Table 3. Selected gradation for wearing course asphalt concrete mixture according to Iraqi specifications

| Sieve Size | Percent Passing (%) |
|------------|---------------------|
|            | Wearing Course       | SCRB (2003) Specifications Limits (Type IIIA) |
| Sieve No.  | Mix A | Mix B | Mix C | Mix D | Mix E | Mix F | Mix G | Mix H | Mix M |
| ¾ in       | 100   | 100   | 100   | 100   | 100   | 100   | 100   | 100   |       |
| ½ in       | 95    | 95    | 95    | 95    | 95    | 95    | 95    | 95    | 95    |
| 3/8 in      | 93    | 83    | 83    | 83    | 83    | 83    | 83    | 83    | 83    |
| No. 4       | 90    | 59    | 53    | 59    | 53    | 59    | 53    | 59    | 59    |
| No. 8       | 87    | 43    | 43    | 43    | 43    | 43    | 43    | 43    | 43    |
| No. 200     | 0.3   | 13    | 13    | 13    | 13    | 13    | 13    | 13    | 13    |
| No. 0.0075  | 4     | 4     | 4     | 4     | 4     | 4     | 4     | 4     | 4     |

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Figure 2. Gradation of wearing coarse at 4% filler content

Figure 3. Gradation of wearing coarse at 6% filler content
2.3. Mineral-Filler

Two types of filler were used in this study, including limestone dust and Portland cement. Limestone was sourced from the lime factory in the Karbala city and cement from the Almas factory in Sulaymaniyah Governorate. The physical properties of these two types of filler are given in Table 4.

| Filler type       | Physical Properties | Specific gravity | Surface area (m²/kg) | % Passing sieve No. 200 (0.075) |
|-------------------|---------------------|------------------|----------------------|---------------------------------|
| Limestone         |                     | 2.84             | 247                  | 95                              |
| Portland cement   |                     | 3.14             | 290                  | 98                              |

2.4. Aspha-min

Aspha-min (Figure 5) is an additive that was hydrothermally crystallized into a fine powder and used in the production of a warm mixture. It was prepared from synthetic sodium aluminium, silicate, or zeolite. It contains approximately 21% (by weight) of water, which is released in the temperature range of 85–180 °C. The addition of Aspha-min to the asphalt mixture is done at a dosage of 0.3% (by weight) of the mixture. During the manufacturing of WMA, the reduction in the production and placement temperature is approximately 30 °C, as demonstrated elsewhere [6]. The physical and chemical features of the Aspha-min are illustrated in Table 5.

Figure 4. Gradation of wearing coarse at 8% filler content

Figure 5. Aspha-min Powder
Table 5. Physical and Chemical Properties of the WMA additive: Aspha-min

| Property          | Result                                      |
|-------------------|---------------------------------------------|
| Ingredients       | Na2O.Al2O3.2SiO2 (Sodium aluminosilicate)   |
| SiO2              | 32.8 percent                                |
| Al2O3             | 29.1 percent                                |
| Na2O              | 16.1 percent                                |
| L.O.I             | 21.2 percent                                |
| Physical state    | Granular powder                             |
| Colour            | White                                       |
| Odor              | Odorless                                    |
| Specific gravity  | 2.03                                        |
| Bulk Density      | 568 kg/m³                                   |
| pH value          | 11.6                                        |
| Solubility in water | Insoluble                               |

2.5. Specimens’ Preparation and Tests

The Marshall compactor was used for the preparation of cylindrical specimens, with the dimensions of 102 mm (diameter) and 64 mm (height). The Pneumatic-repeated loading system (PRLS) (Figure 6) was used to test the Mr by applying repeated indirect compressive load. Nearly 162 specimens were compacted to build the Mr model.

Indirect tension test was applied to measure the Mr of the warm mix in accordance with the ASTM D4123 [28]. The test of the specimens was performed at a different range of temperature, loading duration, and applied loads, and each of the prepared specimens were subjected to 9 tests at 15, 35, and 45°C test temperatures to load durations of 100, 400, and 700 ms with 3 levels of stresses of 10, 20, and 30 Psi. This test consisted of applying a repetitive compressive load with one or more load duration, followed by 0.9-s rest period at 1-Hz frequency interval. The load was applied vertically to the diametric plane of the cylindrical specimen and the horizontal deformation was measured using 2 linear variable differential transducers (LVDTs) (Figure 6). Mr in the indirect tension method was computed using the following Equation 1:

\[
Mr = \frac{P(v+0.27)}{H \times L}
\]

Where, \( Mr \) = resilient modulus (MPa); \( P \): The maximum amount of repeated vertical force (N); \( v \): Poisson ratio of asphalt mixture which is equal to (0.35); \( H \): is the total recoverable deformation in (mm), \( L \): is the specimen thickness in (mm).

Figure 6. Pneumatic repeated load system
3. Results and Discussion

3.1. Effect of Asphalt Content on Mr

Three asphalt contents were used in this research (4.3, 4.8, and 5.3). Figure 7 shows the relationship of resilient modulus with the asphalt content. As illustrated in figure 7, the average Mr increased with the increase in the asphalt content because when the asphalt content increased, complete adhesion was achieved between the aggregate interparticles due to the decreased recoverable strain, which increased the Mr. As the asphalt content increases, the resilient modulus of the specimens increase up to a maximum, then decreases as the asphalt content continue to increase. When the content of asphalt increases from 4.3 to 4.8%, the average resilient modulus increased by 10% whereas when the asphalt content was increased from 4.8 to 5.3 % the average resilient modulus increased by 8.66%. The results agree with Neham (2015) [24] and Puzi (2010) [25].

![Figure 7. Relationship between Asphalt Content and Resilient Modulus](image)

3.2. Effect of Filler Content and Type on Mr

Three content of fillers were used (4, 6, and 8) with 2 types of fillers (limestone and Portland cement). Figure 8 represents the relationship between the Mr and filler content. It has been found that when the filler content increased, the average value of Mr also increased. When the filler content increased from 4 to 6%, the average Mr increased by 6.89%; while, when the filler content increased from 6% to 8%, the average Mr increased by 5.88%. This observation can be attributed to the fact that when the filler content increased, the air voids in the mixture decreased, leading to reduction of the recoverable strain, thereby increasing the Mr.

![Figure 8. Relationship between the resilient modulus and filler content](image)
The effects of filler types are illustrated in Figure 9. When Portland cement was used in the asphalt mixture as mineral filler, the average Mr increased by 10.71% rather than with the use of limestone, which could be because these types of fillers differ in their void content, surface texture, area, shape, and mineral composition. Also the specimens containing Portland cement were prepared in the summer, their homogeneity was better than the limestone because the specimens with limestone were prepared in the winter and as a result of the cold weather and heating of the aggregates to a lesser degree than the hot mixture by 30°C. It led to the difficulty of homogeneity of the mixture and thus gave less stiffness than the specimens contain cement. The results agree with Hilal (2018) [17] and Huan et al. (2011) [26].

![Figure 9. Relationship between Mineral Filler Type and Resilient Modulus](image)

### 3.3. Effect of Load Duration on Mr

Three different levels of load duration were applied in this research (100, 400, and 700 ms) to each of the tested temperature. Figure 10 depicts the effect of load duration on the Mr. When the loading time increased from 100 to 400 ms, it led to a decrease in the Mr by 24.72%; while, when the loading time increased from 400 to 700 ms, it decreased the Mr by 29.28%. This was expected because longer load duration indicated that the asphalt sample was exposed to a high strain, which caused larger deformations with lesser recovery of the deformations, thereby reducing the Mr. Longer load duration means the slow traffic, which has the most damage effect on the asphalt pavement, causing severe rutting and deformations in the structure of pavement. The results agree with Khan et al. (2015) [21], Shafabakhsh and Tanakizadeh, A. (2016) [22], Sarsam and Nihad (2019) [23].

![Figure 10. Effect of Load Duration on Resilient Modulus](image)
3.4. Effect of Testing Temperature on Mr

In this study, three different test temperatures were used (15, 35, and 45°C). For all the load durations for all prepared specimens. Figure 11 displays the relationship between the average Mr values versus the increase in the tested temperature. It can be seen that the temperature greatly affected the decreasing Mr of warm mix; this effect was seen when the test temperature increased from 15 to 45, which led to the reduction of the Mr by 60%. When the temperature increased, the asphalt binder became softer and flowy. At high test temperature and low compaction for warm mix as compared to HAM, bitumen may lose its ability to bind the aggregates together thus increases the shear strain between the particle contacts, this leads to decreases the stiffness of the specimen at an applied deviator stress. The result agree with Hamzah et al. (2014) [15], Goh et al. (2008) [16], Hilal (2018) [17], Albayati (2018) [18].

![Figure 11. Effect of Test Temperature for each Load Duration on Resilient Modulus](image)

**Minitab Vs 17** software was applied to analyze the variables considering in this study. The analysis of variance (ANOVA) for the different effects of these variables is shown in Table 6. The lower value of P or the higher value of F represents the significance of the factor. Also, all p values are lower than 0.05 this indicates that the independent variables had a good explaining the variation in the dependent variable (Resilient Modulus). Table 7 shows the resilient modulus model that predicted from different variables used in this research. It can be observed, through Table 7 the value of $R^2 = 0.964$ was high which indicates a very good relationship obtained means an acceptable correlation between dependent and independent variables. The predicted model indicated that the resilient modulus decreases with the increase of temperature, load duration, and air voids, whereas the resilient modulus increases with the increase of asphalt content and filler types.

![Table 6. ANOVA Test Results for Resilient Modulus Model](image)
Table 7. Summary for Resilient modulus model

|                        | R-sq | R-sq (adj) | R-sq (pred) | SER    | Durbin-Watson |
|------------------------|------|------------|-------------|--------|---------------|
| Regression Model       |      |            |             |        |               |
|                        | 96.46% | 96.42% | 96.36% | 24362.5 | 1.06774       |

4. Conclusions

Based on the analysis of the results, it has been concluded as below:

- Mr of WMA was developed for different test conditions and mixture properties on the PRLS.
- The Mr in the warm mix was greatly influenced by the temperature changes. When the temperature increased from 15 to 45°C, the Mr decreased by 60%.
- Mr decreased by 24.72% when the loading time increased from 100 to 400 ms, and when the loading time increased from 400 to 700 ms, the Mr decreased by 29.28%.
- When the content of asphalt increased from 4.3 to 4.8%, the average Mr increased by 10%; whereas, when the asphalt content increased from 4.8 to 5.3%, the average Mr increased by 8.66%.
- The average value of Mr increased by 6.89% when the filler content increased from 4 to 6%, and when the filler content increased from 6 to 8%, the average Mr increased by 5.88%.
- Mr increased by 10.71% with the use of Portland cement as a mineral filler rather than with the use of limestone as a filler in the mix.
- Mr decreased by 8.53% when the passing sieve no. 4 increased from 53 to 59, but it decreased by 6.72% when the passing sieve no. 4 increased from 59 to 65.
- Mr reduced by 24.72% when the loading time increased from 100 to 400 ms, and when the loading time increased from 400 to 700 ms, the Mr decreased by 29.28%.
- The result of these variables show that the Mr was strongly dependent on the temperature and moderately dependent on the load duration, while it showed low dependence on asphalt content, filler content, passing sieve no. 4, and the types of filler.
- The developed model was nonlinear, with a higher coefficient of determination of $R^2 = 96.46\%$.

5. Conflicts of Interest

The authors declare no conflict of interest.

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A Macro-element for Modeling the Non-linear Interaction of Soil-shallow Foundation under Seismic Loading

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Abstract

This paper presents a macro-element for simulating the seismic behavior of the soil-shallow foundation interaction. The overall behavior in the soil and at the interface is replaced by a macro-element located at the base of the superstructure. The element reproduces the irreversible elastoplastic soil behavior (material non-linearity) and the foundation uplift (geometric non-linearity) at the soil-foundation interface. This new macro-element model with three degrees-of-freedom describes the force-displacement behavior of the footing center. The single element is restrained by the system of equivalent springs and dashpots. The footing is considered as a rigid body. It is solved by a suitable Newmark time integration scheme and implemented in Matlab to simulate the nonlinear behavior of soil-shallow foundation interaction under seismic loading. A reduced scaled soil-foundation system has been tested on a shaking table at the University of Transport and Communications, Hanoi, Vietnam. Five series of earthquake motions were used with maximum acceleration increased from 0.5 m/s² to 2.5 m/s². The comparison of numerical results obtained from the simulation and experiments shows the satisfactory agreement of the model. The proposed macro-element can be used to predict the seismic behavior of a wider variety of configurations.

Keywords: Macro-element; Soil-foundation Interaction; Non-linearity; Seismic Loading.

1. Introduction

In structural design, soil-foundation interaction (SFI) is an important phenomenon that should be taken into account. However, simulating SFI often needs complex models for the soil and the foundation with a great number of degrees-of-freedom (DOF) which requires significant computational costs. That is why various simplified modeling strategies have been recently developed. The macro-element concept consists in condensing all nonlinearities into a finite domain and works with generalized variables (forces and displacements). The macro-element model replaces the soil-foundation system with a single element that allows simulating the behavior of foundations in a simplified way. This approach helps to reproduce the non-linear behavior of foundations considering material and geometric non-linearity. The macro-element reduces the computational effort significantly while preserving the essential dynamic responses of the system.

The term “macro-element” was initially introduced by Nova and Montrasio for studying the settlements of shallow foundations on sand [1]. After that, they proposed an elastic-plastic macro-element for strip and circular footings under quasi-static monotonic loading [2]. Based on this model, Paolucci proposed a numerical tool for studying the response of simple structures under seismic loading. Paolucci’s work took into account the coupling between the non-linear response of SFI and the response of superstructures [3]. Cremer et al. [4] developed the first application of the...
Macro-element for purely cohesive soils with no resistance to tensile stresses. The macro-element could be used not only for static loading but also for dynamic (seismic) loading, considering the plasticity of the soil and the uplift of the foundation. Macro-element models for seismic SFI problems are also available in the literature, such as those proposed by Cremer et al. [5], Chatzigogos et al. [6], Grange et al. [7, 8], Figini et al. [9], Frisco et al. [10], Khebizi et al. [12]. Jin [13] Barari et al. [14], Paroissien et al. [15] and Gorini et al. [16]. For shallow foundations, these authors used the macro element of quasi-static monotonic loading for analyzing the structures under seismic loading. According to Paolucci [11], the superstructure was represented by a single-degree-of-freedom mass and the macro-element introduced nonlinear effects in the calculation of soil reactions through a failure criterion and plastic flow rule. This model is developed further by Figini [9] by considering the uplift-plasticity coupling. However, these models weren’t suitable for earthquake loads because they changed in time and fully recovered once the seismic loadings eccentricity come back. Recently, Khebizi et al. [12] proposed a macro-element to examine the response of shallow foundations under monotonic and cyclic loads. Jin [13] investigated on the response of a caisson foundation in sand with a novel macro-element developed under the framework of hypoplasticity. In the work of Barari et al. [14], the effects of foundation geometry, horizontal load eccentricity and various soil conditions were examined by means of an alternative macro-element model.

Inspired by the above works, this paper proposes a macro element with the material-geometric coupling for seismic analysis of shallow foundation. The next section will describe the new macro-element where the entire soil-foundation system is lumped in a single point at the footing center. The footing is considered as a rigid body. The macro-element is restrained by the system of equivalent springs and dashpots. After the mathematical presentation of the macro-element, the comparison between simulation and experiment results in Section 3 has shown the good performance of the proposed approach.

2. Description of Proposed Macro-element

2.1. The General Structure

The structure of a macro-element model will follow the scheme presented in Figure 1. The soil is divided into two fields: the close field and the far field. The close field is the area where all material and geometric non-linearity are lumped while the far field is the area where the response of the system remains linear. The entire soil-foundation system is replaced by a macro-element located at the base of the superstructure. This model has 3 DOFs (horizontal, vertical and rocking motion), describes the force-displacement behavior of the footing center (Figure 2). In this formulation, the footing is considered as a rigid body. The single macro-element is restrained by the system of equivalent springs and dashpots. After the mathematical presentation of the macro-element, the comparison between simulation and experiment results in Section 3 has shown the good performance of the proposed approach.

![Figure 1. Macro element concept: decomposition in close field and far field](image)
2.2. The Variables of Forces and Displacements

As can be seen in the Figure 2, the entire soil-footing system is lumped in a single point at the footing center. The constitutive equations of the macro-element are written in terms of generalized forces and displacement variables \[6\]. The vector \( F \) of the generalized force variables is defined in Equation 1 as:

\[
F = \begin{bmatrix} V \\ M \\ N \end{bmatrix}
\]

(1)

Whereas, \( N, V, \) and \( M \) are the vertical force, horizontal force and moment applied to the foundation, respectively.

The vector \( u \) of generalized displacement variables is defined in Equation 2 as:

\[
u = \begin{bmatrix} u_x \\ \theta \\ u_z \end{bmatrix}
\]

(2)

In which, \( u_z \) and \( u_x \) are the vertical and horizontal displacements of the footing center of mass; \( \theta \) is its rotation angle. It is worth noting that the corresponding stiffness matrix in the elastic state can be considered as a diagonal matrix (Equation 3) because the soil-foundation system is lumped in a single point.

\[
K_{F0} = \begin{bmatrix} k_0 & 0 & 0 \\ 0 & k_r & 0 \\ 0 & 0 & k_v \end{bmatrix}
\]

(3)

The terms on the diagonal represent the foundation static impedances (\( k_0, k_r \) and \( k_v \) are the stiffness of the equivalent elastic springs to the horizontal direction, vertical direction and rotation, respectively) changed over time during the earthquake process, which can be determined from Gazetas’s formulas \[17\].

2.3. The Yield Function and Flow Rule

Equation 4 is the yields function and flow rule which Paolucci et al. \[11\] employed.

\[
f(F) = h^2 + m^2 - v^2(1 - v)^2 \xi
\]

(4)

Where \( h = V/(\mu N_{\text{max}}), m = M/(\psi BN_{\text{max}}), v = N/N_{\text{max}} \) and \( N_{\text{max}} \) is the ultimate bearing capacity under vertical central load, \( \psi \) is in the range between 0.35 and 0.5; \( \mu = \tan \varphi, \varphi \) is the soil friction angle; \( \xi = 0.95 \), in agreement with the value suggested by Nova and Montrasio \[1\]). The non-associative plastic flow rule from Cremer et al. \[5\] has been adopted (Equation 5):

\[
g(F) = \lambda^2 h^2 + \chi^2 m^2 + v^2
\]

(5)

The optimum parameters \( \lambda = 4 \) and \( \chi = 6 \) were selected.

2.4. The Stiffness Matrix

The elastic stiffness matrix of macro-elements is defined by Equation 3. The nonlinear phase of the seismic
excitation reveals that the instantaneous foundation–soil contact area changes over successive cycles of foundation rotations. This is explained by irrecoverable downward movement of soil beneath the foundation induced by severe foundation rotations during successive seismic loading, resulting in a reduction of the effective foundation width \(B'\) that can be expressed in Equation 6 as follows:

\[
B' = B(1 - \delta)
\]  
   (6)

Where \(B\) is the actual width of the footing and \(\delta\) can be interpreted as a degradation parameter defined in the range \(0 \leq \delta \leq 1\). Initially, \(\delta\) is set to zero. The parameter \(\delta\) is updated throughout the seismic excitation due to accumulation of inelastic foundation tilting. Although the footing has a square shaped, reduction in the footing–soil contact in transverse direction results in a rectangular contact area. Substituting Equation 6 into the approximate static stiffness formulas for a rectangular footing, and supposing that the square-shaped foundation base is in full contact with the soil prior to the seismic excitation, the reduced stiffness factors for each vibration mode are obtained (Equations 7 to 9) as:

\[
k'_0 = k_0\left[0.74(1 - \delta)^0.35 + 0.09 + 0.17(1 - \delta)\right]
\]  
   (7)

\[
k'_r = k_r[\left(1 - 0.2\delta\right)(1 - \delta)^2]
\]  
   (8)

\[
k'_v = k_v[0.66(1 - \delta)^{0.25} + 0.34(1 - \delta)]
\]  
   (9)

Where \(k'_0, k'_r, k'_v\) are the modified stiffnesses in terms of \(\delta\); \(k_0, k_r, k_v\) are the equivalent elastic spring coefficients of the soil–foundation system defined in the previous section. For this purpose, we have selected the following simple degradation function (Equation 10).

\[
\delta(\theta^p) = \frac{\delta_1}{1 + \delta_2\theta^p}
\]  
   (10)

Where \(\delta_1 = 0.75\) and \(\delta_2 = 5000/\text{rad}\) are model parameters related to the ultimate value of \(\delta\) and to the degradation speed, respectively, while \(\theta^p\) the cumulated plastic foundation rotation at a specified instant of time, calculated as:

\[
\theta^p = \sum_\text{n} |\Delta \theta_n - \Delta M_n/k'_r|
\]  
   (11)

In Equation 11, \(n\) and \(M_n\) are the increments of foundation rotation and overturning moment, respectively, calculated at the \(n\)th time step. The elastic stiffness matrix is calculated following (Equation 12):

\[
K'F = \begin{bmatrix}
k'_0 & 0 & 0 \\
0 & k'_r & 0 \\
0 & 0 & k'_v
\end{bmatrix}
\]  
   (12)

The soil behavior is assumed to be linear visco-elastic until the failure surface in Equation 4 is reached. When the failure surface is reached, the plastic flow occurs when \(f(F) \geq 0\) and \(df(F) = 0\) [3]. The elastic stiffness matrix of macro-elements will be reduced by a differential value \(dK^F\) for initial value in Equation 3. This is calculated as a function of the elastic stiffness matrix \(K^{F0}\) and the derivatives of the yield and plastic potential functions (Equation 13).

\[
dK^F = K^{F0}\left(\frac{\partial \phi}{\partial \theta}\right) \left(\frac{\partial \phi}{\partial \theta}\right)^T K^{F0} \left(\frac{\partial \phi}{\partial \theta}\right) K^{F0} \left(\frac{\partial \phi}{\partial \theta}\right)^T \right)^{-1}
\]  
   (13)

Thus, the elastoplastic stiffness matrix of the proposed macro-element in step of \(n^{th}\) is determined by the following formula (Equation 14).

\[
K^F = K'F - dK^F
\]  
   (14)

The flowchart to summarize the defining process of a new macro-element stiffness matrix is shown in Figure 3.
2.5. The Dynamic Equilibrium Equations

The differential equation of motion is presented in Equation 15.

\[ M \ddot{x} + C \dot{x} + F = P \]  

(15)

Where

\[ x = [x_0 \phi x_v]^T \]  

(16)

\[ P = [-m_0 \ddot{x}_g 0 - (m_0)\ddot{z}_g]^T \]  

(17)

\[ F = [V^F M^F N^F]^T \]  

(18)

\[ M = \begin{bmatrix} m_0 & 0 & 0 \\ 0 & f & 0 \\ 0 & 0 & m_0 \end{bmatrix} \]  

(19)

\[ C = \begin{bmatrix} c_0 & 0 & 0 \\ 0 & c_r & 0 \\ 0 & 0 & c_v \end{bmatrix} \]  

(20)

Where \( x \) is vector of the displacements of the basement; \( P \) is vector of base excitations; \( F \) is vector of soil reactions; \( x_0, \phi, x_v \) are horizontal displacements of the basement, rocking motion of the basement and vertical displacements, respectively; \( \ddot{x}_g, \ddot{z}_g \) are horizontal and vertical base excitations, respectively; \( m_0, f \) are mass of the foundation and sum of the centroid moments of inertia of the foundation, respectively; \( c_0, c_r, c_v \) are equivalent dashpot coefficients of the soil-foundation system corresponding to the translational, rocking and vertical modes of vibration, respectively.

The Newmark time integration scheme was used for solving the motion equations Equation 15. Acceleration and velocity are written in Newmark time-stepping method based on the following equations. The equations of motion at time \( i, i + 1 \) and incremental equation of motion are as follows.

\[ M\ddot{x}_i + C\dot{x}_i = P_i \]  

(21)

\[ M\ddot{x}_{i+1} + C\dot{x}_{i+1} = P_{i+1} \]  

(22)

\[ M\Delta\ddot{x}_{i+1} + C\Delta\dot{x}_{i+1} = \Delta P_{i+1} \]  

(23)

Denoting by the subscript \( n \) the quantities calculated at time \( t = n\Delta t \), the motion form of Newmark time integration scheme of Equation 15 can be rewritten as Equation 24.

\[
\left[ M + \frac{C}{\beta \Delta t^2} \right] \ddot{x}_{n+1} + F_{n+1}(x_{n+1}) = p_{n+1} + M \left[ \frac{1-2\beta}{2\beta^2} \ddot{x}_n + \frac{x_n \Delta t + x_{n+1}}{\beta \Delta t^2} \right] + C \left[ \frac{\beta}{\beta^2 - 1} \ddot{x}_n \Delta t + \frac{\beta - 1}{\beta^2} \dot{x}_n + \frac{\beta}{\beta \Delta t} x_n \right]
\]  

(24)
Where $\Delta t$ is the time step; $\beta = 0.25$ and $\gamma = 0.5$ are the Newmark integration parameters; $F_{n+1}^F = F_n^F + K^F (x_{n+1} - x_n)$.

3. Results and Discussion

In order to validate the capability of the numerical strategy, the proposed macro-element is implemented in Matlab by using the motion equation form of Newmark time integration scheme (Equation 24). The experimental investigation was conducted at the University of Transport and Communications, Hanoi, Vietnam to study a shallow foundation lying on sand with a known density. The soil-foundation system was subjected to a series of earthquake base excitations on the shaking table. Due to the limitations of the dimension of shaking table ($2 \times 2$ m), a polycarbonate box of 1.85×1.5×0.7 m was selected and fixed to the table.

![Elevational view of the soil-foundation system](image1)

**Figure 4. Dimensions of the soil-foundation system**

The dry sand was filled in the polycarbonate box and compacted in layers so that nearly homogeneous soil conditions were obtained. The sand relative density $D_r$ was 82%, the mass density $\rho = 2.66 \text{ g/cm}^3$ and the angle of internal friction $\phi = 42.6^\circ$. The shallow foundation model with the dimension of 0.25×0.25×0.1 m (L×W×H) was placed on the sand layers. The recording system consists of 2 accelerometers placed on the foundation model. The overall view of the specimen on the shaking table is shown in Figures 4 and 5.

![Plan view of the soil-foundation system](image2)

![Figure 5. The experimental setup](image3)
The parameters of macro-element model are shown in Table 1.

| $k_0$ (N/m) | $k_r$ (Nm/rad) | $k_v$ (N/m) | $c_0$ (Ns/m) | $c_r$ (Ns/m) | $c_v$ (Ns/m) | $m_0$ (kg) |
|------------|---------------|-------------|--------------|--------------|--------------|-------------|
| $202.68 \times 10^6$ | $201.74 \times 10^3$ | $338.48 \times 10^6$ | $1.34 \times 10^5$ | $1.26 \times 10^3$ | $2.42 \times 10^5$ | $15$ |

The tests were conducted in one horizontally direction (Figure 4). The motion records were derived from the Tolmezzo earthquake. Five earthquake motions, denoted from T1 to T5, were used for the experiments with maximum acceleration increased from $0.5 \text{m/s}^2$ to $2.5 \text{m/s}^2$ ($0.5 \text{m/s}^2$, $1.0 \text{m/s}^2$, $1.5 \text{m/s}^2$, $2.0 \text{m/s}^2$ and $2.5 \text{m/s}^2$). The five motions were applied to the soil-foundation system in chronological order. They have been launched independently in the macro-element model. Figures 7 to 10 shows the comparison of the acceleration at the foundation for all tests, except for test T1 where the values were too small. As can be seen, the simulation results were generally close to the experimental results. No significant shift existed between the simulation and experiment curves.
Table 2 represents the maximum values of acceleration at foundation obtained from test T2 to test T5. It was found that the macro-element was able to simulate correctly the behavior of foundation. The percentage errors reported
permit an assessment of the accuracy of the numerical model. It is noteworthy that the agreement for the T3 and test T4 is in general better than the T2 and T5.

| Table 2. Maximum values of acceleration at foundation |
|-----------------------------------------------|
| Test | Experimentation (m/s²) | Macro-element (m/s²) | Error (%) |
|------|-------------------------|----------------------|-----------|
| T2   | 1.452                   | 1.173                | -19.2%    |
| T3   | 2.244                   | 2.414                | 7.6%      |
| T4   | 2.323                   | 2.525                | 8.7%      |
| T5   | 2.970                   | 3.398                | 14.4%     |

The computational effort involved in the macro-element is orders of magnitudes less than that of 3D FEA analysis by Huynh et al. [18]. The present solutions, implemented in non-compiled MATLAB script files, took between 15-30 seconds to conduct each test. In comparison, the 3D FEA under Cyclic TP software took about 5 hours on the same computer.

4. Conclusion

In this paper, a new macro-element for modeling the behavior of soil-shallow foundation interaction under seismic loading has been represented. The proposed macro-element considered simultaneously the effect of material and geometric nonlinearities on the response of foundation. It used a 3-DOF macro-element and the differential equations of system’s motion. A reduce scaled of soil-foundation system was tested on a shake table to investigate the seismic behavior of this type of interface. The comparison between simulation and experiment results show that this model suited for simulating a couple of material and geometric behaviors of a shallow foundation under seismic loading. The macro-element can be used to investigate numerically the behavior of a wider variety of configurations which are difficult to study experimentally. In the future, possible improvements of the proposed macro-element are necessary, especially concerning the interaction of soil-structure.

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6. Conflicts of Interest

The authors declare no conflict of interest.

7. References

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Truck Driver Behavior and Travel Time Effectiveness Using Smart GPS

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Abstract

The pattern of coal transportation is very dependent on the behaviour of the driver, which influences the effectiveness of travel time. Good driver behaviour will affect the optimization of travel time, and scenarios need to reduce travel time wastage. This study aims to optimize travel time and sensitivity analysis based on the influence of driver behaviour, truck travel movements and the use of travel time on coal haul roads. The research method uses a field survey with a GPS tracker, a smart GPS server 3.3, google earth and statistics. The results showed that the driver's behaviour greatly influenced the pattern of use of travel time and truck travel speed. Coal transportation in the morning can be more optimal than night so that that travel time wastage can reduced by 40%. The proposed optimization scenarios can save 36.7% - 48.61% of the existing travel time and the transport cycle can be increased to four to five times. So that with the addition of the cycle, it will increase the income of the transport company and the driver's income. With smart GPS, companies can improve the performance of transportation services in company management, get coal supplies on time.

Keywords: Drivers Behaviour, Travel Time Effectiveness, Truck, Coal Roads, Scenarios.

1. Introduction

The Borneo Economic Corridor in MP3EI is a National Energy and Mining Product Production and Processing Center, especially the coal sector. The coal commodity is the primary commodity of South Kalimantan according to the results of the Dynamic Location Quotient > 1 and the need for coal production has increased from the 2011-2016 period of 24 million tons. Coal is the primary fuel for electricity, metallurgy, cement, textile, pulp, fertilizer and briquette factories. Coal transportation distribution is a significant thing in coal availability [1].

There have been many studies to analyze driver behaviours such as street characteristics influence, driver category and car performance on urban driving patterns [2]. Davidovic et al. (2018) estimated the professional driver's fatigue as a modern era problem [3]. Dinges (1995) focused on the sleepy behaviour influence; and accidents that occur, exploration studies about long-distance truck drivers [4, 5]. Zicat et al. (2018) estimated young drivers with cognitive function by analyzing the relationship between attitude, driving, cognition and personality [6]. Moreover, Kirti et al. (2019) got the effects of work-rest patterns, lifestyle and payment incentives drivers on long-haul truck driver sleepiness [7]. Meng et al. (2019) reported on the driving fatigue by surveying the taxi drivers and truck-related to accidents in professional drivers [8].

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Transportation is very dependent on the driver behaviour who provides services in the form of timeliness and safety in driving. Reliable driver behaviour, expertise, discipline, work motivation, and professionals can optimize the travel timeliness for each mining transport activity in order to avoid delays and time-wasting that is a loss for the company. Driving is related to factors in the driver who then determine driving behaviour and related to on-going social situations. Bad driver behaviour can affect the use of travel time such as the duration of the rest is too long, the stopping frequency at the food stall or the side road, staying up so that it results in drowsiness and fatigue, thereby reducing the alertness level, unstable speed and working in uncomfortable conditions. The driver behaviour is concerned with dynamic driving characteristics such as road safety, fuel efficiency or good driving patterns.

Modelling and recognizing human driving behaviour has attracted researchers from various scientific disciplines such as physiology, psychology and behaviour for more than fifty years. Significant advances have made from various individual studies on various aspects of human behaviour. The driver model research has made based on the perspective of human factors and vehicle dynamics [9].

Driver behaviour determines vehicle actions in traffic. Research on driver behaviour and vehicle speed approached speed with driver characteristics, traffic conditions and vehicle type with comparing suburban areas and urban [10]. Familiar et al. (2011) analyzed speeding behaviour with a multilevel modelling approach [11]: Gehlert et al. (2012) introduced an evaluation of the different types of dynamic speed display signs [12]. Besides that, Eboli et al. (2017) investigated car users’ driving behaviour through speed analysis, and Galkin et al. (2018) produced modelling trucks that speed on the route considering the driver's state [13, 14]. Likewise, research on travel time from various perspectives such as that conducted by Rahmani et al. (2015) with a non-parametric research for estimation of route travel time distributions [15]. Moghaddam et al. (2017) analyzed the effect of travel time information, reliability, and level of service on driver behaviour using a driving simulator [16]. Uchida (2014) has estimated the travel time value and travel time reliability in road networks [17].

Many methods and models are carried out to optimize travel time, such as the TRIP model for predicting travel time on the Seattle metropolitan area network road, based on large volumes of GPS data [18]. Jenelius (2012) has examined the travel time value variability with flexible scheduling, trip chains and correlated travel times [19]. Westgate et al. (2013) analyzed several approaches exist to predict the probability distribution of travel time on the road network model exclusively link-level variability and assume the independence of travel time on the route [20]. Similar research also conducted by Hunter et al. (2013) with estimates of large-scale cyber-physical systems using streaming data for predicting travel time variability using GPS [21].

This study aims to present an analysis of driver behaviour from the perspective of driving data in detail, such as speed and travel time usage. It is well known that driving a truck is a complex and dynamic task that requires the driver has driving skills. Modelling of driving behaviour and recognition driver characteristics are needed to ease the driver’s workload and improve reliability. This study uses a GPS tracker that connected to a smart GPS server 3.3. Implementation of GPS tracking on trucks has been shown to improve driver behaviour, driver safety, reduce unnecessary time, control fuel, and truck operational costs others. Also, increase vehicle utilization effectively, increase productivity and customer service, also can manage vehicles more effectively and control fleet costs. Operating a fleet is not only about managing vehicles but also requires the management of the people who drive it. That is where the wireless fleet management system (GPS tracker/smart GPS) can provide many benefits for the coal company and its drivers. Using GPS data can positively train and reward drivers for adopting safer and more efficient driving habits. Drivers get essential information, accurate, get roadside assistance (emerging situation), work verification is done on time and existing data that affects many other aspects of driver works. The smart GPS installation in coal trucks can help operators and field supervisors to track trucks, give warnings, monitoring truck locations, provide information, and mark the speed of each truck. Even the field supervisor will call the driver who stops too long somewhere and knows the location if there is damage to the truck so that it is easy and quick to help. In general, smart GPS installed to avoid truck loss and a waste of travel time, so that the use of fuel can also reduce.

2. Research Methodology
2.1. Location of Study

The research was carried out on a private hauling coal road in South Kalimantan Province with an aggregate base course road structure. The distances of the hauling coal route are 56.1 kilometres between the stockpile to Sungai Puting Port, and the road slope is a maximum of 20.3 %, -15.5 %. This research was conducted in the period from September 2018 - March 2019. The location of the study can be explained in Figure 1.
2.2. Participants and Measurement

The discussion in the study divided into two topics, namely (1) the coal truck behaviour with 116 drivers working at the coal transportation company PT. BEM in the Rantau District, South Kalimantan Indonesia and (2) the travel time usage of truck movement. For estimated driver behaviour used driver characteristic questionnaires namely (a) driver characteristics including age, education, population status, income/month, truck driver experience, several mobile phones, cellphone usage while driving, workdays/month, driving frequency, stops frequency, driving duration/day, place to stop, activities at rest, total sleep time/day, activity in social media and cigarette consumption/day. The usage of coal truck travel time using a GPS tracker connected to smart GPS server 3.3 software installed on three Hino 500 FM 260 Ti trucks with codes A, B, and C in a one-month observation. The flowchart of this research method is available in Figure 2.

Figure 2. Research flowchart methodology

The driver demographics characteristics data were analyzed using SPSS version 24 software. The characteristics of data were analyzed using descriptive statistics to investigate the demographic characteristics of the participants. The travel time usage of coal trucks using a smart GPS server 3.3 connected with a GPS tracker will get a route, the truck movement, coordinates of movement and stops, truck speed, and stop location. Smart GPS results will be moved to Google earth so that they display the level of the road, geometric, and height of the road crossing. Collected data are analyzed and compared accordingly. Then sensitivity analysis and optimization scenarios are performed based on the driver’s behaviour patterns and truck movements, so that travel time is more reliable.
3. Results and Discussion

3.1. Characteristics and Behaviour of Coal Driver

The driver’s characteristic is done to find out the driver’s profile so that it will facilitate an understanding of the behaviour of the travel time usage. Characteristics fields were distributed to 116 coal truck drivers. The results of driver characteristics can be seen in Table 1.

Table 1. Driver demographic characteristics

| Variable                      | N | %  | Variable                      | N | %  |
|-------------------------------|---|-----|-------------------------------|---|-----|
| Age                           |   |     | Driving frequency/day         |   |     |
| ≤ 25 years                    | 9 | 8   | ≤ Three times                 | 36| 31  |
| 26-35 years                   | 59| 51  | Four times                    | 67| 58  |
| 36-45 years                   | 33| 28  | Five times                    | 11| 9   |
| ≥ 45 years                    | 15| 13  | > Five times                  | 2 | 2   |
| Education                     |   |     | Stop frequency                |   |     |
| ≤ junior high school          | 5 | 4   | Never                         | 17| 15  |
| Senior High School            | 96| 83  | 1-2 times                     | 29| 25  |
| 3-year diploma               | 12| 10  | > Two times                   | 70| 60  |
| ≥ bachelor                    | 3 | 3   |                               |   |     |
| Population status             |   |     | Driving duration/day          |   |     |
| Local residents               | 81| 70  | Normal, <8 hours              | 38| 33  |
| Outside residents             | 35| 30  | Weight, > 8 hours             | 78| 67  |
| Income/month                  |   |     | Place to stop                 |   |     |
| ≤ 3 million                   | 28| 24  | Food stalls                   | 77| 67  |
| 3-6 million                   | 67| 58  | The side of the road          | 34| 29  |
| ≥ 7 million                   | 21| 18  | Workshop/home                 | 5 | 4   |
| Truck driver experience       |   |     | Activity at rest              |   |     |
| ≤ One year                    | 13| 11  | Sleep                         | 32| 28  |
| 2-4 years                     | 95| 82  | Eat                           | 57| 49  |
| 5-7 years                     | 5 | 4   | Relax/social media            | 4 | 3   |
| ≥ Eight years                 | 3 | 3   | Others                        | 23| 20  |
| Number of cellphones          |   |     | Total sleep time/day          |   |     |
| One                           | 78| 67  | Less (< seven hours)          | 39| 66  |
| Two                           | 33| 29  | Enough (> seven hours)        | 77| 34  |
| > two                         | 5 | 4   |                               |   |     |
| Use of HP/day                 |   |     | Active in social media        |   |     |
| One time                      | 15| 13  | Active                        | 15| 13  |
| 2-3 times                     | 35| 57  | Middle class                  | 67| 58  |
| > 3 times                     | 66| 30  | Not active                    | 34| 29  |
| Working day/month             |   |     | Consumption of cigarettes/day |   |     |
| ≤ four days                   | 65| 56  | Do not smoke                  | 5 | 4   |
| 5-7 days                      | 35| 30  | 1-6 sticks                    | 24| 21  |
| ≥ eight days                  | 16| 14  | 7 - 12 sticks                 | 87| 75  |

Table 1 shows that the highest education qualification, according to recruitment, is a senior high school (83%). The most significant population status of residents is 70%, this aims to empower people local/native, without providing housing and understanding the field situation to reduce conflict during coal-hauling work. The highest income in the range of 3-6 million (58%) and the driving frequency highest/day is four cycles (58%). It means that the driver will get 3-6 million/month if the more four times frequency/day. The average income/month is 4.6 million is higher than the Regional Minimum Wage (UMR) of South Kalimantan Province (2.7 million). Data in the field shows that the driver’s income depends on the driving frequency/day. The revenues of 4.6 million/month based on the driving frequency/day at an average of 4 cycles (calculated from filling in the stockpile to the port and returning to the stockpile). The highest driving experience is in the range of 2-4 years, and the driving duration/day is relatively heavy, namely > 8 hours/day (67%).
The frequency of stopping during the trip is high, which is more than two times (60%) with stops in food stalls (67%), roadside (29%) and workshops/houses (4%). Drivers use the time to stop for breaks, including sleeping, eating, relaxing, social media and others. Most rest periods used for eating and sleeping. Driver behaviour can also be seen from the usage of the total sleep time. From the data produced, the driver has less sleep time (66%) so that it can increase driver fatigue. The work/month holiday that the driver gets is an average of four working days. The driver himself determines the working day because the employment status is freelance.

The use of travel time/day is also influenced by ownership and the use of mobile phones, especially for communication. The average driver has only one mobile phone with the frequency of receiving/making calls 2-3 times and classified as active in social media. In general, someone active in social media will use free time to check or play social media. Most drivers consume cigarettes with a large amount of 7-12 cigarettes (75%), but the procedure during driving is forbidden to smoke to avoid combustible coal fires so that drivers consume cigarettes only outside driving hours.

3.2. The Travel Time Usage

In the map, the results of smart GPS server 3.3 also display stops along the route. If the image zoomed in such a way, it would display lines or trail lines of truck trips that are not the same even though in the same route. The results of the coal trucks on three trucks with numbers BH 5000 (A), 5001 (B) and 5004 (C), which include special lanes along with coordinates, the average speed data, the maximum speed data, and where stops can see as follows Figure 2.

Figure 3. The average speed of coal transport within 28 days of observation (a) trucks A, B, and C with on-loading travel speed (b) trucks with on-loading travel speed and off-loading travel speed

On-loading travel time is travel time, which spends from the stockpile to the port with coal load, and off-loading travel time is the travel time from the port to the stockpile without coal load. In Figure 3(a) shows that the variation in the trucks average speed (trucks A, B and C) in one month of non-stop observation (GPS tracker is not turned off in one month) both during motion/travel time and time temporarily stopped (food stalls, roadside and workshops), but also the time to stop after doing 2 - 4 times the transport cycle. The speed of the truck is different every day. The average speed total in one month of observation is 30 km/hour. The highest average travel speed occurred on February 11, 2019, at 37 km/hour but still below the speed limit of 40 km/hour when on-loading travel.

The minimum average speed occurs on February 14, 2019, at 23 km/hour. In Figure 3(b) shows that the average speed comparison with the condition of on-loading travel speed and the off-loading travel speed with three trucks every day in one month. The maximum speed is 71 km/hour, and the minimum speed is 23 km/hour. The output of the average truck speed is the smart GPS server 3.3 results originating from a GPS tracker installed in each truck. Declining travel speeds can indicate on bends, inclines, and descent, road surface damage, road constriction, and rainy weather.
Figure 4 shows a result comparison of the travel time usage between on-loading travel time and off-loading travel time during the morning afternoon and night conditions. At the time of the morning, it gets the on-loading travel time of 0:50:49, whereas, at night, it is 1:01:28. The value of the off-loading travel time in the morning/afternoon is 0:41:06 and night to 0:47:52. From the results of the travel time usage that was recorded from a smart GPS server 3.3 for one month, it was found that average travel time at night trip is longer than the morning-afternoon trip. It can indicate that there is a decrease in the driver's condition, a decrease in the level of alertness, increased fatigue and lack of street lighting at night. Extended workload and work duration will cause fatigue to the driver with a marked decrease in the safety level and the driver's health condition.

Figure 5 shows that the average duration of travel time usage for one travel cycle time, namely travel time between the stockpile to the port and returning to the stockpile again. The travel time usage consists of the trucks travel time duration with on-loading travel time is 33.4% (2 h 15 m 362 s) and off-loading travel time at 18.2% (1 h 13 m 48 s). The duration usage of the coal loads in the stockpile to the port with a route distance of 56.1 km and normal on-loading travel speed on roads specifically for coal transportation 40 km/hour, then the standard duration is 1 h 24 m 9 s, while the standard duration of off-loading travel speed 60 km/hour is 56 m 6s. From this data, there is a waste of travel time, namely on-loading travel time with 57 minutes and return time of 51 m 27 s. The waste of travel time usage on coal haul road indicated rainy weather, rough road conditions, dusty roads, drowsy, tired driver behaviour, reduced alertness, long periods of rest, and stopping and obstacles to vehicle conditions.

The use of travel time duration when coal loading in the stockpile is 13.2% (53 m 32 s) and at the coal unloading time at the port is 10.6% (42 m 54 s), and it can be reduced by proper port management, arrangements for entering/exiting ports, reducing queuing time, increasing conveyor belts and repairing port roads. Whereas the duration of use in the food stall is 9.4% (38 m 19 s) and on the roadside, 5.3% (21 m 31 s) can be reduced by
providing regular meals for drivers, provision of drinking water to trucks, counselling on staffing procedures and transportation of coal. Long stops can damage the condition of vehicles and roads, especially in trucks with coal loads, because, in general, the load ranges from 28 - 30 tons (exceeding the load). The duration of time spent in the workshop of 9.9% (39 m 58 s) indicated that because of vehicle damage, vehicle checking, refuelling, and transportation management. So that if the cause can resolve, then the travel time will be more optimal and profitable.

Figure 6. Sensitivity scenario using average travel time in one travel cycle

Figure 6 shows three comparisons of situations, namely the existing situation, scenario 1 and scenario 2. The optimization sensitivity includes two scenarios, namely:

1. **Scenario 1** was changed the coal trucks travel speed with on-loading travel using a planned speed of 40 km/hour and off-loading travel speeds of 60 km/hour, the duration of loading time in stockpiles and unloading at ports fixed because the mining system has three different authorities, namely the owner of the mine, road owners of transport and port owners. In the scenario, one only changes the travel time associated with the transport road only. For a stop at the food stalls, it is used one hour to rest. Because, on average, one day is three cycles, then one hour is divided into three cycles, which is twenty minutes. To stop at the workshop and on the roadside is eliminated. The results obtained were a reduction in waste of travel time by 48.61%.

2. **Scenario 2** was changed travel time on the coal hauling, loading in the stockpile and unloading at the port. The trucks speed with on-loading travel speed using 40 km/hour and off-loading travel speed 60 km/hour. The use of travel time in the stockpile and port is changed in half from the existing conditions by the entrance management to reduce the queue, add the conveyor belt, repair the port road and enlarge the entrance/exit. The stop was fixed for twenty minutes and stopped at the food stalls, and the roadside eliminated. So the results that can be optimized are 36.72%.

With the results of scenario 1 and 2, the transport cycle can be increased to four to five times. So that with the addition of the cycle, it will increase the income of the transport company, the driver's income and the availability of coal stock is guaranteed. Trucks are coal-hauling units that provide relatively low hauling costs and flexible because of their high travel speeds. The high travel speeds allow for quicker hauling of coals when travelling on established roads.

4. **Conclusion and Research Implications**

The use of smart GPS in each truck is significant to improve and control the pattern of coal driver behaviour. Driver characteristic data can illustrate driver behaviour that affects travel time performance. The high income and driving experience affect the work motivation of drivers. The frequency of stopping during the trip, time to stop for breaks, the less sleep time, driver fatigue, and duration of mobile phone / social media usage significantly affect travel time. From the results of the characteristics of the driver can be compared with the survey results of truck movements as primary data so that there is a match between the characteristics of the driver’s data and the movement of the truck, which results in inefficient travel time. Sensitivity analysis and optimization are implemented by reducing stop times during trips, queuing at stockpiles and ports, changing sleep and rest patterns and adjusting workloads to reduce driver fatigue.
Optimizing travel time can be done with several scenarios requiring cooperation between drivers, transport owners, road entrepreneurs, mining owners, and ports. The transportation of coal in the morning can be more optimum than a night and can reduce by 40% of the current travel time. Even though the scope of hauling coal is local and uses local drivers, standardization of transport must be applied towards more enormous profits. By changing driver behaviour in the use of time, travel time reliability can be achieved. The next research that can be done to analyze the coal transportation system policy covering drivers, vehicle and road conditions. Also, research on the effects of topography and the quality of road can be analyzed so that all aspects related to the transportation of coal can be analyzed. The South Borneo because of the geographical and geological conditions of the area.

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6. Conflicts of Interest
The authors declare no conflict of interest.

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Influence of Natural Zeolite and Paraffin Wax on Adhesion Strength Between Bitumen and Aggregate

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Abstract

Asphalt mixture that is used for the construction of flexible pavements is mainly composed of two constituents i.e. bitumen and aggregate. Sturdy adhesion among bitumen and aggregate is the sign of durability of asphalt pavements. Adhesion is considered as one of the most important factors for sustainable asphalt pavement. This is the motive why its miles utmost important to deeply understand the phenomenon of adhesion considering the effect of alternate in temperature, moisture conditions. In this study softer binder 80/100 was selected that has less adhesion compared to hard pen grades. Limestone aggregates which is commonly used for the construction of asphalt pavements has also been selected. Two types of modifiers (Zeolite and Paraffin Wax) were selected because of the extensive use in asphalt foaming and the polymer modified asphalt mixtures as temperature reducing agent. To investigate the strength of adhesive bond, Bitumen Bond Strength (BBS) was performed at different temperatures, in dry, and wet conditions. To quantify the effect of modifiers on penetration grade and softening point conventional testing is performed. For performance grading, the PG test was performed using Dynamic Shear Rheometer. The comparisons were developed among pull of tensile strength at dry and after 72hrs water conditioning while preserving the temperature at 25°C. To check the effect of temperature BBS is performed at 15°C. The results illustrate that 2% zeolite shows best results in terms of adhesion and performance grade while Paraffin wax has less adhesion and poor performance grade.

Keywords: Bitumen; Aggregates; Adhesion; Pen Grade; Softening Point; BBS; DSR; Performance Grade.

1. Introduction

Most of the pavement are constructed in the world are asphalt pavements. During the life period, these pavements must bear climate impact in terms of moisture, temperature and loads. The major reason for pavements deformation is moisture damage [1]. Introduction of moisture into asphalt pavements leads to adhesion loss between the binder and aggregates. The deformation of asphalt pavements mainly is due to adhesion loss [2]. Diffusion of water into pavement layers weakens the adhesive bond between aggregate and bitumen. The occurrence of stripping is due to debonding, which is caused by water ingress. Studies have done on properties of asphalt pavements shows that the mechanical properties of flexible pavement depend on the bond between the binder and aggregate. The strength of the interface bond between binder and aggregate defines the life of pavement and its potential to withstand against heavy loading and climate condition.

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The moisture damage is not only causing the reduction in stiffness but also strength of asphalt pavements as well as leads to various types of distresses like stripping, ravelling, hydraulic scour, rutting and alligator cracking. So, it is important to quantify the adhesion properties and effect of water on interfacial bond in asphalt mixtures [3, 4]. Factors like aggregate mineralogy, chemical properties of binder and surface of aggregates control the moisture damage in asphalt pavements [5]. According to studies, aggregate with basic nature shows more adhesion than acidic aggregates and have greater resistance against moisture damage [6]. 548 billion are spent on maintenance of road pavements in America because of moisture damage. About 82% of American Transportation Agencies recommend the use of adhesion promoters in low-performance job mix formulas [7-9]. Zhang has used the Rediset [10] Nano-charcoal and coconut shell ash [11] and, Hamedi and Tahami (2018) has used Zycosoil as adhesion promoter [2]. There are two types of modification against moisture damage: additives are mixed in bitumen or aggregates are modified. Because of ease in modification in bitumen, method of mixing of anti-stripping agents in bitumen is adopted [2]. The zeolites are used in asphalt foaming technologies as water containing group. The zeolites consist of microporous aluminosilicate minerals. The crystalline structure of zeolites continuously releases the water at 400°C without damaging their structure [12]. The pen grade and softening point are also improved by zeolite. When zeolite is added in asphalt mixtures, it decreases the mixing temperature. Because of this property, there is the saving of energy. Moreover, by the addition of the zeolites, the potential of asphalt pavements is increased against permanent deformation [13].

The polymer-modified asphalts are developed to reduce rutting, fatigue and thermal cracking which leads to reduce maintenance costs. High working temperature is required for polymer-modified asphalt mastic. At the same time, high temperature makes bitumen brittle material which has a bad impact on performance. High working temperature required more energy and cause the emission of bitumen fumes and CO₂ than conventional HMA works. To meet the allowed working temperature conditions and emission, the wax is used to decrease mixing temperature and emission as flow agent [14, 15]. Numerous test methodologies were developed by researchers to investigate adhesion between bitumen and aggregates. The EN 1297-11 provides three methods to quantify affinity in asphalt mixture. These tests are rolling-bottle-test, static water storage and detachment in boiling water. Whereas, in the Lithuanian standard LST 1362.23 – boiling water test method is used. The Rolling-bottle testing is considered most suitable but the mechanical strain by rolling process shows bad impact of accuracy of results. There is no differentiation of results in static water storage, and the boiling water test doesn’t provide accurate results [16]. The Pneumatic Adhesion Tensile Testing Instrument (PATTI) instruments which is known as most suitable device for newly proposed Bitumen Bond strength test. It is a portable device and can be used easily for adhesion testing. Procedure to perform this test is quite easy and quick [10].

The waxes are used in PMAs as flowing agent and Zeolites are used in asphalt foaming as water agents. Due to environmental limitations, waxes and zeolites are extensively used in asphalt pavements to reduce energy emission and CO₂. Because of their use in asphalt pavements, it is necessary to investigate their effect on adhesion. The major aim of this study is to quantify the effect of Waxes and Zeolite on adhesion between bitumen and aggregate.

In Pakistan, flexible pavements are facing severe issues of adhesion failure especially in Rainy and high-temperature areas. Due to adhesion loss, the maintenance cost of pavements has been increased as well as service life is decreased too. To sort out this problem, this study was done by using modifiers. So that this research will help highway agencies to uses this research in asphalt pavements.

The material that is used in this study is easily available throughout Pakistan. The modifier Natural Zeolite and Paraffin wax are cheap and commonly available. There is ease of mixing of these additives in bitumen. The methodology of investigating adhesion strength is quite simple and portable. This test can be performed at any desired temperature into a controlled temperature chamber. The outcomes of this study are very helpful and adaptable in the field. By using this research, the maintenance cost of asphalt pavements will minimize.

2. Materials

2.1. Bitumen

80/100 was selected as Binder. The Penetration Test (BS EN 1426) and Softening Point Test (BS EN 1427) was performed to verify the pen grade and calculate softening point of this bitumen. According to results, the Pen Grade was 87 and the softening point was 44°C. The name of bitumen was given “B” in this study.

2.2. Aggregates

As limestone shows better adhesion due to its basic nature that’s why limestone was selected. Lime-stone is selected to investigate how the Zeolite and Wax modified bitumen affect adhesion bond with basic aggregates because the limestone is considered a suitable aggregate with respect to adhesion. The properties of this aggregate are presented in the following Table 1.
Table 1. Aggregate nature and type

| Materials   | Type       | Component                  | Rock Type          | Nature       |
|-------------|------------|----------------------------|--------------------|--------------|
| Aggregate   | Lime Stone | Calcite 65%, Silica 30%    | Fossiliferous Limestone | Basic       |

Figure 1. Crushed limestone

2.3. Additives

Two additives were selected based on their use in Asphalt technologies. One was Natural Zeolite (Z) which easily available in Pakistan a 2nd is Paraffin Wax (P). The chemical composition of zeolite is given in Table 2.

Table 2. Chemical composition of zeolite

| Chemical Component | Quantity (%) |
|--------------------|--------------|
| Silica as SiO₂     | 67.72        |
| Aluminum as Al₂O₃  | 16.29        |
| Sodium Oxide as NaO₂| 1.49         |
| Iron as Fe₂O₃      | 0.62         |
| Potassium Oxide as K₂O | 3.68    |
| Calcium Oxide      | 3.14         |
| Manganese Oxide    | 0.01         |
| Magnesium Oxide    | 0.00         |

The Paraffin Wax is colourless or white material extracted from petroleum, coal or shale oil. The Waxes are hydrocarbons containing twenty to fourth atoms with formula CₙH₂ₙ₊₂. These additives were used in 0.5, 2 and 3.5 percent by weight of bitumen.

3. Experimental Methodology

Figure 2 shows the flowchart methodology which has been followed in this study while performing laboratory testing.

3.1. Physical Properties Testing

The softening point was determined under British Standard (BS EN 1426) test. That is commonly known as Ring Ball Test. To find penetration grade, Penetration Test was performed under BS EN 1427. The results are presented in Table 3.
The results illustrate by increasing dosages of Z in bitumen the softening points are increased and pen grade decreased. This means that Z has made the B stiffer than virgin B. While in the case of P, as the dosages are increased the bitumen B becomes softer than Base bitumen.

3.2. Mixing of Additive into Bitumen

To mix additives into bitumen, 200 gr of bitumen was heated at 130 °C to 150 °C until it converted in liquid form. Then prescribed ratios of additives were added into liquid bitumen. For homogenous mixing of bitumen, the mixture was put under stirrer with rpm 500 to 700 for five minutes. The homogenous mixture was poured into cans with a proper seal. Then these cans were kept in a dark place at 25 °C [9].

3.3. Bitumen Bond Strength Test (BBS)

Basically, BBS is a modification of the PATTI test. This test is performed under specification of (ASTM D-4541). This test is used to determine the bond strength between aggregate and binder in dry and after water conditioning. The BBS device consists of a metallic pull-off stub, reaction plate, pressure hose, piston, and a portable pneumatic adhesion tester. In this test the metallic stubs are pulled off by pressure. If the applied stress is greater than the cohesive and adhesive strength of bond, the failure occurs. Equation 1 is used to calculate the Pull of Tensile Strength (POTs).

\[
POTs = \frac{(BP - Ag) - c}{ApS}
\]  

Where BP is burst pressure in kPa, \(Ag\) is contact area between reaction plate and gasket, \(ApS\) is area of pulled-off metallic stubs and \(c\) is the piston constant. The outer and inner diameters of metallic stubs are 22 mm and 20 mm respectively with 800 µm edge thickness. The systematic diagram is given in Figure 3.

![Figure 3. Test assembly of bitumen bond strength test](image)

For sample preparation, the limestone substrates of size 300 mm \(\times\) 150 mm \(\times\) 25 mm were selected as shown in Figure 4. To clean this plate and to remove impurities, it was washed with de-ionized water and then place into oven at 60°C for 60 minutes to evaporate surface water. The metallic stubs first cleaned with acetone and then they were heated in oven at 75 °C. The bitumen was heat at 160 °C for 5 minutes to convert it into liquid form. Then bitumen was poured onto stubs surface with spoon and then firmly put on substrate [17].

![Figure 4. Lime-stone substrate](image)
After that, the specimens were kept in a dark and dry place to cool down at 25°C. This test was performed at different temperatures 15°C and 25°C to observe the effect of temperature on adhesion. To investigate the effect of water, the samples were kept in d-ionized water for 72 hrs. After performing a test, POTs were calculated using Equation 1. The BBS specimen is shown in Figure 5.

3.4. Performance Grade Testing

Penetration grading or viscosity grading have limited ability to fully characterize asphalt binder to use in Hot Mix Asphalt (HMA) pavements. To overcome this problem, performance grade was developed. In performance grading system, the bitumen is categorized according to their failure temperature. This characterization is more accurate than conventional Penetration Grading. This reliability of PG Testing enhances the quality of the binder which is used in HMA pavements.

The core theme behind this testing is to correlate the HMA asphalt binder properties with the conditions under which it will be used. High-Temperature Grade: To calculate the upper limit of performance grade, Dynamic Shear Rheometer was used. The test was performed under specification of AASHTO M320. In DSR testing, high-temperature grade is measure in strained-controlled mode. Where strain was kept 10% and frequency was fixed at 10 rad/s. Complex shear modulus (G*) and phase angle (θ) were measured in response to a sinusoidal stress for each sample [18]. The results have been summarized in Table 4.

Table 4. Summary of DSR test results for virgin and modified binders

| Sample          | 52°C  | 58°C  | 64°C  | 70°C  | 76°C  | 82°C  | Failure Temperature |
|-----------------|-------|-------|-------|-------|-------|-------|---------------------|
| G*/sin(θ) kPa   | ---   | ---   | ---   | ---   | ---   | ---   | ---                 |
| Virgin 80/100   | 4.43  | 2.46  | 1.10  | 0.536 | ---   | ---   | 64.8°C              |
| 0.5% P          | 3.41  | 1.70  | 0.670 | ---   | ---   | ---   | 62.4°C              |
| 2% P            | 2.89  | 1.42  | 0.610 | ---   | ---   | ---   | 61.1°C              |
| 3.5% P          | 2.77  | 1.21  | 0.565 | ---   | ---   | ---   | 59.6°C              |
| 0.5% Z          | 4.83  | 2.47  | 1.05  | 0.542 | ---   | ---   | 64.9°C              |
| 2% Z            | 5.19  | 2.75  | 1.15  | 0.581 | ---   | ---   | 65.8°C              |
| 3.5% Z          | 5.52  | 2.92  | 1.25  | 0.614 | ---   | ---   | 70°C                |

4. Results and Discussion

4.1. Results

The specimens were prepared under the specification of ASTM-4541 and the test was performed in a dry condition at 25°C. To investigate the effect of temperature, the samples were also tested at 15°C. All tests were performed in the temperature-controlled chamber. To examine the effect of moisture, the samples were conditioned by keeping in de-ionized water for 72 hrs at 25°C. For each combination of bitumen and aggregate, 4 specimens were tested for their average results. The POTs were calculated by using Equation 1.

In Figure 6 the results show that 2% of Z Bitumen has the highest pull of tensile strength (POTs), which is 509 psi than that of virgin B with POTs 400 psi. The results illustrate with an increase of dose of Z, the adhesion increases but after 2% of Z further addition of Z decrease the adhesion. While P shows the decrease in adhesion as the quantity of P increase in B. 3.5% of P bitumen has lowest POTs that is 156 psi. The 0.5% of P bitumen shows a slight decrease in adhesion in dry condition. To quantify the effect of moisture the BBS was performed at 15°C on 80/100 Bitumen with lime-stone.
The results are presented in Figure 7 and it reveals that with a decrease in temperature the adhesion is improved. The 2% of Z bitumen has the highest POTs that are 1545 psi while 3.5% of P bitumen has the lowest POTs that is 707 psi. The virgin has 1397 psi Pull of Tensile strength which is lower than 0.5% of Z modified bitumen but higher than P modified bitumen.

Figure 8 represents the results of BBS was performed on virgin and modified bitumen with Lime-stone after 72hrs water conditioning. According to results, 2% of Z in bitumen stands at highest position with 361 psi POTs. The virgin B have 261 psi POTs that is higher than other ratios of P and Z, but it is lower than 2% of Z modified B. While 3.5% of P modified B have lowest POTs that are 167 psi.
4.2. Discussion

Chemical and physical properties, aggregate mineralogy and compatibility of bitumen with type of aggregate in term of polarity and composition are the major factors which governed the adhesion among binder and aggregates. The introduction of modifiers into binder enhances the physical and chemical properties of bitumen. The results are presented in section 0. In the discussion section, the behaviour of bitumen either virgin or modified will be discussed against the adhesive bond between binder and aggregate. In Figure 9, the correlation indicates that with an increase in stiffness of binder, the adhesion increases. When 0.5% of Z was added to bitumen, the adhesion has increased 2.2% than that of virgin B. But, as dose of Z was increased to 2% of Z, the adhesion has increased 20.3% than that of base B. Further increment in Z quantity in B shows the 22.75% decrease in adhesion. In the case of P, with an increase in dosage of P into bitumen, adhesion has decreased. For 0.5% of P in B, adhesion has reduced to 1% than that of base B. When 3.5% of P is added into bitumen, the adhesion has dropped to 57% than that of virgin B. The behaviour of Z modified bitumen shows that the adhesion increases due to stiffness till a certain limit and beyond this limit the adhesion start decreasing and this trend is observed in the case of 3.5% of Z. The reason behind this behaviour is that when bitumen becomes stiffer it behaves like a solid brittle material. On the other hand, the introduction of P makes bitumen softer which cause a reduction in adhesion.

![Figure 9. Correlation between BBS results and softening point and pen-grade of B](image)

Effect of moisture: in Figure 10, if BBS after 72 hrs water conditioning is examined, the results illustrate that 2% shows highest resistance against moisture that is 27.7% more than that of base B. While the reduction in adhesion after 72hrs water conditioning for 2% of Z into bitumen with limestone is 29.21% of 2% of Z into bitumen in dry state. The reduction in adhesion for virgin B is 34.75% of virgin B in dry state. If reduction for 2% of Z and virgin B is compared, reduction in adhesion for virgin B is 5.53% more than that of 2% of Z modified bitumen. Now, if results of P modified bitumen are compared before water conditioning and after 72hrs. For 0.5% of P bitumen, the adhesion has dropped to 37.87% after water conditioning. While in the case of 3.5% of P, there is a slight decrease in adhesion that is only 3%. This behaviour shows that 0.5% of P modified bitumen has poor performance against moisture damage.

![Figure 10. BBS results at 25 °C and 15 of virgin and modified B with lime-stone](image)
In Figure 10, the comparison is developed between BBS results at 25 and 15°C of virgin and modified Bitumen by using limestone. The core theme behind this comparison is to observe the effect of temperature on adhesion. At 15°C, the adhesive bond of 0.5% of Z bitumen becomes 72.3% stronger than that of at 25°C. For 2% of Z bitumen, the adhesion has increased to 67% than that of at 25°C. For virgin B, the adhesion has increased to 71.3% than at 25°C. For P modification, the decrease in temperature has improved the adhesion. For 0.5% of P bitumen, the adhesive bond has become 70.9% stronger than at 25°C. For 3.5% of P modified bitumen, the adhesion has increased to 75.6% than at 25°C. These behaviours illustrate that at lower temperature the adhesion between binder and aggregate is improved. So, not only physicochemical properties or mineralogy of aggregates the temperature also affect the adhesion. At high temperature, the adhesion decreases.

In Asif Sa et al. (2018) [17] researches Bitumen Bond strength test was performed to evaluate adhesion properties of binder and aggregate. Only virgin bitumen B2 (91 Pen Grade) was tested with different types of aggregates in dry and after 72 hrs water conditioning in that research. While in this research two types of modifier were used to quantify their effect on adhesive properties of bitumen. The pull of tensile strength of B2 with limestone was 345 psi while in present research (B with limestone) that is 400 psi. After 72 hrs water conditioning of B2 specimen, the pull of tensile strength was dropped to 285 psi while in present research that is 261 psi. Due to performing BBS testing at 15°C, 25°C and after 72 hrs water conditioning with two type of modifier in this study has created greater difference between past study where only virgin bitumen were tested by using time as parameter.

In the above discussion, the adhesion is discussed according to temperature and pen grading. Now adhesion will be discussed according to physicochemical properties and mineralogy of aggregate. The Z has proved itself the best additive in terms of adhesion, as Z has an excess of cations in the form of SiO$_2$ (67.72%). When it is mixed with bitumen, it increased the polarity of bitumen by increasing positive ions. On the other side, the limestone has excess of anions due to CaCO$_3$ (65%). Because of this polarity difference, the bond between Z modified bitumen and limestone becomes stronger than that of virgin B and limestone. In the results of strong bonding, Z modified bitumen shows great potential against moisture damage. For the high polarity of aggregate, different types of aggregate can be used and to increase bitumen polarity, it is modified with organic and inorganic additives [19, 20]. The phase angle is increased due to enhancement in P content. The increase in phase angle decreases the viscosity of bitumen. This property of P damages the wettability mechanism of bitumen. As the phase angle is increased, the reduction in adhesion occurs. This reduction in adhesion is significant sign of moisture damage [21]. Due to these problems, the P modified bitumen shows lower adhesion than virgin and Z modified B. The viscosity of bitumen has a vital role in stripping. The less viscous bitumen gives better coating, but more viscous bitumen shows more resistance against stripping. So, P modified bitumen has poor performance against adhesion while Z modified has better performance against adhesion.

![Figure 11. Performance grade of virgin and modified B](image)

Figure 11 is a graphical representation of the performance grading of bitumen. The results show that the modification of P in bitumen decreases the failure temperature. At 3.5% of P in bitumen, the failure temperature has dropped to 8% of virgin bitumen. While when Z is mixed in bitumen the failure temperature has increased. With an addition of 3.5% of Z in bitumen, the failure temperature has raised to 7.4% than the virgin. This raising in failure temperature is a sign of improvement in rutting at high temperatures. And, the fall in failure temperature due modification of P in bitumen reflects the potential to resist fatigue cracking.
5. Conclusions

- Modification of bitumen with Zeolite shows that Zeolite can be used to make bitumen stiff as 0.5% addition of Z in Bitumen change the grade 87 to 74 and 3.5% of Z change the grade 87 to 57. While paraffin wax can be used to make the bitumen soft as 0.5% addition of paraffin wax convert the grade 87 to 94 and 3.5% of paraffin wax improves the grade to 134.

- As many factors control adhesion like viscosity, phase angle, contact angle, surface energy, physiochemical properties, chemical nature of aggregates and bitumen grade. The domination of these factors on adhesion properties is not straight forward. Sometimes one factor dominates while the other dominates under the other conditions. In this study, 3.5% Z should show maximum adhesion in case of limestone with B bitumen, but it shows less. Though it’s chemically compatible with limestone at the same time, it makes bitumen stiffer. So, the bond becomes weak.

- The 2% of Zeolite dosage in Bitumen shows maximum adhesion strength with limestone as the POTs increase to 20.3% of virgin POTS. So, when there is moisture damage the combination of 2% Zeolite in B with limestone should be used.

- The modification of Paraffin wax in B shows inverse behaviour. As dosages are increased, the adhesion loss is started. At 3.5% of Paraffin into bitumen the adhesion drops to 43% of the virgin bitumen specimen in dry state and it is dropped to 64% of virgin bitumen after 72hrs water conditioning. So, the use of Paraffin as a flowing agent in Polymer modified Asphalts may affect the adhesion.

- The performance grading is showing that the modification of Zeolite makes bitumen harder. The 3.5% of Zeolite into bitumen changed the failure temperature from 64.8 to 70°C So, Zeolite modified bitumen is useful in hot areas of Pakistan. Where temperature rises up-to 50°C.

- The results of testing after 72 hrs water condition illustrate 2% of Zeolite in bitumen has increased adhesion (361 psi) as compared to virgin (261 psi) and Paraffin wax modified bitumen (167 psi). Thus, Zeolite is also suitable Rainy Areas of Pakistan for adhesion purposes.

- The performance grading shows that Paraffin wax modified bitumen shows better results at lower temperature 15°C. The addition of 3.5% of Paraffin wax dropped the failure temperature from 64.8 to 59.6°C. Therefore, it can be used in cold areas of Pakistan like Northern Areas.

- The use of PATTI for Bitumen Bond Strength is very helpful. It is a portable device and can be used at any temperature to investigate adhesion either at lower temperature or at higher temperatures as compared to other techniques to investigate adhesion.

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7. Conflicts of Interest

The authors declare no conflict of interest.

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Approximation of the Multidimensional Optimal Control Problem for the Heat Equation (Applicable to Computational Fluid Dynamics (CFD))

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Abstract

This work is devoted to finding an estimate of the convergence rate of an algorithm for numerically solving the optimal control problem for the three-dimensional heat equation. An important aspect of the work is not only the establishment of convergence of solutions of a sequence of discrete problems to the solution of the original differential problem, but the determination of the order of convergence, which plays a very important role in applications. The paper uses the discretization method of the differential problem and the method of integral estimates. The reduction of a differential multidimensional mixed problem to a difference one is based on the approximation of the desired solution and its derivatives by difference expressions, for which the error of such an approximation is known. The idea of using integral estimates is typical for such problems, but in the multidimensional case significant technical difficulties arise. To estimate errors, we used multidimensional analogues of the integration formula by parts, Friedrichs and Poincare inequalities. The technique used in this work can be applied under some additional assumptions, and for nonlinear multidimensional mixed problems of parabolic type. To find a numerical solution, the variable direction method is used for the difference problem of a parabolic type equation. The resulting algorithm is implemented using program code written in the Python 3.7 programming language.

Keywords: Approximation of a Three-Dimensional Parabolic Problem; Optimal Control; Convergence of the Gradient Method; Integral Estimates; Functional Convergence Estimation, CFD.

1. Introduction

The heat equation is used to find the dependence of the temperature of the medium on the spatial coordinates and time, for given coefficients of heat capacity and heat conductivity. This is a second order partial differential equation, which is a parabolic type equation. Since the need to determine temperatures in the whole space is often absent, when setting the problem, additional conditions are introduced that determine the restrictions on the solution of the problem for a given area. For example, one of these conditions is to set the temperature distribution at the boundary of the region (the Dirichlet problem).
The process of finding the temperature distribution at given times is a laborious task. Since differential problems of a continuous nature cannot be programmed due to the limited capabilities of computer technology, such problems, by discretizing them, reduce to similar difference problems. Such a transition is carried out using difference schemes.

The main task of approximation is to find such an approximate function that least, in a certain sense, deviates from a given continuous function. Due to the fact that when solving continuous problems, the differential operators are replaced by finite-difference analogues, which are written in the form of algebraic equations, problems arise for determining the convergence and approximation error.

Note that when switching from a differential operator to a finite-difference analogue, a numerical solution is obtained that differs from the original solution. In such cases, an analysis is performed that determines the approximation order. For example, in Godunov and Ryabenkii (1987) study, the one-dimensional optimal control problem of the heat conduction process and the gradient descent method are considered, on the basis of which the approximation order of the finite-difference problem was obtained [1]. The optimality criterion is based on the gradient descent method, ideas leading to the assertion of the type of maximum principle by L. S. Pontryagin [2–4], lead to significant complications and are not considered in this paper. Approximation of optimization problems is considered by many researchers. An important work is Serovaïskii (2013) [5], from which methods for obtaining estimates of the boundedness of the target functional are used.

In modern works, attention is paid to the convergence of functionals in optimization problems of different nature. A hyperbolic boundary value problem with a quadratic cost functional is considered in Edalatzadeh et al. (2020) study [6]. An important point is the use of a similar technique of integral estimates to obtain optimal control in an explicit form. Criteria for the existence of optimal forms in Banach spaces were established in Edalatzadeh (2016 and 2019) studies [7, 8]. For a differential operator in divergent form and for an integro-differential operator in Deligiannidis et al. (2020) and Mukam and Tambue (2020) researches [9, 10] using integral estimates in suitable spaces, weak convergence of the numerical method was established and the order of convergence of the functional sequence to the solution was found.

The technique developed in this paper will be transferred to parabolic problems with variable coefficients, as well as to nonlinear cases. The possibility of such a step is considered plausible due to the Guillén-González et al. (2020) and Biccari et al. (2020) works [11, 12].

The aim of this work is to estimate the approximation of a finite-difference analogue for the heat equation of three spatial variables. The solution to the difference problem is constructed using the variable direction method.

Note that the original result on the convergence estimation of the sequence of the target functional in 3-dimensional space is established and the constants in the O symbols are directly calculated. We can briefly formulate the sequence of actions and steps that are used in the work:

- Statement of the differential problem;
- Analysis of the differential problem, obtaining an estimate of the norm of the solution depending on the control function;
- Building a sequence of discrete tasks;
- Obtaining expressions for errors between solutions to differential and discrete problems;
- Estimation of errors using the technique of Sobolev spaces and the establishment of target inequality.

Based on the discretization of the three-dimensional heat conduction problem, a numerical algorithm is developed, with the help of which a software package is created to determine the time required for uniform distribution of heat in the rod.

2. The Problem Statement

The following is a third-order differential heat equation that describes the process of heating a body in space:

\[
\frac{\partial f}{\partial t} = a^2 \left( \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \right) + u(x, y, z, t)
\]

\[(x, y, z, t) \in Q = Q_3 \times (0, T), Q_3 = (0, l_x) \times (0, l_y) \times (0, l_z)\]  

For which the following boundary conditions are given:

\[
\left. \frac{\partial f}{\partial Q} \right|_{_{\partial Q}} = \psi(x, y, z, t), \quad 0 < t < T;
\]

\[
f|_{_{t=0}} = \varphi(x, y, z), 0 \leq x \leq l_x, 0 \leq y \leq l_y, 0 \leq z \leq l_z,
\]

\[
f|_{_{x=0}} = \varphi(x, y, z), 0 \leq x \leq l_x, 0 \leq y \leq l_y, 0 \leq z \leq l_z,
\]

\[
f|_{_{y=0}} = \varphi(x, y, z), 0 \leq x \leq l_x, 0 \leq y \leq l_y, 0 \leq z \leq l_z,
\]

\[
f|_{_{z=0}} = \varphi(x, y, z), 0 \leq x \leq l_x, 0 \leq y \leq l_y, 0 \leq z \leq l_z,
\]
Where \( f(x, y, z, t) \) is the solution of the boundary value problem, \( u(x, y, z, t) \) is a control function that shows the temperature at the point \((x, y, z)\), at the moment of time \(t\), \(\alpha^2\) is the thermal conductivity coefficient, \(\varphi(x, y, z)\) is the temperature of the rod at the initial moment of time at each point, \(\psi(x, y, z, t)\) is a given function from \(L_2[(0, l_x) \times (0, l_y) \times (0, l_z)]\). Questions of representation of solutions, existence and uniqueness are stated in Vladimirov (1981) and Shubin (2003) works [13, 14].

We denote that the control belongs to the following set:

\[
U = \left\{ u(x, y, z, t) \in L_2(Q) : \int_0^T u^2(x, y, z, t)dx dy dz dt \leq R^2 \right\},
\]

(3)

Where \( R = \text{const} > 0 \).

Such a problem is called the Dirichlet problem or the first boundary value problem. We find a numerical solution to this problem using numerical methods, namely, the finite difference method. By expanding the function in a Taylor series, the first and second partial derivatives are expressed, and the boundary conditions are used to determine the value of the nodes on the boundary region.

The task is to find a function \( f(x, y, z; t; u) \), such that on the whole region \( L_2[(0, l_x) \times (0, l_y) \times (0, l_z)] \) by the time \( T \) we get the distribution function heat close to the given function \( b(x, y, z) \). The criterion for this difference problem has the form:

\[
f(u) = \int_0^{l_x} \int_0^{l_y} \int_0^{l_z} |f(x, y, z, t; u) - b(x, y, z)|^2 dx dy dz \rightarrow \inf, u \epsilon U
\]

(4)

And the boundary conditions are rewritten as follows:

\[
\frac{\partial f}{\partial Q_3} = 0, 0 < t < T
\]

(5)

\[
f|_{t=0} = 0, 0 \leq x \leq l_x, 0 \leq y \leq l_y, 0 \leq z \leq l_z
\]

In this case, it is necessary to go to the finite-difference analogue of the function \( f(x, y, z, T; u) \) and evaluate the approximation order.

3. Equation of a Parabolic Type

In this paper, we consider the process of temperature distribution over a three-dimensional rod with a length, height, and width equal to \( l_x, l_y, l_z \), respectively, for the time interval \( T \), which is described by the heat equation. An inhomogeneous equation is considered:

\[
\frac{\partial f}{\partial t} = \left( \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \right) + u(x, y, z, t),
\]

(6)

Which has coefficient \( \alpha^2 = 1 \) and boundary conditions (5).

We will seek a generalized solution to the original problem in the form of an expansion into a triple Fourier series. Let:

\[
f(x, y, z, t) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \sum_{k=1}^{\infty} X_n(x) \cdot Y_m(y) \cdot Z_k(z) \cdot T_{nmk}(t)
\]

(7)

\[
u(x, y, z, t) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \sum_{k=1}^{\infty} X_n(x) \cdot Y_m(y) \cdot Z_k(z) \cdot U_{nmk}(t)
\]

(8)

Substituting these series in Equation (6), we can conclude that (6) is certainly satisfied if the terms of the series are equal for the corresponding indexes of the number series of the left and right sides of the equation:

\[
X_n(x) \cdot Y_m(y) \cdot Z_k(z) \cdot T'_{nmk}(t) =
\]

\[
= \left( X_n''(x)Y_m''(y)Z_k''(z) + X_n''(x)Y_m'(y)Z_k'(z) + X_n'(x)Y_m'(y)Z_k''(z) \right) T_{nmk}(t) + X_n(x)Y_m(y)Z_k(z) U_{nmk}(t)
\]

(9)

By removing the inhomogeneous additive in Equation (9), divide it into \( X_n(x) \cdot Y_m(y) \cdot Z_k(z) \cdot T_{nmk}(t) \) and rewrite it in the following form:
\[
\begin{align*}
X''(x) + \lambda^2 X(x) &= 0 \\
Y''(y) + \mu^2 Y(y) &= 0 \\
Z''(z) + p^2 Z(z) &= 0 \\
T''(t) + (\lambda^2 + \mu^2 + p^2)T(t) &= 0
\end{align*}
\] (10)

We find a solution to the three Sturm-Liouville problems. We start with the problem \(X''(x) + \lambda^2 X(x) = 0\), with \(X(0) = X_x(1) = 0\). Consider 3 cases of solving a linear differential equation.

For \(\lambda^2 < 0\), the general form of the solution takes the form \(X_n(x) = C_1 e^{-\lambda x} + C_2 e^{\lambda x}\). Due to the boundary conditions, the solution becomes trivial. This solution does not fit.

For \(\lambda^2 = 0\), the general solution is \(X_n(x) = C_1 + C_2 x\). The solution, by analogy with the case \(\lambda^2 < 0\) also does not fit.

For \(\lambda^2 > 0\), the general solution is \(X_n(x) = C_1 \cos(\lambda x) + C_2 \sin(\lambda x)\). It follows from the boundary conditions that \(C_2 = 0\) and \(C_1 \sin(l_x) = 0\). It follows that \(\lambda l_x = \pi n\). Consequently, the general decision takes the following form.

\[
X_n(x) = C_1 \cos\left(\frac{\pi n}{l_x} x\right), n = 1, 2, ...
\] (11)

To obtain a complete orthonormal system, we define \(C_n\). To do this, take the scalar product from (9), equate it to 1 and find the integral.

\[
\int_0^{l_x} C_n^2 \cos^2\left(\frac{\pi n}{l_x} x\right) dx = 1
\]

We get that \(C_n = \frac{2}{\sqrt{l_x}}\) and:

\[
X_n(x) = \frac{2}{\sqrt{l_x}} \cos\left(\frac{\pi n}{l_x} x\right), n = 1, 2, ...
\] (12)

Similarly, we find a generalized solution for \(Y(y)\) and \(Z(z)\).

\[
Y_m(y) = \frac{2}{\sqrt{l_y}} \cos\left(\frac{\pi m}{l_y} y\right), m = 1, 2, ...
\] (13)

\[
Z_k(z) = \frac{2}{\sqrt{l_z}} \cos\left(\frac{\pi k}{l_z} z\right), k = 1, 2, ...
\] (14)

We find the general solution of the differential equation based on \(\lambda^2, \mu^2\) and \(p^2\).

\[
T_{nmk}'(t) + \left(\frac{\pi n}{l_x}^2 + \frac{\pi m}{l_y}^2 + \frac{\pi k}{l_z}^2\right) T_{nmk}(t) = U_{nmk}(t)
\] (15)

We apply the variational constant method. We solve the corresponding homogeneous equation and find a generalized solution in which \(C_n\) is an arbitrary constant on \(t\).

\[
T(t) = C_n(t) e^{-\delta^2 t} \\
T'(t) = C_n'(t) e^{-\delta^2 t} - \delta^2 C_n(t) e^{-\delta^2 t}, \text{ where } \delta^2 = \left(\frac{\pi n}{l_x}\right)^2 + \left(\frac{\pi m}{l_y}\right)^2 + \left(\frac{\pi k}{l_z}\right)^2
\] (16)

We put this in Equation (9) and we obtain that for the unknown function \(C_n(t)\) the equality \(C_n'(t) e^{-\delta^2 t} = U_{nmk}(t)\) must be satisfied. We get that.

\[
C_n(t) = \int_0^t e^{\delta^2 \tau} U_{nmk}(\tau) d\tau
\] (17)

Whence the solution of the Cauchy problem is given by the formula:

\[
T_{nmk}(t) = \int_0^t e^{\delta^2 (t-\tau)} U_{nmk}(\tau) d\tau, t > 0
\]

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We obtain a formula for calculating the expansion coefficients \( u(x, y, z, t) \) in eigenfunctions. Given the orthogonality of the Sturm-Liouville problem, we obtain:

\[
U_{nmk}(t) = \frac{8}{l_x l_y l_z} \int_{D} U(x, y, z, t) \cos \left( \frac{\pi n x}{l_x} \right) \cos \left( \frac{\pi m y}{l_y} \right) \cos \left( \frac{\pi k z}{l_z} \right) \, dx \, dy \, dz
\]  
(18)

Hence, on the basis of (7), (9), (11) and (12), we obtain:

\[
f(x, y, z, t) = \frac{8}{l_x l_y l_z} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \sum_{k=1}^{\infty} \cos \left( \frac{\pi n x}{l_x} \right) \cos \left( \frac{\pi m y}{l_y} \right) \cos \left( \frac{\pi k z}{l_z} \right) f_N \left( \frac{x}{l_x}, \frac{y}{l_y}, \frac{z}{l_z} \right) \, dx \, dy \, dz
\]  
(19)

Where \( \delta^2 = \left( \frac{\pi n}{l_x} \right)^2 + \left( \frac{\pi m}{l_y} \right)^2 + \left( \frac{\pi k}{l_z} \right)^2 \), and \( U_{nmk}(t) \) is equal to (14).

4. Discretization of the Problem

The difference minimization problem has the following form. It is necessary to minimize the objective function \( f(x, y, z, t) \) on the four-dimensional domain \( \bar{D} = [0, l_x] \times [0, l_y] \times [0, l_z] \times [0, T] \), where \( x, y, z \) are spatial variables and \( t \) is time variable. The grid \( \omega_{hxhyhz} = \{(x_i, y_j, z_k, t_p) : x_i = ih_x, y_j = jh_y, z_k = kh_z, t_p = pr, i = 0...X_h, j = 0...Y_h, k = 0...Z_h, p = 0...P\} \), where \( h_x, h_y, h_z, \tau \) are grid steps, \( h_xX_h = l_x, h_yY_h = l_y, h_zZ_h = l_z, \tau P = T \). Following works [15] and [16] we perform discretization and obtain difference problems.

We define the function \( f_{hxhyhz} = \{f_{ijkp} : i = 0...X_h, j = 0...Y_h, k = 0...Z_h, p = 0...P\} \) on the grid partition \( \omega_{hxhyhz} \), which will correspond to separate differences

\[
\begin{align*}
&f_{hxijkp} = \frac{1}{h_x}(f_{i+1,jkp} - f_{ijkp}) \quad f_{hxijkp} = \frac{1}{h_x}(f_{ijkp} - f_{i-1,jkp}) \\
&f_{hyijkp} = \frac{1}{h_y}(f_{ij+1,kp} - f_{ijkp}) \quad f_{hyijkp} = \frac{1}{h_y}(f_{ijkp} - f_{ij-1,kp}) \\
&f_{hzijkp} = \frac{1}{h_z}(f_{ij+1,kp} - f_{ijkp}) \quad f_{hzijkp} = \frac{1}{h_z}(f_{ijkp} - f_{ijk-1,kp}) \\
&f_{hijzkp} = \frac{1}{h_z}(f_{hij+1,kp} - f_{hij,kp}) = \frac{1}{h_z}(f_{ij+1,kp} - 2f_{ijkp} + f_{i-1,jkp}) \\
&f_{hijyp} = \frac{1}{h_y}(f_{hij+1,kp} - f_{hij,kp}) = \frac{1}{h_y}(f_{ij+1,kp} - 2f_{ijkp} + f_{ij-1,kp}) \\
&f_{hxijzp} = \frac{1}{h_z}(f_{hxij+1,kp} - f_{hxij,kp}) = \frac{1}{h_z}(f_{hij+1,kp} - 2f_{ijkp} + f_{ijk-1,kp}) \\
&f_{hijkp} = \frac{1}{\tau}(f_{ijkp} - f_{ijkp-1})
\end{align*}
\]  
(20)

We rewrite items (3)-(5) taking into account the discretization of the original problem. The grid function \( f_{hxhyhz} = f_{hxhyhz}(u_{hxhyhz}) \) will be the difference analogue of the function \( f(x, y, z, t; u) \). Also, the function \( u_{hxhyhz} = \{u_{ijkp} : i = 1...X_h-1, j = 1...Y_h-1, k = 1...Z_h-1, p = 1...P\} \), which belongs to:

\[
U_{hxhyhz} = \left\{ u_{ijkp} : \sum_{p=1}^{M} \sum_{l=1}^{X_h-1} \sum_{j=1}^{Y_h-1} \sum_{k=1}^{Z_h-1} h_x h_y h_z \tau u_{ijkp}^2 \leq R^2 \right\}
\]  
(21)

Will be the difference analogue for the control \( u(x, y, z, t) \). Then the criterion (4) for the minimization problem taking into account the function \( f_{hxhyhz} \) takes the following form:

\[
\begin{align*}
&f_{hxhyhz}(u_{hxhyhz}) = \sum_{i=1}^{X_h-1} \sum_{j=1}^{Y_h-1} \sum_{k=1}^{Z_h-1} h_x h_y h_z |f_{ijkp} - b_{ijkp}|^2 \rightarrow \inf,
\end{align*}
\]  
(22)
\( u_{h_x h_y h_z} \in U_{h_x h_y h_z} \)

Equation (6) taking into account (16) and boundary conditions:
\[
\begin{align*}
 f_{i j k p} &= \left( f_{h_x h_y h_z i j k p} + f_{h_y h_z i j k p} + f_{h_z i j k p} \right) + u_{i j k p}, \\
 i &= 1..X_h - 1, j = 1..Y_h - 1, k = 1..Z_h - 1, p = 0..P; \\
 f_{h_x i j k p} &= f_{h_x X_h i j k p} = f_{h_x i j k P} = f_{h_x i j 1p} = f_{h_x i j 2p} = 0, \\
 p &= 1..P; \\
 f_{i j k 0} &= 0, i = 0..X_h, j = 0..Y_h, k = 0..Z_h. 
\end{align*}
\] (23)

5. Theoretical Information

In the course of performing mathematical analysis, a number of theorems, equations, and inequalities were used that play a fundamental role or are often used in mathematical calculations and simplifications.

Partial Summation Formula:
\[
\sum_{n=p}^{q} a_n b_n = - \sum_{n=p}^{q-1} A_n (b_{n+1} - b_n) + A_q b_q - A_{p-1} b_p, \\
A_n = \sum_{k=0}^{n} a_k, \text{ at } n \geq 0
\] (24)

Cauchy-Bunyakovsky inequality for sums and integrals:
\[
\sum_{i=1}^{n} |x_i y_i| \leq \left( \sum_{i=1}^{n} |x_i|^2 \right)^{\frac{1}{2}} \left( \sum_{i=1}^{n} |y_i|^2 \right)^{\frac{1}{2}} \] (25)

\[
\int_{a}^{b} f(x) g(x) dx \leq \left( \int_{a}^{b} f^2(x) dx \right)^{\frac{1}{2}} \left( \int_{a}^{b} g^2(x) dx \right)^{\frac{1}{2}}
\]

Lemma 1. [1] If some quantities \( \varphi_i, i = 0, ..., N \) satisfy the inequalities:
\[
0 \leq \varphi_0 \leq a, 0 \leq \varphi_{i+1} \leq a + b \sum_{m=0}^{i} \varphi_m, i = 1, ..., N - 1, b \geq 0,
\]
Then the estimate \( 0 \leq \varphi_i \leq a (1 + b)^i \) is fair, at \( i = 0, ..., N \). If
\[
0 \leq \varphi_{i-1} \leq a + b \sum_{m=0}^{N-1} \varphi_m, i = 1, ..., N - 1, 0 \leq \varphi_{N-1} \leq a,
\]
Then the estimate \( 0 \leq \varphi_{i-1} \leq a (1 + b)^{N-i-1} \) is fair, at \( i = 0, ..., N - 1 \).

Elementary Inequalities:
\[
|ab| \leq \frac{\varepsilon}{2} a^2 + \frac{1}{2 \varepsilon} b^2, (a + b)^2 \leq 2a^2 + 2b^2,
\]
\[
(a + b + c)^2 \leq 3(a^2 + b^2 + c^2) \forall a, b, c \in \mathbb{R} \forall \varepsilon > 0.
\] (26)

6. Analysis of the Differential Problem

We begin the analysis of the differential problem by deriving two estimates for sufficiently smooth classical solutions to problem (5), (6), which will be emphasized in future work. Further actions are based on functional inequalities, which are sufficiently developed in Vasilev (2002) study [17].

We multiply equation (1.6) by \( f(x, y, z, t; \mu) \) and integrate the resulting equality over the rectangle
\[ Q_\tau = \{(x, y, z, t) : 0 \leq x \leq l_x, 0 \leq y \leq l_y, 0 \leq z \leq l_z, 0 \leq t \leq \tau\} \]

Where \( \tau \) — arbitrary fixed point in time, \( 0 \leq \tau \leq T \).

\[
\int_{Q_\tau} \frac{\partial f}{\partial t} f \, dxdydzdt - \int_{Q_\tau} \Delta f \cdot f \, dxdydzdt = \int_{Q_\tau} uf \, dxdydzdt
\tag{27}
\]

In view of conditions (2), we transform the first term from the left-hand side:

\[
\int_{Q_\tau} \frac{\partial f}{\partial t} f \, dQ_\tau = \int_{Q_3} \left( \int_0^\tau \left( \int_0^t (f^2) \, dt \right) \, dQ_3 \right) = \int_{Q_3} f^2(x, y, z, \tau) \, dQ_3
\tag{28}
\]

To estimate the second term, we introduce each term of the Laplace operator under the differential sign, after which we apply the boundary conditions (5). As a result, we have:

\[
\int_{Q_\tau} \Delta f \cdot f \, dQ_\tau = \int_{Q_\tau} \left( \frac{\partial f}{\partial x} \right)^2 + \left( \frac{\partial f}{\partial y} \right)^2 + \left( \frac{\partial f}{\partial z} \right)^2 \, dQ_\tau
\tag{29}
\]

We use the Cauchy-Bunyakovsky formula (21) for the right-hand side of equality (27), after which we pass to the maximum in time for the classical solution of problem (5), (6). We have:

\[
\int_{Q_\tau} uf \, dQ_\tau \leq \int_0^\tau \left( \int_{Q_3} u^2 \, dQ_3 \right) \left( \int_{Q_2} f^2 \, dQ_3 \right)^{\frac{1}{2}} \left( \int_{Q_1} f^2 \, dQ_3 \right)^{\frac{1}{2}} \, dt \leq
\]

\[
\leq \max_{0 \leq t \leq T} \left( \int_{Q_2} f^2 \, dQ_3 \right)^{\frac{1}{2}} \left( \int_{Q_1} f^2 \, dQ_3 \right)^{\frac{1}{2}} \int_0^\tau \left( \int_{Q_3} u^2 \, dQ_3 \right) \, dt \leq \max_{0 \leq t \leq T} \left( \int_{Q_3} f^2 \, dQ_3 \right)^{\frac{1}{2}} \left( \int_{Q_1} f^2 \, dQ_3 \right)^{\frac{1}{2}} \sqrt{T} \| u \|_{L^2(Q)}
\]

\[
\int_{Q_\tau} uf \, dQ_\tau \leq \max_{0 \leq t \leq T} \left( \int_{Q_3} f^2 \, dQ_3 \right)^{\frac{1}{2}} \sqrt{T} \| u \|_{L^2(Q)}
\tag{30}
\]

We replace the terms in Equation (27) in accordance with formulas (28), (29) and (30), we have:

\[
\frac{1}{2} \int_{Q_3} f^2(x, y, z, \tau) \, dQ_3 + \int_{Q_\tau} \left( \frac{\partial f}{\partial x} \right)^2 + \left( \frac{\partial f}{\partial y} \right)^2 + \left( \frac{\partial f}{\partial z} \right)^2 \, dQ_\tau \leq
\]

\[
\leq \max_{0 \leq t \leq T} \left( \int_{Q_3} f^2 \, dQ_3 \right)^{\frac{1}{2}} \sqrt{T} \| u \|_{L^2(Q)}
\tag{31}
\]

Let us estimate this inequality. To do this, we remove each term from the right-hand side in turn. Based on this, we evaluate the first term.

\[
\int_{Q_3} f^2(x, y, z, \tau) \, dQ_3 \leq \max_{0 \leq t \leq T} \left( \int_{Q_3} f^2 \, dQ_3 \right)^{\frac{1}{2}} 2\sqrt{T} \| u \|_{L^2(Q)} \quad \forall \tau \in [0, T]
\]

Therefore, if we take the integral of the square of the function \( f \) with respect to the maximum \( \tau \) on the interval \([0, T]\), square and extract the square root, and then use the estimate for the first term, we obtain the following inequality:

\[
\max_{0 \leq t \leq T} \left( \int_{Q_3} f^2 \, dQ_3 \right)^{\frac{1}{2}} 2\sqrt{T} \| u \|_{L^2(Q)}
\]

Or:

\[
\max_{0 \leq t \leq T} \int_{Q_3} f^2 \, dQ_3 \leq \max_{0 \leq t \leq T} \int_{Q_3} f^2 \, dQ_3 \quad \forall \tau \in [0, T]
\]

\[
\max_{0 \leq t \leq T} \int_{Q_3} f^2 \, dQ_3 \leq \max_{0 \leq t \leq T} \int_{Q_3} f^2 \, dQ_3 \quad \forall \tau \in [0, T]
\]

\[
\max_{0 \leq t \leq T} \int_{Q_3} f^2 \, dQ_3 \leq \max_{0 \leq t \leq T} \int_{Q_3} f^2 \, dQ_3 \quad \forall \tau \in [0, T]
\]

\[
\max_{0 \leq t \leq T} \int_{Q_3} f^2 \, dQ_3 \leq \max_{0 \leq t \leq T} \int_{Q_3} f^2 \, dQ_3 \quad \forall \tau \in [0, T]
\]
\[
\max_{0 \leq t \leq T} \int f^2(x, y, z, t) dQ_3 \leq 4T\|u\|_{L^2(Q)}^2 \quad (32)
\]

From (31) we make an estimate for the second term, taking into account the estimate (32), we have:

\[
\int_{\tilde{Q}_t} \left( \left( \frac{\partial f}{\partial x} \right)^2 + \left( \frac{\partial f}{\partial y} \right)^2 + \left( \frac{\partial f}{\partial z} \right)^2 \right) dQ_t \leq \max_{0 \leq t \leq T} \left( \int f^2 dQ_t \right)^{\frac{1}{2}} \sqrt{T\|u\|_{L^2(Q)}} \leq 2T\|u\|_{L^2(Q)} \quad (33)
\]

Based on inequality (31) and estimates (32) and (33), we obtain the first estimate for a sufficiently smooth solution to problem (31) and (32):

\[
\max_{0 \leq t \leq T} \int f^2(x, y, z, t) dQ_3 + \int_{\tilde{Q}_t} \left( \left( \frac{\partial f}{\partial x} \right)^2 + \left( \frac{\partial f}{\partial y} \right)^2 + \left( \frac{\partial f}{\partial z} \right)^2 \right) dQ_t \leq 6T\|u\|_{L^2(Q)} \quad (34)
\]

Multiply equation (32) by \(\frac{\partial f}{\partial t}\) and integrate over the domain \(Q_t\):

\[
\int_{\tilde{Q}_t} \left( \frac{\partial f}{\partial t} \right)^2 dQ_t = \int \Delta f \cdot \frac{\partial f}{\partial t} dQ_t + \int u \frac{\partial f}{\partial t} dQ_t \quad (35)
\]

We estimate the first scalar product from the right-hand side. To do this, we introduce each term of the Laplace operator under the differential sign. As a result, we get:

\[
\int_{\tilde{Q}_t} \left( \frac{\partial f}{\partial t} \right)^2 dQ_t = \frac{1}{2} \int_{\tilde{Q}_t} \left( \frac{\partial f}{\partial x} \right)^2 + \left( \frac{\partial f}{\partial y} \right)^2 + \left( \frac{\partial f}{\partial z} \right)^2 \right) dQ_t
\]

Taking into account the boundary conditions (5), only the last integral does not vanish. If we introduce the derivative of the function with respect to each variable under the differential sign and use the main theorem of mathematical analysis, we get:

\[
= \int_{\tilde{Q}_t} \left( \int_0^1 \frac{1}{2} \frac{\partial}{\partial t} \left( \left( \frac{\partial f}{\partial x} \right)^2 + \left( \frac{\partial f}{\partial y} \right)^2 + \left( \frac{\partial f}{\partial z} \right)^2 \right) \right) dQ_3
\]

\[
= -\frac{1}{2} \left( \left( \frac{\partial f(x, y, z, t)}{\partial x} \right)^2 + \left( \frac{\partial f(x, y, z, t)}{\partial y} \right)^2 + \left( \frac{\partial f(x, y, z, t)}{\partial z} \right)^2 \right) dQ_3
\]

As a result, we obtain the following equality:

\[
\int_{\tilde{Q}_t} \left( \frac{\partial^2 f}{\partial x^2 \partial t} + \frac{\partial^2 f}{\partial y^2 \partial t} + \frac{\partial^2 f}{\partial z^2 \partial t} \right) dQ_t \quad (36)
\]

\[
= -\frac{1}{2} \int_{\tilde{Q}_t} \left( \left( \frac{\partial f(x, y, z, t)}{\partial x} \right)^2 + \left( \frac{\partial f(x, y, z, t)}{\partial y} \right)^2 + \left( \frac{\partial f(x, y, z, t)}{\partial z} \right)^2 \right) dQ_3
\]

Based on formula (36) and the elementary inequality of paragraph 1.4 for the product from formula (35), we have:

\[
\frac{1}{2} \int_{\tilde{Q}_t} \left( \left( \frac{\partial f(x, y, z, t)}{\partial x} \right)^2 + \left( \frac{\partial f(x, y, z, t)}{\partial y} \right)^2 + \left( \frac{\partial f(x, y, z, t)}{\partial z} \right)^2 \right) dQ_3 + \]
\[ + \int_{Q_\tau} \left( \frac{\partial f}{\partial t} \right)^2 dQ_\tau = \int_{Q_\tau} u \frac{\partial f}{\partial t} Q_\tau \leq \frac{1}{2} ||u||_{L^2(Q)}^2 + \frac{1}{2} \int_{Q_\tau} \left( \frac{\partial f}{\partial t} \right)^2 dQ_\tau \]

Or:

\[ \int_{Q_\tau} \left( \frac{\partial f}{\partial t} \right)^2 dQ_\tau + \int_{Q_\tau} \left( \left( \frac{\partial f(x, y, z, \tau)}{\partial x} \right)^2 + \left( \frac{\partial f(x, y, z, \tau)}{\partial y} \right)^2 + \left( \frac{\partial f(x, y, z, \tau)}{\partial z} \right)^2 \right) dQ_3 \leq ||u||_{L^2(Q)}^2 \]

\forall \tau \in [0,T]

Hence we have 2 inequalities:

\[ \int_{Q} \left( \frac{\partial f}{\partial t} \right)^2 dQ \leq ||u||_{L^2(Q)}^2 \]

\[ \max_{0 \leq t \leq T} \int_{Q_3} \left( \left( \frac{\partial f(x, y, z, \tau)}{\partial x} \right)^2 + \left( \frac{\partial f(x, y, z, \tau)}{\partial y} \right)^2 \right) \leq \]

\[ + \left( \frac{\partial f(x, y, z, \tau)}{\partial z} \right)^2 \right) dQ_3 \leq ||u||_{L^2(Q)}^2 \forall \tau \in [0,T]. \tag{37} \]

In addition, if we integrate equation (6) over the domain Q taking into account (37), we have:

\[ \int_{Q} (\Delta f)^2 dQ = \int_{Q} \left( \frac{\partial f}{\partial t} - u \right)^2 dQ \leq 2 \int_{Q} \left( \frac{\partial f}{\partial t} \right)^2 dQ + 2 \int_{Q} u^2 dQ \]

\[ \leq 4 ||u||_{L^2(Q)}^2 \tag{38} \]

Adding inequalities (37) and (38) we obtain the second estimate for a sufficiently smooth solution:

\[ \max_{0 \leq t \leq T} \int_{Q_3} \left( \left( \frac{\partial f(x, y, z, \tau)}{\partial x} \right)^2 + \left( \frac{\partial f(x, y, z, \tau)}{\partial y} \right)^2 + \left( \frac{\partial f(x, y, z, \tau)}{\partial z} \right)^2 \right) dQ_3 + \]

\[ + \int_{Q} \left( \frac{\partial f}{\partial t} \right)^2 dQ + \int_{Q} (\Delta f)^2 dQ \leq 6 ||u||_{L^2(Q)}^2 \tag{39} \]

We use the Friedrichs inequality and inequalities (37), and also taking the maximum in time for differentials with respect to spatial variables, we estimate the square of the solution with respect to the control function:

\[ 4 \int_{Q} f^2 dQ \leq \frac{R^2}{2} \max_{0 \leq t \leq T} \int_{Q_3} \left( \left( \frac{\partial f}{\partial x} \right)^2 + \left( \frac{\partial f}{\partial y} \right)^2 + \left( \frac{\partial f}{\partial z} \right)^2 \right) dQ_3 + \frac{\tau^2}{2} \int_{Q} \left( \frac{\partial f}{\partial t} \right)^2 dQ \leq \]

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\[
\frac{l^2_{\text{max}}}{2} \|u\|_{L^2(Q)}^2 + \frac{T^2}{2} \|u\|_{L^2(Q)^r}^2 \leq \sum_{i,j,k=1} \tau_f f_{i,j,k}^2 - \sum_{i,j,k=1} \tau(f_{i,j,k}^2 + f_{j,i,k}^2 + f_{j,i,k}^2) f_{i,j,k} = \]
\[
\frac{\sum_{i,j,k=1} \tau u f_{i,j,k}^2}{\sum_{i,j,k=1} \tau} \]
\[
\forall (x, y, z, t) \in Q, l_{\text{max}} = \max\{l_x, l_y, l_z\}.
\]

From here we get the energy estimate:

\[
\max_{(x, y, z) \in Q} \int_Q f^2 dQ \leq C \|u\|_{L^2(Q)}^2
\]
\[
C = \left( \frac{l^2_{\text{max}} + T^2}{8} \right), l_{\text{max}} = \max\{l_x, l_y, l_z\}
\]

7. Analysis of a Discrete Task

Using analogues with estimates (34) and (39), we derive the corresponding estimates for the discrete problem. We multiply Equation (19) by \(h_i h_j h_k \tau f_{i,j,k} = \tau f_{i,j,k} \) and sum over \(i, j, k\) from 1 to \(X_h - 1 = X_h,\) from 1 to \(Y_h - 1 = Y_h,\) and make the maximum transition in time for a discrete solution, from 1 to \(Z_h - 1 = Z_h,\) respectively:

\[
\sum_{i,j,k=1} \tau f_{i,j,k} f_{i,j,k} \geq \frac{1}{2} (f_{i,j,k}^2 f_{i,j,k}^2 - f_{i,j,k}^2 f_{i,j,k}^2), \]
\[
i = 1..X_h - 1, j = 1..Y_h - 1, k = 1..Z_h - 1, p = 1..M
\]

From here:

\[
\sum_{i,j,k=1} \tau f_{i,j,k} f_{i,j,k} \geq \frac{1}{2} \sum_{i,j,k=1} f_{i,j,k}^2 - \frac{1}{2} \sum_{i,j,k=1} f_{i,j,k}^2 f_{i,j,k}^2, p = 1..P
\]

In order to transform the second term from the left side of Equation (41), we use the summation formula by parts (20) and the boundary conditions (19):

\[
\sum_{i,j,k=1} \tau f_{i,j,k} f_{i,j,k} = \sum_{i,j,k=1} \tau f_{i,j,k}^2
\]

Similarly, the formula is applicable to the spatial variables \(x, y, z\).

We substitute formulas (43) and (44) in the formula (41):

\[
\frac{1}{2} \sum_{i,j,k=1} (h_{i,j,k}^2 f_{i,j,k}^2 - h_{i,j,k}^2 f_{i,j,k}^2) + \sum_{i,j,k=1} \tau(f_{i,j,k}^2 + f_{j,i,k}^2 + f_{j,i,k}^2) f_{i,j,k} \leq
\]
\[
\sum_{i,j,k=1} \tau u f_{i,j,k} f_{i,j,k} , p = 1..P
\]

Inequality (45) is summed over \(p\) from 1 to some \(p\), where \(p\) on the interval \(1 \leq p \leq P\). We use the boundary condition \(f_{i,j,k} = 0, i = 0..X_h, j = 0..Y_h, k = 0..Z_h.\) Then, if we expand the right-hand side of inequality (45) according to the Cauchy-Bunyakovsky formula (21) and make the maximum transition in time for a discrete solution, we obtain a difference analogue of the inequality (30):
\[
\sum_{i,j,k=1}^{\frac{1}{2}} \frac{\sum_{i,j,k=1}^{\frac{1}{2}}}{\sum_{i,j,k=1}} h f_{ijkp}^2 + \frac{\sum_{i,j,k=1}^{\frac{1}{2}}}{\sum_{i,j,k=1}} h \tau u_{ijkp} f_{ijkp} \leq \max_{1 \leq p \leq P} \left( \sum_{i,j,k=1}^{\frac{1}{2}} \frac{\sum_{i,j,k=1}^{\frac{1}{2}}}{\sum_{i,j,k=1}} h f_{ijkp}^2 \right)^{\frac{1}{2}}.
\]

Then, if we carry out mathematical transformations similar to those carried out when estimating inequality (30), we obtain the following estimates for the left and right terms:

\[
\max_{1 \leq p \leq P} \sum_{i,j,k=1}^{\frac{1}{2}} h f_{ijkp}^2 \leq 4T \sum_{i,j,k=1}^{\frac{1}{2}} h \tau u_{ijkp} f_{ijkp}
\]

\[
\sum_{i,j,k=1}^{\frac{1}{2}} \frac{\sum_{i,j,k=1}^{\frac{1}{2}}}{\sum_{i,j,k=1}} h \tau \left( f_{xijkp}^2 + f_{yijkp}^2 + f_{zijkp}^2 \right) \leq 2T \sum_{i,j,k=1}^{\frac{1}{2}} h \tau u_{ijkp}^2 f_{ijkp}
\]

If we add inequalities (47) and (48), we obtain a difference estimate similar to the integral estimate (34) up to a constant:

\[
\max_{1 \leq p \leq P} \sum_{i,j,k=1}^{\frac{1}{2}} h f_{ijkp}^2 + \sum_{i,j,k=1}^{\frac{1}{2}} h \tau \left( f_{xijkp}^2 + f_{yijkp}^2 + f_{zijkp}^2 \right) \leq
\]

\[
2T \sum_{i,j,k=1}^{\frac{1}{2}} h \tau u_{ijkp} f_{ijkp} \leq 6T \sum_{i,j,k=1}^{\frac{1}{2}} h \tau u_{ijkp}^2 f_{ijkp}
\]

Find the difference analogue for the estimate (39). To do this, we multiply the equation from (19) by \( h \tau f_{xijkp} \) and summarize the resulting expression by \( i,j,k \) by 1 \( \leq \) \( X_h - 1; 1 \leq j \leq Y_h - 1; 1 \leq k \leq Z_h - 1 \):

\[
\sum_{i,j,k=1}^{\frac{1}{2}} h f_{xijkp}^2 = \sum_{i,j,k=1}^{\frac{1}{2}} h \tau \left( f_{xijkp} + f_{yijkp} + f_{zijkp} \right) f_{xijkp} =
\]

\[
= \sum_{i,j,k=1}^{\frac{1}{2}} h \tau u_{xijkp} f_{xijkp}, p = 1, ..., P
\]

We use the summation formula in parts (20) in accordance with formula (44) and the boundary conditions (19) to estimate the second term from the left-hand side. We get:

\[
- \sum_{i,j,k=1}^{\frac{1}{2}} h \tau \left( f_{xijkp} + f_{yijkp} + f_{zijkp} \right) f_{xijkp} =
\]

\[
= \sum_{i,j,k=1}^{\frac{1}{2}} h \tau \left( f_{xijkp} f_{xijkp} + f_{yijkp} f_{yijkp} + f_{zijkp} f_{zijkp} \right),
\]

\[
p = 1, ..., P
\]

We use formula (42) to estimate the right-hand side of the equality (51):

\[
\sum_{i,j,k=1}^{\frac{1}{2}} h \tau \left( f_{xijkp} f_{xijkp} + f_{yijkp} f_{yijkp} + f_{zijkp} f_{zijkp} \right) \geq
\]

\[
\frac{1}{2} \sum_{i,j,k=1}^{\frac{1}{2}} h \left( f_{xijkp}^2 + f_{yijkp}^2 + f_{zijkp}^2 - f_{xijkp}^2 - f_{yijkp}^2 - f_{zijkp}^2 \right)
\]

Substitute this estimate in (50). We have:
\[
\sum_{i,j,k=1}^{X_h,Y_h,Z_h} \frac{1}{2} \sum_{i,j,k=1}^{X_h,Y_h,Z_h} h(f_{\xi ij k p}^2 + f_{\eta ij k p}^2 + f_{\zeta ij k p}^2) +
\]
\[
\sum_{i,j,k=1}^{X_h,Y_h,Z_h} h(f_{\xi ij k p-1}^2 + f_{\eta ij k p-1}^2 + f_{\zeta ij k p-1}^2) \leq \sum_{i,j,k=1}^{X_h,Y_h,Z_h} h\mu_{ij k p} f_{\xi ij k p},
\]

\( p = 1, ..., P \)

The left side of inequality (53) is summed over \( p \) from 1 to some \( P \), where \( P \) is in the interval \( 1 \leq p \leq P \). Given \( f_{ij k0} = 0, t = 0 \), \( X_h = 0 \), \( Y_h = 0 \), \( Z_h = 0 \), we obtain:

\[
\sum_{i,j,k=1}^{X_h,Y_h,Z_h} \frac{1}{2} \sum_{i,j,k=1}^{X_h,Y_h,Z_h} h(f_{\xi ij k p}^2 + f_{\eta ij k p}^2 + f_{\zeta ij k p}^2) \leq \sum_{i,j,k=1}^{X_h,Y_h,Z_h} h\mu_{ij k p} f_{\xi ij k p}.
\]

Or, if we transfer the first amount from the right to the left:

\[
\sum_{i,j,k=1}^{X_h,Y_h,Z_h} h\mu_{ij k p} f_{\xi ij k p} \leq \sum_{i,j,k=1}^{X_h,Y_h,Z_h} \frac{1}{2} \sum_{i,j,k=1}^{X_h,Y_h,Z_h} h(f_{\xi ij k p}^2 + f_{\eta ij k p}^2 + f_{\zeta ij k p}^2)
\]

Finally, by squaring Equation (19) we apply the elementary inequality for the square of the sum from (4) and estimate the result with (56):

\[
\sum_{i,j,k=1}^{X_h,Y_h,Z_h} \frac{1}{2} \sum_{i,j,k=1}^{X_h,Y_h,Z_h} h(f_{\xi ij k p}^2 + f_{\eta ij k p}^2 + f_{\zeta ij k p}^2) \leq \sum_{i,j,k=1}^{X_h,Y_h,Z_h} h\mu_{ij k p} f_{\xi ij k p}.
\]

If we add inequalities (55)-(57), then we get the difference analogue of estimate (39):

\[
\sum_{i,j,k=1}^{X_h,Y_h,Z_h} \frac{1}{2} \sum_{i,j,k=1}^{X_h,Y_h,Z_h} h(f_{\xi ij k p}^2 + f_{\eta ij k p}^2 + f_{\zeta ij k p}^2) + \sum_{i,j,k=1}^{X_h,Y_h,Z_h} h\mu_{ij k p} f_{\xi ij k p}
\]

\[+ \sum_{i,j,k=1}^{X_h,Y_h,Z_h} h\mu_{ij k p} f_{\xi ij k p} \leq 6 \sum_{i,j,k=1}^{X_h,Y_h,Z_h} h\mu_{ij k p}.
\]
8. Evaluation of the Difference of Differential Decision and Discrete Analogue

We introduce the Hilbert space $L_{2h,\gamma_0,\mu,\tau} = L_{2h}$, which is the difference analogue of the space $L_2(Q)$. The elements of this space will be the grid functions $f_{h,\gamma_0,\mu,\tau} = f_{ht} = \{f_{ijkp}, i = 1..X_h, j = 1..Y_h, k = 1..Z_h, p = 1..P\}$, and the scalar and vector spaces are defined as follows:

$$
\langle f_{ht}, g_{ht} \rangle = \sum_{p, i, j, k = 1}^{} htf_{ijkp}g_{ijkp} \quad (59)
$$

$$
\|f_{ht}\|_{L_{2ht}} = \left( \sum_{p, i, j, k = 1}^{} htf_{ijkp}^2 \right)^{\frac{1}{2}}
$$

By $b_{ht}f_{ht}$ we denote the piecewise constant continuation of the grid function $f_{ht}$ according to the rule:

$$
b_{ht}f_{ht} = (b_{ht}f_{ht})(x, y, z, t) = f_{ijkp}
$$

$$
(x, y, z, t) \in Q_{ijkp} = [(x, y, z): x_i \leq x \leq x_{i+1}, y_j \leq y \leq y_{j+1}, z_k \leq z \leq z_{k+1}]
$$

$$
\leq z_{k+1}, t_{p-1} \leq t \leq t_p, (x, y, z) \in Q_{ijk} = [(x, y, z): x_i \leq x \leq x_{i+1}, y_j \leq y \leq y_{j+1}, z_k \leq z \leq z_{k+1}]
$$

$$
, i = 1..X_h, j = 1..Y_h, k = 1..Z_h, p = 1..P;
$$

The domain of the function $b_{ht}f_{ht}$ is denoted by $Q_h = [(x, y, z, t): h_x \leq x \leq l_x, h_y \leq y \leq l_y, h_z \leq z \leq l_z, 0 \leq t \leq T]$. We note that:

$$
\int_{Q_h} b_{ht}f_{ht}dQ_h = \sum_{p, i, j, k = 1}^{} htf_{ijkp}\|b_{ht}f_{ht}\|_{L_{2ht}} = \|f_{ht}\|_{L_{2ht}} \quad (61)
$$

$$
\langle b_{ht}f_{ht}, b_{ht}g_{ht} \rangle_{L_{2ht}} = \sum_{p, i, j, k = 1}^{} htf_{ijkp}g_{ijkp} = \langle f_{ht}, g_{ht} \rangle_{L_{2ht}}
$$

Based on (60), (61), we rewrite the differential equation (16):

$$
b_{ht}f_{ht} - b_{ht}(f_{xht} + f_{yht} + f_{zht}) = b_{ht}u_{ht}, (x, y, z, t) \in Q_h
$$

(62)

Subtract (62) from equation (6), multiply the resulting equality by $f - b_{ht}f_{ht}$ and integrate over the domain $Q_h$:

$$
\int_{Q_h} \left( \frac{\partial f}{\partial t} - b_{ht}f_{ht} \right)(f - b_{ht}f_{ht})dQ_h -
$$

$$
\int_{Q_h} \left( \Delta f - b_{ht}(f_{xht} + f_{yht} + f_{zht}) \right)(f - b_{ht}f_{ht})dQ_h =
$$

$$
\int_{Q_h} (u - b_{ht}u_{ht})(f - b_{ht}f_{ht})dQ_h =
$$

$$
(63)
$$

We estimate the first term from the left side of the equality (63). We replace the integration over the entire domain with summation in accordance with the formula (61):

$$
\sum_{p, i, j, k = 1}^{} \int_{Q_{ijkp}} \left( \frac{\partial f}{\partial t} - b_{ht}f_{ht} \right)(f - b_{ht}f_{ht})dQ_{ijkp} =
$$

$$
\sum_{p, i, j, k = 1}^{} \left( \frac{1}{2} \frac{\partial}{\partial t}(f - (t - t_p)f_{ijkp} - f_{ijkp})^2 +
$$

$$
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$$
\[
+ \left( \frac{\partial f}{\partial t} - f_{ijkp} \right) (t - t_p) f_{ijkp} \int Q_{ijkp} =
\]

For the first term, we substitute the limiting value for integration over the time variable, and we open the first bracket for the second:

\[
\sum_{p,i,j,k=1} \sum_{q_{ijk}} \left[ \frac{1}{2} \sum_{p=1}^p \left( (f(x, y, z, t_p) - f_{ijkp})^2 - (f(x, y, z, t_p) - f_{ijkp})^2 \right) \right] dQ_{ijk} +
\]

\[
\sum_{p,i,j,k=1} \sum_{q_{ijk}} \left( f(t - t_p) f_{ijkp} t_p - \int f_{ijkp} dt - f_{ijkp} (t - t_p) dt \right) dQ_{ijkp}
\]

For the first sum, we go through the cycle in the time variable, opening the squares of the difference and using the boundary condition \( f_{ijk0} = 0 \), and for the second, we calculate the time integral for the third term, substitute the limit values in the first and third elements of the term bracket. Then the final inequality takes the following form:

\[
\int \left( \frac{\partial f}{\partial t} - b_h f_{ih} \right) (f - b_h f_{ih}) dQ_h \geq
\]

\[
\sum_{p,i,j,k=1} \sum_{q_{ijk}} \left( f(x, y, z, t_p) - f_{ijkp} \right)^2 dQ_{ijk} +
\]

\[
\sum_{p,i,j,k=1} \sum_{q_{ijk}} (f(x, y, z, t_p - 1) - f) f_{ijkp} dQ_{ijkp}
\]

We transform the second term from the left-hand side of (64). We note that:

\[
\sum_{p,i,j,k=1} \sum_{q_{ijk}} \left[ \frac{\partial^2 f}{\partial x^2} - f_{xx}(x, y, z, t) \right] (f - f_{ijkp}) dQ_{ijk} =
\]

\[
\sum_{p,i,j,k=1} \sum_{q_{ijk}} \left[ \frac{\partial^2 f}{\partial x^2} - f_{xx}(x, y, z, t) \right] (f - f_{ijkp}) dQ_{ijk} +
\]

\[
\sum_{p,i,j,k=1} \sum_{q_{ijk}} \left( f_{xx}(x, y, z, t) - f_{xx}(x, y, z, t) \right) (f - f_{ijkp}) dQ_{ijk} +
\]

\[
\sum_{p,i,j,k=1} \sum_{q_{ijk}} (f(x, y, z, t) - f_{ijkp})(f(x, y, z, t) - f_{ijkp}) dQ_{ijkp}
\]

\[
\forall t, t_{p-1} < t \leq t_p, p = 1, ..., P
\]

We transform the first term from the right-hand side of (65). To do this, we take out the differential from the first bracket, we apply integration by parts. For the part of the expression in which the limit values are substituted, we will go through the cycle in the variable \( x \). Then, having completed the mathematical operations, we arrive at the following inequality:

\[
\sum_{p,i,j,k=1} \sum_{q_{ijk}} \int \frac{\partial f}{\partial x} \left( \frac{\partial f}{\partial x} - (x - x_i) f_{xx}(x, y, z, t) - f_{xx}(x, y, z, t) \right) (f - f_{ijkp}) dQ_{ijkp} =
\]

\[
\sum_{p,i,j,k=1} \sum_{q_{ijk}} \left( \frac{\partial f}{\partial x} (x, y, z, t) - f_{xx}(x, y, z, t) \right) (f - f_{ijkp}) dQ_{ijkp} =
\]

\[
\frac{\partial f}{\partial x} (x, y, z, t) - f_{xx}(x, y, z, t)
\]

\[
(f - f_{ijkp}) dQ_{ijkp} \int Q_{ijkp} =
\]
\[
\begin{align*}
&\frac{1}{2} \sum_{i,j,k=1}^{\overline{x}_n,\overline{y}_n,\overline{z}_n} \int_{Q_{jk}} \left[ f(x, y, z, t) - f_{i j k p} \right]^2 dQ_{ijk} + \\
&+ \sum_{p,i,j,k=1}^{p_\overline{x}_n,\overline{y}_n,\overline{z}_n} \int_{Q_{ijkp}} \left[ (f(x_i, y, z, t) - f_{x i j k p})^2 + (f(x, y_j, z, t) - f_{y i j k p})^2 \right] dQ_{ijkp} \\
&+ \sum_{i,j,k=1}^{x_n,\overline{y}_n,\overline{z}_n} \int_{Q_{ijk}} \left[ (f(x_i, y, z, t) - f_{x i j k p})^2 + (f(x, y_j, z, t) - f_{y i j k p})^2 \right] dQ_{ijkp} \leq \sum_{i=1}^{10} F_i
\end{align*}
\]

Where:

\[
F_1 = \sum_{p,i,j,k=1}^{p_\overline{x}_n,\overline{y}_n,\overline{z}_n} \int_{Q_{ijkp}} \left( f - f(x, y, z, t_{p-1}) \right) f_{i j k p} dQ_{ijkp}
\]

The third term from the right-hand side of (65), and using the formula for summing by parts (17), can be represented as follows:

\[
\begin{align*}
&\sum_{i,j,k=1}^{x_n,\overline{y}_n,\overline{z}_n} \int_{Q_{jk}} \left[ (f_{x x i j k p}(x_i, y, z, t) - f_{x x i j k p}) (f(x_i, y, z, t) - f_{i j k p}) \right] dQ_{ijk} = \\
&= \sum_{i,j,k=1}^{x_n,\overline{y}_n,\overline{z}_n} \int_{Q_{jk}} h_x (f(x_i, y, z, t) - f_{i j k p}) \left( f(x_i, y, z, t) - f_{i j k p} \right) dQ_{ijk} = \\
&= \sum_{j,k=1}^{y_n,\overline{z}_n} \int_{Q_{jk}} \left( - \sum_{i=1}^{x_n} h_x (f(x_i, y, z, t) - f_{x i j k p})^2 + \\
&+ (f_x(x_{x_i}, y, z, t) - f_{x x i j k p}) \cdot \\
&\cdot \left( f(x_{x_i}, y, z, t) - f_{x x i j k p} \right) \cdot \\
&\cdot \left( f(0, y, z, t) - f_{0 j k p} \right) \right) dQ_{jk}, \forall t, t_{p-1} < t \leq t_p, p = \overline{1..P}
\end{align*}
\]
\[ F_2 = \sum_{p=1}^{\ell_p} \int \sum_{i,k=1}^{\bar{r}_h} \int_{Q_{ikp}} \left( \frac{\partial f(x_{i,k}, y, z, t)}{\partial x} - f(x_i, y, z, t) \right) \cdot (f(x_{i,k}, y, z, t) - f(x_i, y, z, t)) \cdot \sum_{i,k=1}^{\bar{r}_h} \int_{Q_{ikp}} \left( \frac{\partial f(x_{i,k}, y, z, t)}{\partial y} - f_y(x_{i,k}, y, z, t) \right) \cdot (f(x_{i,k}, y, z, t) - f_y(x_{i,k}, y, z, t)) + \sum_{i,k=1}^{\bar{r}_h} \int_{Q_{ikp}} \left( \frac{\partial f(x_{i,k}, y, z, t)}{\partial z} - f_z(x_{i,k}, y, z, t) \right) \cdot (f(x_{i,k}, y, z, t) - f_z(x_{i,k}, y, z, t)) + (f_{x_{i,k}}(x_{i,k}, y, z, t) - f_{x_{i,k}}(x_{i,k}, y, z, t)) + \sum_{i,k=1}^{\bar{r}_h} \int_{Q_{ikp}} \left( \frac{\partial f(x_{i,k}, y, z, t)}{\partial x} - f(x_{i,k}, y, z, t) \right) \cdot (f_{x_{i,k}}(x_{i,k}, y, z, t) - f(x_{i,k}, y, z, t)) + \sum_{i,k=1}^{\bar{r}_h} \int_{Q_{ikp}} \left( \frac{\partial f(x_{i,k}, y, z, t)}{\partial y} - f_y(x_{i,k}, y, z, t) \right) \cdot (f_{y_{i,k}}(x_{i,k}, y, z, t) - f_y(x_{i,k}, y, z, t)) + \sum_{i,k=1}^{\bar{r}_h} \int_{Q_{ikp}} \left( \frac{\partial f(x_{i,k}, y, z, t)}{\partial z} - f_z(x_{i,k}, y, z, t) \right) \cdot (f_{z_{i,k}}(x_{i,k}, y, z, t) - f_z(x_{i,k}, y, z, t)) \]
\[ + \left( f(y, y_j, z, t) - f(y_{j, k, p}) \right) \left( f - f(x, y_j, z, t) \right) + \\
+ \left( f(x, y, z_k, t) - f_{x, z_k, t} \right) \left( f - f(x, y, z_k, t) \right) dQ_{i, j, k, p} \]

\[ F_0 = - \sum_{p=1}^{P} \sum_{i,k,j=1}^{I} \int_{Q_{i, j, k, p}} \left( f_x(x_{X_n, Y_n, Z_n}, y, z, t) - f_{x_{X_n, Y_n, Z_n}} \right) \left( f(x, y, z, t) - f(0, y, z, t) \right) \]

\[ - f_{y_{j, k, p}} dQ_{i, j, k, p} \]

\[ F_9 = - \sum_{p=1}^{P} \sum_{i,j,k=1}^{I} \int_{Q_{i, j, k, p}} \left( f_y(x_{Y_n, Y_n, Z_n}, y, z, t) - f_{y_{Y_n, Y_n, Z_n}} \right) \left( f(x, y, z, t) - f(0, y, z, t) \right) \]

\[ - f_{y_{j, k, p}} dQ_{i, j, k, p} \]

\[ F_{10} = \sum_{p, i, j, k=1}^{P, I, J, K} \int_{Q_{i, j, k, p}} (u - u_{i, j, k, p}) (f - f_{i, j, k, p}) dQ_{i, j, k, p} \]
\[ \forall (y, z, t) \in [0, l_y] \times [0, l_z] \times [0, T], \]

\[ \forall j = 1, \ldots, Y_h, \forall k = 1, \ldots, Z_h, \forall p = 1, \ldots, P \]

We also note that:

\[
\sum_{p, a, b, c = 1}^{p, X_h, Y_h, Z_h} \int (f(x_a, y, z, t) - f_{abc})^2 dQ_{abc} = \sum_{p, a, b, c = 1}^{p, X_h, Y_h, Z_h} \int \left( (f(x_i, y, z, t) - f) + (f - f(x, y, z, t_p)) \right) + \\
+ (f(x, y, z, t_p) - f_{abc})^2 dQ_{abc} \leq 
\]

Using the elementary inequality from (22) for the square of the trinomial, as well as the property that the square of the integral does not exceed the integral of the square, we pass to the inequality:

\[
\leq 3 \sum_{p, a, b, c = 1}^{p, X_h, Y_h, Z_h} \int \int h_k \left( \frac{\partial f}{\partial x} \right)^2 d\xi + \int t_p \left( \frac{\partial f}{\partial t} \right)^2 d\eta + \\
+ f(x, y, z, t_p) - f_{abc}) dQ_{abc} \leq 3 \left( h_k \left( \frac{\partial f}{\partial x} \right)^2 + \tau \left( \frac{\partial f}{\partial t} \right)^2 + \sum_{p, a, b, c = 1}^{p, X_h, Y_h, Z_h} \int \left( f(x, y, z, t) - f_{abc} \right) dQ_{abc} \right) 
\]

If we write down similar estimates for the spatial variables \( y \) and \( z \), then add them up and apply estimate (39), we obtain:

\[
\sum_{p, a, b, c = 1}^{p, X_h, Y_h, Z_h} \int \left( f(x_a, y, z, t) - f_{abc} \right)^2 + \left( f(x, y, z, t_p) - f_{abc} \right)^2 dQ_{abc} \leq C(h_k^2 + h_y^2 + h_z^2 + 3\tau^2) \cdot 
\]

\[
\|u\|_{L_2(Q)} + \sum_{p, a, b, c = 1}^{p, X_h, Y_h, Z_h} \int 3\tau(f(x, y, z, t_p) - f_{abc}) dQ_{abc} 
\]

Based on formulas (80)-(81) it follows that

\[
\sum_{p, i, j, k = 1}^{p, X_h, Y_h, Z_h} \int (f(x_i, y, z, t) - f_{ijk})^2 dQ_{jk} + \\
+ \sum_{p, i, k, j = 1}^{p, X_h, Y_h, Z_h} \int (f(x, y_j, z, t) - f_{ijk})^2 dQ_{ik} + \\
+ \sum_{p, i, j, k = 1}^{p, X_h, Y_h, Z_h} \int (f(x, y, z_k, t) - f_{ijk})^2 dQ_{ijp} \leq 
\]

\[
\leq C \left( \sum_{p, a, b, c = 1}^{p, X_h, Y_h, Z_h} \int \int t_p \left( f_k(x_a, y, z, t) - f_{abc} \right)^2 + \\
+ f(x, y, z, t_p) - f_{abc})^2 dQ_{abc} \leq C(h_k^2 + h_y^2 + h_z^2 + 3\tau_\tau) \left( \|u\|_{L_2(Q)} \right) 
\]

\[ i = 1, \ldots, X_h, j = 1, \ldots, Y_h, k = 1, \ldots, Z_h \]

Further note that
\[
\frac{\partial f}{\partial x} - f_x(x_i, y, z, t) = \frac{1}{h_x} \int_{x_{i-1}}^{x_i} \left( \frac{\partial f}{\partial x} - \frac{\partial f(\xi, y, z, t)}{\partial x} \right) d\xi =
\]
\[
= \frac{1}{h_x} \int_{x_{i-1}}^{x_i} \left( \int \frac{\partial^2 f(\eta, y, z, t)}{\partial x^2} d\eta \right) d\xi
\]
\[
\forall x \in [0, l_x], (y, z, t) \in [0, l_y] \times [0, l_z] \times [0, T], i = 1, \ldots, X_h
\]
Hence, for all \( s, s_i \leq s \leq s_i+1, i = 1, \ldots, X_h \), we have:
\[
\sum_{p, j, k=1}^{p, Y_h, Z_h} \int_{Q_{j+k}} \left( \frac{\partial f}{\partial x} - f_x(x_i, y, z, t) \right)^2 dQ_{j+k} \leq
\]
\[
\leq \sum_{p, j, k=1}^{p, Y_h, Z_h} \int_{Q_{j+k}} \left( \frac{1}{h_x} \int_{x_{i-1}}^{x_i} \int_{x_{i-1}}^{x_{i+1}} \left| \frac{\partial^2 f(\eta, y, z, t)}{\partial x^2} \right| d\eta \right) d\xi \right)^2 dQ_{j+k} \leq
\]
\[
\leq 2h_x \sum_{p, j, k=1}^{p, Y_h, Z_h} \int_{Q_{j+k}} \int_{Q_{j+k}} \left| \frac{\partial^2 f(\eta, y, z, t)}{\partial x^2} \right|^2 d\eta dQ_{j+k}
\]
If you perform similar operations for other spatial variables, then add up the estimates and change the integration region from the interval to the entire region \([0, l_x] \times [0, l_y] \times [0, l_z] \times [0, T] \), and use estimate (39), and for \( h_{\text{max}} \) take \( \max\{h_x, h_y, h_z\} \), then we pass to the following inequality:
\[
\sum_{p, j, k=1}^{p, Y_h, Z_h} \int_{Q_{j+k}} \left( \frac{\partial f}{\partial x} - f_x(x_i, y, z, t) \right)^2 dQ_{j+k} +
\]
\[
+ \sum_{p, j, k=1}^{p, Y_h, Z_h} \int_{Q_{j+k}} \left( \frac{\partial f}{\partial y} - f_y(x, y_j, z, t) \right)^2 dQ_{j+k} +
\]
\[
+ \sum_{p, j, k=1}^{p, Y_h, Z_h} \int_{Q_{j+k}} \left( \frac{\partial f}{\partial z} - f_z(x, y, z_k, t) \right)^2 dQ_{j+k} \leq
\]
\[
\leq 2h_{\text{max}} \left( \left\| \frac{\partial^2 f}{\partial x^2} \right\|_{L_2(Q)}^2 + \left\| \frac{\partial^2 f}{\partial y^2} \right\|_{L_2(Q)}^2 + \left\| \frac{\partial^2 f}{\partial z^2} \right\|_{L_2(Q)}^2 \right) \leq h_{\text{max}} C \| u \|_{L_2(Q)}^2
\]
In addition, taking into account (84), (39) by performing similar operations, we can obtain:
\[
\sum_{p, j, k=1}^{p, Y_h, Z_h} \int_{Q_{j+k}} \left( \left( \frac{\partial f}{\partial x} - f_x(x_i, y, z, t) \right)^2 + \left( \frac{\partial f}{\partial y} - f_y(x, y_j, z, t) \right)^2 +
\]
\[
+ \left( \frac{\partial f}{\partial z} - f_z(x, y, z_k, t) \right)^2 \right) dQ_{j+k} \leq
\]
\[
\leq 2h_{\text{max}}^2 \left( \left\| \frac{\partial^2 f}{\partial x^2} \right\|_{L_2(Q)}^2 + \left\| \frac{\partial^2 f}{\partial y^2} \right\|_{L_2(Q)}^2 + \left\| \frac{\partial^2 f}{\partial z^2} \right\|_{L_2(Q)}^2 \right) \leq h_{\text{max}}^2 C \| u \|_{L_2(Q)}^2
\]
If we write the function \( f_x(x_i, y, z, t) \) in \( x_i \) and go from the difference via Newton-Leibniz back to the integral, and also use the estimate (39), then we can obtain the following estimate:
\[
\sum_{p, j, k=1}^{p, Y_h, Z_h} \int_{Q_{j+k}} \left( f_x(x_i, y, z, t) \right)^2 dQ_{j+k} =
\]
\[
\sum_{p, l, i, k=1} P_{ijkl} Q_{ijkl} + \int \left( \int \left( \int \frac{\partial^2 f(\eta, y, z, t)}{\partial x^2} d\eta \right) \right) dQ_{ijkl} \leq 2 \int \left( \int \left( \int \frac{\partial^2 f(\eta, y, z, t)}{\partial x^2} d\eta \right) \right) dQ_{ijkl} \leq 2 \left( \left\| \frac{\partial^2 f}{\partial x^2} \right\|_{L^2(Q)} \right)^2
\]

If we perform the mathematical transformations for the functions \( f_{xy}(x, y, z, t) \) and \( f_{yy}(x, y, z, t) \), in a similar way, and then sum them all up, we can obtain the inequality:

\[
\sum_{p, l, i, k=1} P_{ijkl} Q_{ijkl} + \left( f_{xy}(x, y, z, t) \right)^2 + \left( f_{yy}(x, y, z, t) \right)^2 dQ_{ijkl} \leq C \left\| u \right\|_{L^2(Q)}^2
\]

(87)

Now we can proceed to estimates of the quantities \( F_i, i = 1, ..., 10 \) from (68). Let's start by evaluating \( F_1 \). To do this, we pass from the difference, through Newton - Leibniz, to integration, use the elementary inequality from (22) for the product, and also take into account estimates (39) and (58):

\[
|F_1| \leq \sum_{p, l, i, k=1} P_{ijkl} Q_{ijkl} + \int_{t_{p-1}}^{t_p} \left( \int \frac{\partial f(x, y, z, t)}{\partial t} dt \right) f_{ijkl} dQ_{ijkl} \leq 2 \left( \left\| \frac{\partial f}{\partial t} \right\|_{L^2(Q)} + \left\| f_{ijkl} \right\|_{L^2(Q)} \right)^2 \leq \tau C \left( \left\| u \right\|_{L^2(Q)}^2 + \left\| u \right\|_{L^2(Q)} \right)
\]

(88)

To estimate \( F_2 \), using the Cauchy-Bunyakovsky formula (21), we represent the sums of the products in the form of the product of the sums, after which we apply the elementary inequality from (22) for the product, and estimate the resulting terms using formulas (82) and (85). We get the following estimate:

\[
|F_2| \leq \frac{\varepsilon}{2} C \left( \sum_{p, l, i, k=1} P_{ijkl} Q_{ijkl} + \int_{t_{p-1}}^{t_p} \left( \int \left( f_{xy}(x, y, z, t) - f_{ijkl} \right)^2 + \left( f_{yy}(x, y, z, t) - f_{ijkl} \right)^2 \right) dt + 3 \tau f(x, y, z, t_p) - f_{ijkl} dQ_{ijkl} + C(h_x + h_y + h_z + 3\tau) \left\| u \right\|_{L^2(Q)}^2 + \frac{h_{\max}}{2E} C \left\| u \right\|_{L^2(Q)}^2 \right)
\]

(89)

Similarly to the estimate \( F_2 \), we obtain the estimate \( F_3 \):

\[
|F_3| \leq \frac{\varepsilon}{2} C \left( \sum_{p, l, i, k=1} P_{ijkl} Q_{ijkl} + \int_{t_{p-1}}^{t_p} \left( \int \left( f_{xy}(x, y, z, t) - f_{ijkl} \right)^2 + \left( f_{yy}(x, y, z, t) - f_{ijkl} \right)^2 \right) dt + 3 \tau f(x, y, z, t_p) - f_{ijkl} dQ_{ijkl} + C(h_x + h_y + h_z + 3\tau) \left\| u \right\|_{L^2(Q)}^2 + \frac{h_{\max}}{2E} C \left\| u \right\|_{L^2(Q)}^2 \right)
\]

(90)

To estimate \( F_4 \), we break each term by the Cauchy-Bunyakovsky formula (21). In each case, we reduce the second factor to the control norm in the space \( L_{2\gamma t} \), taking into account formula (58). In the first factor, add and subtract \( f_{x}(x_{i+1}, y, z, t), f_{x}(x_{i+1}, y, z, t), f_{x}(x, y, z_{i+1}, t) \) in accordance with the spatial variable, we apply the elementary inequality from (22) for the square of the trinomial, we use estimates (39), (86) and (87). We obtain the following inequality:
\[ |F_4| \leq C \max \|u\|_{L^2(\Omega)} \|u_{hr}\|_{L^2(\Omega)} \leq h_{\text{max}} C (\|u\|_{L^2(\Omega)}^2 + \|u_{hr}\|_{L^2(\Omega)}^2) \]  

(91)

To estimate \( F_4 \), we break each term by the Cauchy-Bunyakovsky formula (21), and then evaluate them individually using formulas (34) and (86). We have:

\[ |F_4| \leq h_{\text{max}} C \|u\|_{L^2(\Omega)}^2 \]  

(92)

To estimate \( F_6 \), we divide each term by the Cauchy-Bunyakovsky formula (21), integrate the first factor of each term with respect to the corresponding spatial variable, and use estimates (34), (39) and (87). We have:

\[ |F_6| \leq h_{\text{max}} C \|u\|_{L^2(\Omega)}^2 \]  

(93)

To estimate \( F_7 \), we use the Cauchy-Bunyakovsky formula (21). The left factor is estimated using (39),(58) and (87), in the right we pass from the difference to integration, apply the Cauchy-Bunyakovsky formula (21) and evaluate it using the formula (34). We have:

\[ |F_7| \leq h_{\text{max}} C (\|u\|_{L^2(\Omega)}^2 + \|u_{hr}\|_{L^2(\Omega)}^2) \]  

(99)

To estimate \( F_8 \) and \( F_q \), we note that \( f_x(x_i,y,z,t) - f_{xX_k} = f_x(x_i,y,z,t) - \partial f_x(x_i,y,z,t)/\partial x \) due to the boundary conditions (5) and (19) both for the variable \( x \), and for other spatial variables \( y \) and \( z \). Given these conditions, we estimate \( F_8 \) and \( F_q \) similarly to the estimates \( F_2 \) and \( F_3 \):

\[ |F_8| \leq \frac{\varepsilon}{2} C \sum_{p,i,j,k=1}^{n_p} \sum_{q_{ijk}} \left( \int_{t_{p-1}}^{t_p} \left( \left| f_x(x_i,y,z,t) - f_{xX_k} \right|^2 \right) dt + \right. \]
\[ + \left. \left( \left| f_y(x_i,y,z,t) - f_{yX_k} \right|^2 \right) dt + \right. \]
\[ + \left. \left( \left| f_z(x_i,y,z,t) - f_{zX_k} \right|^2 \right) dt + \right. \]
\[ \left. + C(h_x + h_y + h_z + 3\varepsilon) \|u\|^2_{L^2(\Omega)} + \frac{h_{\text{max}} C}{2\varepsilon} \|u\|^2_{L^2(\Omega)} \right) \]  

(100)

To evaluate \( F_{10} \), we use Cauchy-Bunyakovsky (21) and (39):

\[ \|F_{10}\| = \sum_{p,i,j,k=1}^{n_p} \sum_{q_{ijk}} \int (u - u_{ijk}) (f - f_{ijk}) dQ_{ijk} \leq \]

\[ \leq \|u - b_{hr} u_{hr}\|_{L^2(\Omega)}^2 + \sum_{p,i,j,k=1}^{n_p} \sum_{q_{ijk}} \left( \int_{t_{p-1}}^{t_p} \frac{\partial f(x,y,z,t)}{\partial t} dt \right)^2 + \]
\[ + \left( f(x,y,z,t_p) - f_{ijk} \right)^2 dQ_{ijk} \leq \frac{1}{2} \|u - b_{hr} u_{hr}\|_{L^2(\Omega)}^2 + \]
\[ + \tau^2 C \|u\|^2_{L^2(\Omega)} + \tau \sum_{p,i,j,k=1}^{n_p} \sum_{q_{ijk}} \left( f(x,y,z,t_p) - f_{ijk} \right)^2 dQ_{ijk} \]  

(102)

We substitute all the obtained estimates (88)-(102) into the inequality (68):
\[
\frac{1}{2} \sum_{i,j,k=1}^{x_n,y_n,z_n} \int_{Q_{ijk}} \left| f(x, y, z, t_p) - f_{ijkp} \right|^2 \, dQ_{ijk} \\
+ \sum_{p,i,j,k=1}^{p,x_n,y_n,z_n} \int_{Q_{ijk}} \left( \left( f(x, y, z, t) - f_{xijkp} \right)^2 + \left( f(x, y, z, t) - f_{yijkp} \right)^2 \right) \, dQ_{ijk} + \\
+ \epsilon C (h_x + h_y + h_z + 3 \tau) \left( 1 + \epsilon + \frac{1}{\epsilon} \right) \left( \|u\|_{L^2(Q)}^2 + \|u\|_{L^2_{\partial R}}^2 \right) \\
\cdot \sum_{p,i,j,k=1}^{p,x_n,y_n,z_n} \int_{Q_{ijk}} \left( f(x, y, z, t) - f_{xijkp} \right)^2 + \left( f(x, y, z, t) - f_{yijkp} \right)^2 \right) \, dQ_{ijk} \leq \|u - b_{htu_{ht}}\|_{L^2(Q_h)}^2 \\
+ \tau (1 + 3 \epsilon C) \sum_{p,i,j,k=1}^{p,x_n,y_n,z_n} \int_{Q_{ijk}} \left( f(x, y, z, t_p) - f_{ijkp} \right)^2 \, dQ_{ijk} + \\
+ \epsilon C (h_x + h_y + h_z + 3 \tau) \left( 1 + \epsilon + \frac{1}{\epsilon} \right) \left( \|u\|_{L^2(Q)}^2 + \|u\|_{L^2_{\partial R}}^2 \right)
\]  

Or, if we group the elements, we get:

\[
\left( \frac{1}{2} - \tau (1 + 3 \epsilon C) \right) \sum_{i,j,k=1}^{x_n,y_n,z_n} \int_{Q_{ijk}} \left| f(x, y, z, t_p) - f_{ijkp} \right|^2 \, dQ_{ijk} + (1 - \epsilon C) \cdot \sum_{p,i,j,k=1}^{p,x_n,y_n,z_n} \int_{Q_{ijk}} \left( f(x, y, z, t) - f_{xijkp} \right)^2 + \left( f(x, y, z, t) - f_{yijkp} \right)^2 \right) \, dQ_{ijk} + \\
\leq \|u - b_{htu_{ht}}\|_{L^2(Q_h)}^2 \\
+ \tau (1 + 3 \epsilon C) \sum_{p,i,j,k=1}^{p,x_n,y_n,z_n} \int_{Q_{ijk}} \left( f(x, y, z, t_p) - f_{ijkp} \right)^2 \, dQ_{ijk} + \\
+ \epsilon C (h_x + h_y + h_z + 3 \tau) \left( 1 + \epsilon + \frac{1}{\epsilon} \right) \left( \|u\|_{L^2(Q)}^2 + \|u\|_{L^2_{\partial R}}^2 \right)
\]

We introduce some conditions. We fix \( \epsilon > 0 \) so small that the inequality \( 1 - \epsilon C > 0 \) holds. In addition, we assume that \( \tau \) is so small that \( 1/2 - \tau (1 + 3 \epsilon C) \geq 1/4 \). Then from inequality (103) we come to:

\[
\sum_{i,j,k=1}^{x_n,y_n,z_n} \int_{Q_{ijk}} \left| f(x, y, z, t_p) - f_{ijkp} \right|^2 \, dQ_{ijk} \leq \|u - b_{htu_{ht}}\|_{L^2(Q_h)}^2 \\
+ 4 \tau (1 + 3 \epsilon C) \sum_{p,i,j,k=1}^{p,x_n,y_n,z_n} \int_{Q_{ijk}} \left( f(x, y, z, t_p) - f_{ijkp} \right)^2 \, dQ_{ijk} + \\
+ \epsilon C (h_x + h_y + h_z + 3 \tau) \left( 1 + \epsilon + \frac{1}{\epsilon} \right) \left( \|u\|_{L^2(Q)}^2 + \|u\|_{L^2_{\partial R}}^2 \right)
\]

For inequality (104), we use Lemma 1, introduce the constants \( C_1 = 4(1 + 3 \epsilon C) \) and \( C_2 = C(1 + \epsilon + 1/\epsilon) \). We have:
\[
\frac{X_{n,Y_{n,Z_{n}}}}{\sum_{i,j,k=1}^{Q_{ijk}}} \int |f(x,y,z,t_p) - f_{ijkp}|^2 dQ_{ijk} \leq (1 + \tau C_1). \tag{105}
\]

\[
\cdot \left(\|u - b_{hr}u_{hr}\|_{L_2(Q_{n})}^2 + C_2(h_x + h_y + h_z + 3\tau)(\|u\|_{L_2(Q)}^2 + \|u\|_{L_2(Q_{hr})}^2)\right)
\]

Note that when expanding the function \(e^{\tau C_1}\) in a Taylor series, the first 2 terms of the expansion correspond to \(1 + \tau C_1\), whence we can obtain the inequality \(1 + \tau C_1 \leq e^{\tau C_1}\), and it follows \((1 + \tau C_1)^p \leq e^{\tau C_1}\). Based on this:

\[
\frac{X_{n,Y_{n,Z_{n}}}}{\sum_{i,j,k=1}^{Q_{ijk}}} \int |f(x,y,z,t_p) - f_{ijkp}|^2 dQ_{ijk} \leq \tag{106}
\]

\[
\leq C \left(\|u - b_{hr}u_{hr}\|_{L_2(Q_{n})}^2 + (h_x + h_y + h_z + 3\tau)(\|u\|_{L_2(Q)}^2 + \|u\|_{L_2(Q_{hr})}^2)\right)
\]

Using estimate (106), we prove that problem (17)-(19) approximates problem (3)-(6) with respect to function.

Theorem 2. Let the step function correspond to problem (17)-(19):

\[
b_{ijk} = \frac{1}{h} \int_{Q_{ijk}} b(\xi,\eta,\phi)d\xi d\eta d\phi, \tag{107}
\]

\[
i = 1..X_n - 1, j = 1..Y_n - 1, k = 1..Z_n - 1
\]

Then \(\lim_{(h_x,h_y,h_z)\to 0} J_{hr} = J\).

Let us prove this theorem. Let us evaluate the difference \(J(u) - J_{hr}(u_{hr})\), assuming that \(u \in U, u_{hr} \in U_{hr}\). Taking into account estimates (34),(39),(49),(58) and (106), the definition of the sets (3) and (17), the inequality:

\[
\frac{X_{n,Y_{n,Z_{n}}}}{\sum_{i,j,k=1}^{Q_{ijk}}} h b_{ijk}^2 = \sum_{i,j,k=1}^{Q_{ijk}} h \left(\frac{1}{h} \int_{Q_{ijk}} b(\xi,\eta,\phi)d\xi d\eta d\phi \right)^2 \leq \sum_{i,j,k=1}^{Q_{ijk}} \int_{Q_{ijk}} b^2(\xi,\eta,\phi)d\xi d\eta d\phi \leq \|b\|_{L_2(Q_{n})}^2 \tag{108}
\]

Then if we subtract the discrete criterion (4) from the criterion of the differential problem (18) and estimate the difference:

\[
|J(u) - J_{hr}(u_{hr})| = \int_0^h |f(x,y,z,T;u) - b(x,y,z)|^2 dQ_3 +
\]

\[
+ \sum_{i,j,k=1}^{Q_{ijk}} \int (f(x,y,z,t_p;u) - f_{ijkp}) + (b(x,y,z) - b_{ijk}) \cdot
\]

\[
( f(x,y,z,t_p;u) + b_{ijk} - f_{ijkp} - b(x,y,z) ) dQ_3 \leq
\]

\[
\leq 2 \left( \int_0^h (f^2(x,y,z,T;u) - b^2(x,y,z)) dQ_3 \right) +
\]

\[
\left[ \sum_{i,j,k=1}^{Q_{ijk}} \int (f(x,y,z,t_p;u) - f_{ijkp})^2 dQ_3 \right]^{\frac{1}{2}} +
\]

\[
+ \left[ \sum_{i,j,k=1}^{Q_{ijk}} \int (b(x,y,z) - b_{ijk})^2 dQ_3 \right]^{\frac{1}{2}} \times \left[ \int Q_3 (f^2(x,y,z,t_p;u) dQ_3 \right]^{\frac{1}{2}} +
\]

765
\[
\left(\sum_{i,j,k=1}^{\infty} h f_{ijk}^2\right)^{\frac{1}{2}} + \|b\|_{L_2(Q)}^2 + \left(\sum_{i,j,k=1}^{\infty} h b_{ijk}^2\right)^{\frac{1}{2}} \leq 2 \int_0^h b^2(x, y, z) \, dQ_3 + C \left(\|u - b_{ht}u_{ht}\|_{L_2(Q)} + \sqrt{h_x + h_y + h_z + 3\tau}\right) + \\
hCR^2 + \left(\sum_{i,j,k=1}^{\infty} \int_{Q_{ijk}} \left(b(x, y, z) - b_{ijk}\right)^2 \, dQ_3\right)^{\frac{1}{2}}
\]

We can obtain the following inequality:
\[
|f(u) - f_{ht}(u_{ht})| \leq hCR^2 + 2 \int_0^h b^2(x, y, z) \, dQ_3 + \\
+ C \left(\|u - b_{ht}u_{ht}\|_{L_2(Q)} + \sqrt{h_x + h_y + h_z + 3\tau}\right) + \\
+ \left(\sum_{i,j,k=1}^{\infty} \int_{Q_{ijk}} \left(b(x, y, z) - b_{ijk}\right)^2 \, dQ_3\right)^{\frac{1}{2}}
\]

(109)

We estimate the differential function and its step analogue to show that as \((h_x, h_y, h_z) \to 0\) due to the average continuity of the function \(b(x, y, z) \in L_2(Q_3)\), its square is the difference with the step function \(b_{ijk}\) tends to 0. For this, we integrate the square of the difference of functions over the variables and use the definition (107), we obtain:
\[
\sum_{i,j,k=1}^{\infty} \int_{Q_{ijk}} \left(\frac{1}{h} \int_{Q_{ijk}} \left(b(x, y, z) - b(\xi, \eta, \phi)\right) \, d\xi d\eta d\phi\right)^2 \, dQ_{ijk} \leq \\
\sum_{i,j,k=1}^{\infty} \int_{Q_{ijk}} \left(\frac{1}{h} \int_{-h}^h (\Delta b)^2 \, da dc de\right) \, dQ_{ijk} = \\
\frac{1}{h} \int_{-h}^h \left(\sum_{i,j,k=1}^{\infty} \int_{Q_{ijk}} \left(\Delta b\right)^2 \, dQ_{ijk}\right) \, da dc de \leq \max_{(a,b,c) \in \mathcal{H}} \int_{Q_3} |\Delta b|^2 \, dQ_3 \to 0,
\]
\(\Delta b = b(x + a, y + c, z + e) - b(x, y, z)\)

Since problem (5), (6) and (19) have a solution, i.e., \(U_* \neq \emptyset, U_{ht} \neq \emptyset\), we fix some \(u_*\) and \(u_{ht*}\), so that \(u_* \in U_*\), \(u_{ht*} \in U_{ht}\). Since \(\|b_{ht}u_{ht*}\|_{L_2(Q)} = \|u_{ht*}\|_{L_2(Q)} \leq R\), taking \(b_{ht}u_{ht*} = 0\) outside \(Q_h\), we can assume that \(b_{ht}u_{ht*} \in U\). For the control function \(u_* \in U_*\) we construct its discrete analog \(Q_{ht}u_* = \{u_{ijkp} \mid i = 1..X_{ht}, \, k = 1..Y_{ht}, \, p = 1..P\}\) by the rule:
\[
u_{ijkp} = \frac{1}{h} \int_{Q_{ijk}} u_*(x, y, z, t) \, dQ_{ijkp}
\]

(111)

We show that \(Q_{ht}u_* \in U_{ht}\). For this we show:
\[
\|Q_{ht}u_*\|_{L_2(Q)}^2 \leq \sum_{p,i,j,k=1}^{\infty} \int_{Q_{ijk}} u_{ijkp}^2(x, y, z, t) \, dQ_{ijkp} \leq \|u_*\|_{L_2(Q)}^2 \leq R
\]

(112)

Having performed mathematical transformations similar to formula (110), we obtain:
We find the upper and lower limits of the difference in the criteria of the differential and discrete problems in order to determine an estimate of the rate of convergence. Let’s start with the upper limit:

\[
J_r - J_{ht*} \leq J(b_{ht}u_r) - J_{ht}(u_{ht*}) \leq hCR^2 + C\sqrt{(h_x + h_y + h_z + 3\tau)} + \\
\frac{h}{\sqrt{2}} \int_0^h R^2(x, y, z) dQ_3 + C \left( \sum_{i,j,k=1}^{\mathcal{X}_h, \mathcal{Y}_h, \mathcal{Z}_h} \int_{Q_{ijk}} (b(x, y, z) - b_{ijk})^2 dQ_3 \right)^{\frac{1}{2}}
\]

(114)

We begin by estimating the last term from the right-hand side. Based on the formula (112), we discard it, since it tends to 0 with decreasing step. The second term with a sufficiently small difference in the arguments of a certain integral will give an insignificant value. The first term, in comparison with the third, has a larger order of smallness; therefore, the upper limit is determined by such a quantity as \(C\sqrt{(h_x + h_y + h_z + 3\tau)}\).

We perform the same operations to determine the lower limit, but change the arguments for the criteria of the differential and discrete problems. We get:

\[
J_r - J_{ht*} \geq J(u_r) - J_{ht}(Q_{ht}u_r) \geq -C\sqrt{(h_x + h_y + h_z + 3\tau)} - \\
- \sum_{i,j,k=1}^{\mathcal{X}_h, \mathcal{Y}_h, \mathcal{Z}_h} \int_{Q_{ijk}} (b(x, y, z) - b_{ijk})^2 dQ_3 \right)^{\frac{1}{2}} - 2 \int_0^h b(x, y, z) dQ_3 - \\
-\|u_r(x, y, z, t) - b_{ht}Q_{ht}u_r\|_{L^2(Q_h)} - hCR^2
\]

(116)

Based on the formula (113), the first term is neglected due to its lesser influence on the right side in comparison with others. For the remaining elements of the right-hand side, the conclusions remain similar to the conclusions for the formula (114).

The limits of (115), (117) imply the statement of Theorem 2. Inequalities (114), (116) estimate the rate of convergence for \(J_r - J_{ht*}\). If \(b(x, y, z, u_r) = u_r(x, y, z, t)\) are sufficiently smooth, then it follows from (114), (116) that:

\[
|J_r - J_{ht*}| = O\left(\sqrt{(h_x + h_y + h_z + 3\tau)}\right)
\]

(118)

9. Conclusion

The problem of determining the approximation order of the optimal control problem for the spatial process of heat conduction is considered in the paper. Using the methods of integral inequalities and the method of difference approximation, a difference problem is obtained, an algorithm for finding its solution is described, and an estimate is obtained for the deviation of the value of the difference functional from the continuous functional. The established inequality Equation (118) gives an idea of the time complexity of the process of calculating an approximate solution when the accuracy of calculations is given in advance. The time steps and spatial variables are not independent, additional restrictions must be imposed to ensure stability. The methodology for obtaining an approximation estimate can be used for implicit approximations, hybrid schemes. The methods used in this article can be successfully applied for similar parabolic problems with bounded coefficients, as well as for problems of large dimensions.

10. Conflicts of Interest

The authors declare no conflict of interest.
11. References

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Experimental Study of Large-scale RC Beams Shear-Strengthened with Basalt FRP Sheets

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Abstract

Over the last three decades, many experimental studies have been conducted to investigate the behavior of Reinforced Concrete (RC) beams, shear strengthened with externally bonded Fiber-Reinforced Polymer (FRP) composite. However, the majority of experimental studies have focused on small- to medium-scale beam specimens. As a result, most design equations that have been developed as part of these studies may thus not be accurate at predicting the shear strength of large-scale RC beams shear-strengthened with FRP sheets. This study thus involved performing tests on six specimens to study the effect of the larger scale, along with new variables such as beam width, new varieties of FRP sheets (basalt FRP (BFRP)), and the strengthening configuration (U-jacketing), on the prediction of the ultimate load of RC beams strengthened with externally bonded FRP composite. The experimental results were analyzed and showed that all these variables affected the lateral strain along the bottom and the top of the beams. It was found that variations in the depth to width ratio of the beams caused the failure angle to vary as well. For beams strengthened with BFRP sheets, both the cracking and ultimate load increased to 1.19 and 1.94 times the cracking and ultimate load of the control beams under identical conditions.

Keywords: Large-scale RC Beams; BFRP Sheets; Shear Strengthened; Beam Width; Lateral Strain.

1. Introduction

The technique of applying various types of Fiber-Reinforced Polymer (FRP) sheets to strengthen concrete structures has become a well-recognized method, particularly for strengthening Reinforced Concrete (RC) beams. This is clearly shown by the development of design codes associated with the technique [1]. This technique is used to strengthen RC beams in the shear zone. However, studying the shear behavior of these RC beams is complicated because the mechanisms are complex making the prediction of the shear strength and behavior of these beams difficult. For this reason, in the last three decades, many experimental and numerical studies have been conducted on RC beams strengthened with externally bonded FRP sheets to provide data through which design equations and models can be developed that can predict shear force as accurately as possible [1-3].

Some previous research has taken into account the effect of debonding between the concrete surface and the FRP in suggesting models [4-6]. Several models have also been proposed based on an analytical study carried out on many experimental and numerical tests to provide a database through which to verify the accuracy of the models [7-9]. Because the RC beams in the resistance to shear are complex, therefore many researchers have focused on studying the behavior of RC beams in the shear zone [10-12]. Also from the useful and new properties of basalt BFRP, many

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researches have focused on the use of this type of FRP in the strengthening operations, whether in the shear zone [13-15] or in the flexural zone [16-18] or both together [19] with different forms of BFRP, whether sheets or bars [20, 21]. However, these experimental and numerical studies have not considered all the parameters that influence the shear behavior of RC beams strengthening with FRP sheets; such as the beam width, the effect of scale (large-scale dimensions), new types of FRP sheets (such as basalt FRP (BFRP)), and the applied strengthening configuration (U-jacketing). Therefore, using these models to predict shear behavior sometimes does not yield accurate values. The reason for the inaccuracy is that these design equations and models have been proposed based on a limited number of experimental test results on small-scale RC beams. Additionally, they have neglected some of the variables mentioned above.

In previous studies by Sayed et al. (2014) [22] and Deniaud and Cheng (2001) [23], a database of experimental results from more than 300 RC beams was collecting from 40 experimental studies using different types of strengthening configurations. However, in this database, it was observed that the tests were performed only on small-scale RC beams with a total depth and width of less than 500mm and 300mm, respectively. In addition, not many tests took the actual lengths of the RC beam span into account, as is necessary for bridge girders. Additionally, the effect of the actual dimensions of the RC beams on the prediction of shear behavior was rarely taken into account [24-27]. As a result, none of the existing analytical models and design equations directly considers the effect of scale on the calculation of the shear strengthening with externally bonded BFRP composite. Therefore, the shear behaviour of large-scale RC beams strengthened in the shear zone with BFRP sheets will be investigated in this study. Many parameters will be included in the experimental study, such as the effect of larger scales, beam width, type of FRP sheets (BFRP), and strengthening configuration (U-jacketing), in order to provide more realistic data that can be used to predict the shear behavior with higher accuracy.

2. Materials and Methods

2.1. Specimen Details

Six rectangular RC beams were tested. They were simply supported and were of a large scale, with a total height of 1000 mm and beam width varying from 300 to 500 mm with a shear span to depth ratio $a/d$ of 1.90, as shown in Figure 1. The beams, under equal two-point static loads 800 mm apart placed symmetrically about the mid-span, were tested up to the point of failure. The concrete standard cubic compressive strength $f_{cu}$ for each beam is shown in Table 1. It was found that these strengths ranged from 48.75 to 49.88 MPa. Two types of steel bars were used to reinforce the RC beams. These were namely deformed steel bars, which were used for longitudinal reinforcement, and plain steel bars, which were used for web vertical reinforcement. Four bar sizes; 10, 16, 25, and 32 mm diameter bars, were used to obtain the same main reinforcement ratio of 3.0% of the concrete cross-sectional area for all beams. The web rebars consisted of 8.0 mm diameter stirrups with yield and ultimate strengths of 430 and 590 MPa, respectively, at a spacing of 200 mm at the shear span zone, and 150 mm at the flexural span, as shown in Figure 1. The main reinforcement yield and ultimate strengths were 488 and 674MPa, respectively, while Young’s modulus was 206 GPa.

Figure 1. Geometrical details of the large-scale RC beams (all dimensions in mm)
### Table 1. Summary of details for the beam specimens analyzed in the present study

| Beam specimen | Geometric data | Concrete data | Area of steel reinforcement | External shear reinforcement |
|---------------|----------------|---------------|----------------------------|-----------------------------|
|               | $b$ (mm) | $h$ (mm) | $d$ (mm) | $a$ (mm) | $f_{cu}$ (MPa) | $n \times t_f$ (mm) | $h_f$ (mm) | $f_{fu}$ (MPa) | $E_f$ (GPa) | Type |
| C-1000/300    | 300    | 1000 | 915   | 1750  | 48.75 | 8042 | 1472 | 0 | 0 | 0 | 0 |
| C-1000/400    | 400    | 1000 | 915   | 1750  | 48.75 | 11259 | 1963 | 0 | 0 | 0 | 0 |
| C-1000/500    | 500    | 1000 | 915   | 1750  | 49.88 | 13672 | 2454 | 0 | 0 | 0 | 0 |
| U-B-1000/300  | 300    | 1000 | 915   | 1750  | 48.75 | 8042 | 1472 | 4 $\times$ 0.157 | 1000 | 2100 | 100 | BFRP |
| U-B-1000/400  | 400    | 1000 | 915   | 1750  | 48.75 | 11259 | 1963 | 4 $\times$ 0.157 | 1000 | 2100 | 100 | BFRP |
| U-B-1000/500  | 500    | 1000 | 915   | 1750  | 49.88 | 13672 | 2454 | 4 $\times$ 0.157 | 1000 | 2100 | 100 | BFRP |

Three specimens that were not strengthened (C-1000/300, C-1000/400, and C-1000/500) were used as control beams to compare with the three beams that were strengthened with continuous BFRP sheets applied at the shear span, as shown in Figure 2. These beams were strengthened with four layers of BFRP sheet as the U-jacketing vertical fiber which possessed a tensile strength, ultimate tensile strain, and an elastic modulus of 2100 MPa, 2.1%, and 100 GPa, respectively. The bond at the BFRP and concrete interface was made with epoxy adhesive material which possessed an elastic modulus and tensile strength of 3.43 and 51.9 MPa, respectively. A curvature of at least 20 mm had to be provided at the cross-sectional corners of the beam when beam strengthening with externally bonded U-jacket BFRP laminate.

![Figure 2. Geometrical details of the RC beams strengthened by U-jacketing with BFRP sheets](image)

**2.2. Instrumentation and Test Setup**

All beams were tested using a loading machine with a 10000 kN capacity to apply monotonic loads at two symmetrically positioned load points. A computer-aided data acquisition system was used to monitor the load, strains, and displacements throughout the loading tests at selected time intervals. The load was applied until the failure load was reached. The typical measurements taken were: vertical deflection of the beam at mid-span, the horizontal displacement of the beam at shear span (out-of-plane), the strain on the BFRP sheets, and the strain on the concrete at the top surface of the beam at mid-span.

To measure the concrete and BFRP sheet strains, electrical resistance strain gauges were attached to the concrete and BFRP sheet surfaces. The deflection at the beam mid-span was measured using linear variable displacement transducers (LVDTs). The main components of the testing equipment included the LVDTs, the strain gauges, the hydraulic jack equipment, and the frame used for testing the control and strengthened beams as shown in Figures 3 and 4. For all specimens, including both control and strengthened beams, five LVDTs were installed on both faces of the beam set 25 mm apart along the diagonal strut to record out-of-plane displacement, as shown in Figure 5.
3. Experimental Test Results and Discussion

The results presented were expressed in terms of cracking and ultimate load capacities, mid-span load, deflection, concrete compression strain relationships, out-of-plane displacement, load-BFRP strain relationships, and failure modes. Detailed analysis and discussion of the results will be presented in this section.

3.1. Pattern of Cracks, Shear Capacity and Modes of Failure

The pattern of cracks, shear capacity, and modes of failure was analyzed for all beams in the various beam series as follows:

3.1.1. Large-scale Beam Series (1000/300)

The first crack in the large-scale control beam C-1000/300 was observed at the bottom concrete surface at the mid-span of the beam while it was exposed to a cracking load of 300 kN. By increasing the applied load, the crack increased and the first crack formed at the shear zone at a cracking load equal of 360 kN. The final failure mode was
observed to be a shear-type with an inclination of 43° to the horizontal axis, as shown in Figure 6. The beam test specimen failed at a corresponding applied load of 1260 kN.

The first crack in beam U-B-1000/300 strengthened with four layers of BFRP sheet U-jacketing, started at the bottom concrete surface in the flexural zone under a load application point at a cracking load of 360 kN and propagated vertically up to two-thirds of the height of the beam, as shown in Figure 7. The ultimate load of U-B-1000/300 was 2440 kN, 1.94 times greater than that of the control beam C-1000/300. The mode of failure was noted to be tensile rupture failure of the BFRP sheet, as shown in Figure 7.

3.1.2. Large-scale Beam Series (1000/400)

The first crack in control beam C-1000/400 was observed at the mid-span of the beam at the bottom concrete surface under a cracking load of 440 kN. Increasing the applied load caused the crack to increase and the first crack formed at the shear zone under a cracking load of 620 kN. The final mode of failure was noted to be a shear-type failure with an angle of inclination of 36° to the horizontal axis, as shown in Figure 8. The ultimate load capacity of C-1000/400 was 1600 kN.

The first crack in beam U-B-1000/400 strengthened with four layers of BFRP sheet U-jacketing, started at the bottom concrete surface in the flexural zone under a load application point at a cracking load of 540 kN, and propagated vertically up to two-thirds of the height of the beam, as shown in Figure 9. The ultimate load capacity was 3050 kN, 1.91 times greater than that of the control beam C-1000/400. The mode of failure was noted to be a BFRP debonding failure, as shown in Figure 9.
3.1.3. Large-scale Beam Series (1000/500)

The first crack in control beam C-1000/500 was observed at the mid-span of the beam at the bottom concrete surface under a cracking load of 630 kN. Increasing the applied load caused the crack to increase and the first crack was observed at the shear zone under a cracking load of 810 kN. The final mode of failure was noted as being shear-type with an angle of inclination of 30° to the horizontal axis, as shown in Figure 10. The beam test specimen failed at an applied ultimate load of 1950 kN.

The first crack in beam U-B-1000/500, strengthened with four layers of BFRP sheet U-jacketing, started at the bottom concrete surface in the flexural zone at the mid-span under a cracking load of 720 kN and propagated vertically up to two-thirds of the height of the beam, as shown in Figure 11. The ultimate load was 3860 kN, 1.98 times greater than that of control beam C-1000/500. The mode of failure was noted as being BFRP tensile rupture failure, as shown in Figure 11.

It was observed that the angle of crack failure in the control beam changed depending on the ratio between its depth and width. It was found that by decreasing the ratio, the angle decreased in the order: 43°, 36°, and 30°, for depth to width ratios of 3.33, 2.50, and 2.00, respectively. Table 2 shows the cracking and ultimate shear load capacities for the control and strengthened beams along with the ratio between them and the failure modes for the different beam series.
Table 2. Summarized experimental test results for the present study

| Beam specimen | $b$ (mm) | $h$ (mm) | Cracking load (kN) | % Increases | Ultimate load (kN) | % Increases | Failure mode |
|---------------|---------|----------|-------------------|------------|-------------------|------------|-------------|
| C-1000/300    | 300     | 1000     | 300               | ---        | 1260              | ---        | S           |
| C-1000/400    | 400     | 1000     | 440               | ---        | 1600              | ---        | S           |
| C-1000/500    | 500     | 1000     | 630               | ---        | 1950              | ---        | S           |
| U-B-1000/300  | 300     | 1000     | 360               | 20.00%     | 2440              | 93.65%     | TR          |
| U-B-1000/400  | 400     | 1000     | 540               | 22.70%     | 3050              | 90.63%     | BF          |
| U-B-1000/500  | 500     | 1000     | 720               | 14.29%     | 3860              | 97.95%     | TR          |

* S= shear failure, BF = debonding failure, and TR = tensile rupture failure.

3.2. Load–Deflection Relationships

At the point of maximum deflection, the measured values at the bottom surface were plotted against the applied load from zero loads up to the point of failure for all tested beams. All measured and plotted values indicated that the deflection increased as the applied load increased. The relationship between the applied load and corresponding maximum deflection was approximately linear at the beginning of the relationship up to a point near to the cracking load, and was predominantly non-linear at higher loads, as shown in Figures 12 to 14. The slope of the linear relationship was predominantly dependent upon the various parameters included in this study.

It is a well-known fact that the deflection under any load level for a strengthened beam is typically smaller than that of a control beam under the same load. However, the maximum measured loads and deflections at failure for strengthened beams are typically bigger than those of control beams.

From the figures, it can be seen that the plots showing the relationship between load and deflection do not indicate a yielding stage because the observed failure mode was a shear failure; whereas for the control beams, the curve showed a smooth deflection. This is the reason for the occurrence of the sudden failure in strengthened beams.

Figure 12. Load deflection curves for strengthened and control beams from beam series (1000/300)
3.3. Maximum Deflection

Figures 12 to 14 clearly show that for all beams and beam widths, increasing the applied load will typically increase the maximum deflection. The rate of increase was mainly dependent on the beam width and the shear zone strengthening, an increase in either of which caused a reduction in the rate of increase. This decrease can be seen in the cracking load at maximum deflection, which was measured at mid-span as shown in Figure 15. From the figure, it can be seen that by increasing the width of the beams, the deflection at the cracking load decreased. However, the ultimate measured value of the deflection at the point of failure for the strengthened beams was larger than that of the control beams, as shown in Figure 16. This could be ascribed to an increase in the stiffness of the beams due to the increase in the width of the beam and to shear zone strengthening. Also, the presence of strengthening by BFRP sheets increases the ductility of the RC beams. This is evident from the ultimate deflection for the strengthened RC beams when compared to without strengthened.
3.4. Relationship between the Load and Concrete Strain

The concrete strain was measured at the top surface mid-span point and the measured values were plotted against the applied load from zero loads up to failure for the various tested beams. The relationship between the applied shear force and the concrete strain for all beams is shown in Figure 17.

For beam series 1000/300, the rate of decrease was considered high for the strengthened beam under any load when compared to the control beam. Additionally, the measured maximum concrete strain at failure load for the strengthened beam U-B-1000/300 was found to be nearly identical to that of the control beam C-1000/300.

The characteristics of the relationship between load and concrete strain for all large-scale beam series (1000/400 and 1000/500) were similar to those of beam series 1000/300, as shown in Figure 17. For all beam series, it was clear that the effect of beam width and the bonded sheet strengthening on concrete compression strain was typically nearly identical to their effect on the deflection relationship. Additionally, the measured maximum mid-span concrete strain at failure load for the strengthened beams was considered low; it was thus deduced that no crushing will occur at the concrete compression zone at the top surface of the beams.
3.5. Out-of-Plane Displacement (Lateral Displacement)

Out-of-plane displacements along the diagonal strut were measured for all beam specimens and plotted as shown in Figures 18 to 20. The beam specimens were tested without load eccentricity. In order to ignore the eccentricity, an average value was taken for both sides at every point.

From these figures, it can be observed that the value of the out-of-plane displacements of the strengthened beams was smaller than those of the control beams under the same load, such as the failure load for the control beam. This deficiency in out-of-plane displacements is caused by the presence of U-jacketing strengthening by BFRP sheets. However, the ultimate value of the out-of-plane displacements for the strengthened beams was larger than that of the control beams at the failure load. This was deemed to be due to the sides not being added with BFRP sheets. The horizontal part of the BFRP sheets was thus unable to control lateral movement in the beam.
For beams strengthened with U-jacketing confinement, debonding failure can occur at the top surface of the beam, as shown in Figure 21. For the bottom surface of the beam, since out-of-plane displacements are controlled by the horizontal part of the BFRP sheets, no debonding will occur. This allows the value of the shear load capacity to be increased up to the tensile rupture failure capacity of the BFRP sheets, as shown in Figure 22.
3.6. Influence of the Beam Width

The width of the beam had a significant, direct influence on the out-of-plane displacement, as shown in Figure 23, as well as on the lateral strain, as shown in Figure 24. This lateral strain on the edges of the beam can be controlled by the horizontal part of the FRP sheets by using U-jacketing strengthening or completely wrapped. The relationship between the beam height and lateral concrete strain for different beam widths at failure is shown in Figure 24. When the width of the beam increased, the lateral strain decreased, which led to slow debonding failure or a change to fiber rupture failure.
3.7. Effective Strain on BFRP Sheets

The strains in the fiber direction of the vertical BFRP sheet were measured using 9 strain gages positioned in the test region, as shown in Figure 25. The results were plotted at the failure load levels (25%, 50%, 75%, and 100% of ultimate load), as shown in Figures 26 to 28. From these figures, it can be seen that in the case of tensile rupture failure, the BFRP sheet strain distribution can be seen to be spread across all locations for any load level. This implied that the BFRP sheet was very efficient at distributing strain. The BFRP sheet strain distribution effect did not have to create an even distribution at every location in the case of debonding failure and therefore fell behind tensile rupture failure in terms of efficiency. This implied that the strain was concentrated in one location, so debonding failure was bound to happen earlier than tensile rupture. Therefore, if the FRP sheets as a completely wrapped strengthened are used around the cross-section, then the occurrence of the tensile rupture of the FRP, as a result, happens and thus it can obtain the maximum efficiency of the FRP material.

Figure 25. Typical number, location, and direction of strain gauges mounted on the BFRP sheet for the strengthened beams

Figure 26. Vertical BFRP sheet strain distribution over the shear span for strengthened beam U-B-1000/300

Figure 27. Vertical BFRP sheet strain distribution over the shear span for strengthened beam U-B-1000/400

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Figure 28. Vertical BFRP sheet strain distribution over the shear span for strengthened beam U-B-1000/500

4. Conclusions

Based on the experimental test results conducted on large-scale RC beams strengthened with BFRP sheets, it was evident that the BFRP sheets provided appreciable enhancement and increased both the toughness and ultimate strength of the strengthened beams in comparison to the control beams.

- For beams with widths of 300, 400, and 500mm, it was observed that by using BFRP sheets for strengthening, both the cracking and ultimate load increased in comparison to the control beams under the same conditions. The cracking load of the 300, 400, and 500mm wide strengthened beams was 1.20, 1.23, and 1.14 times greater than that of the control beams, respectively. Additionally, the ultimate load of the 300, 400, and 500 mm wide strengthened beams was 1.94, 1.91, and 1.98 times greater than that of the control beams, respectively.

- Varying the depth to width ratio of the beam caused variation in the failure angle as well. By increasing this ratio, the angle of failure likewise increased. Ratios of 2.00, 2.50, and 3.33 yielded failure angles of 30°, 36°, and 43°, respectively.

- Variations in beam width caused variations in the lateral strain as well, in an inversely proportional relationship.

- The BFRP sheet strain was very well distributed in the case of tensile rupture, but this was not so in the case of debonding failure where the BFRP sheet strain was concentrated at a specific location.

5. Acknowledgements

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6. Conflicts of Interest

The authors declare no conflict of interest.

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Seismic Performance of Clay Bricks Construction

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Abstract

The extensive use of masonry construction accompanied by the seismic hazard in Iraq requires comprehensive studies to assess the seismic performance of such construction. This study aims to evaluate the seismic performance of URM and CM buildings by their nonlinear time-history responses. ANSYS 18.2 software has been used to perform the nonlinear dynamic analyses. The mechanical properties have been investigated as the first step of the study. A simple mechanical instrument was improvised to determine the tensile strength of masonry directly. Ground motions were chosen in a manner so that their peak ground accelerations and site soils are as similar as possible to those in the South of Iraq. The computer software terminated all the analyses before the ends of the applied earthquake duration because the solutions did not converge. In the numerical models, severe cracks have been observed in both URM and CM models, indicating their unsafe seismic performance. The minor cracks in confining concrete in the CM model compared to the severe ones in the masonry walls of the same model show the capability of the confinement to prevent the disintegration of collapsed masonry walls, at least in damaging cases like the building state at the solution termination.

Keywords: Masonry; Confined; Earthquake; ANSYS; Cracks.

1. Introduction

Masonry is the oldest construction type used throughout the world. It was used in Mesopotamia about 5000 B.C. [1]. However, the existing Iraqi monuments denote its old usage in construction. It is still widely used in Iraq in the form of URM or CM buildings. Stones besides other building types are used in the northern and western portions of the country, while clay bricks and concrete blocks are used in the middle and southern portions. However, clay bricks masonry is mainly used in the south region. URM structures are reliable for supporting gravity loads, but their resistance is weak under the effect of lateral loads. The post-earthquake observations demonstrate how they are seismically vulnerable and how their collapse causes the majority of casualties if they represent the most buildings in the affected area. Since masonry buildings exist in regions that have effective seismicity, experimental and theoretical studies have been implemented to assess their seismic performance and to propose suitable retrofitting techniques that enhance their seismic response. In this study, the nonlinear time-history response of URM and CM buildings has been investigated by ANSYS 18.2 using the William-Waranke plasticity model to simulate the material nonlinearity. Solid65 has been used for the simulation. This element is capable of cracking in tension and crushing in compression, which is a characteristic of the mechanical behavior of brittle materials such as masonry and concrete. The element has eight nodes with three degrees of freedom at each node.

The analysis with ANSYS Mechanical APDL has three main stages: preprocessor, solution, and postprocessor. In the first stage, the model geometry is built, and the mechanical properties are input. The second stage (solution)
includes the definition of the boundary conditions, load application, and analysis running. In the postprocessor stage, analysis results are viewed in terms of graphs, figures, animations, or numbers. The mechanical properties of clay brick masonry have been determined through the experimental part of the study. No previous studies were found in the study area for the same purpose except the one implemented by Al-Chaar et al. [2], in which the tensile strength of masonry has not been involved in the experimental program.

The current study is not a parametric study; its primary purpose is to reveal whether the masonry models overcome the applied ground motions or not, and this is the essential criterion to evaluate their seismic performance. The mechanical properties of the numerical models should be as precise as possible. Therefore, the study headlines are the determination of masonry mechanical properties, the macro-modeling of masonry buildings, the selection of seismic waves, and applying the seismic waves to the masonry models to obtain their nonlinear time-history responses. Finally, the seismic performance of a masonry building is considered good if its model overcomes the applied ground motion. Otherwise, it is unsafe under the effect of earthquakes.

2. Literature Reviews

The structural vulnerability of masonry buildings and the dangerous effects of their damage during earthquakes lead to present many theoretical and experimental studies to assess their seismic performance and to propose suitable retrofitting techniques that enhance their structural response in 2015, Yaseen [3] investigated the seismic fragility of the URM buildings in the North of Iraq (Kurdistan region), which represent approximately 87% of all buildings in this region. The macro-modeling and the incremental dynamic analysis were performed using the TREMURI program to perform a nonlinear time-history analysis. The study indicated that the seismic safety of the studied, low-rise URM buildings in the concerned region is questionable, denoting the need for strengthening such structures to mitigate the potential economic and life losses that probably happen during future earthquakes.

Abdulla et al. (2017) [4] described a simplified micro-model for the simulation of masonry utilizing the extended finite element method and a combination of plasticity-based models. The detailed micro-modeling gives accurate and complete results, but it takes intensive computations, and thus, it is used for small masonry models. As an alternative, the researchers have proposed a simplified micro-model in which the brick units are expanded to compensate for the vanished mortar volume. Discontinuous elements model the interaction between enlarged units. The validity of the proposed method was verified by comparison to the results of experimentally tested masonry walls, which subjected to in-plane cyclic loads, out-of-plane monotonic loads, and in-plane monotonic loads. The comparison showed good accuracy for the analysis method. In 2018, Chacara et al. [5] proposed a modeling approach for unreinforced masonry structures, by which the masonry panels are simulated with quadrilateral macro-elements having rigid edges and connected by hinges and a diagonal nonlinear link. Each element has seven degrees of freedom; six degrees of freedom represent the panel translations and rotations as a rigid body, and the seventh corresponds to the shear deformation of the panel itself. The proposed modeling was performed to obtain the seismic response of two masonry models. The results of the analyses are in good agreement with those provided by finite element simulations. Also, the modeling reduces the computation cost.

Kallioras et al. (2018) [6] presented the results of an experimental test carried out on a full-scale, single-story URM building. A unidirectional-table test was implemented on the building, which is consisted of double-wythe, clay-brick URM walls including large openings and a floor made of timber beams and planks composing a flexible diaphragm. Its sharply inclined roof is composed of timber trusses. The parts of the perimeter walls above the floor (the gables) are the weaker when affected by an out-of-plane excitation. Therefore, the direction of shaking was chosen to be perpendicular to these walls. It was observed that only minor damage occurred for the affected building up to an input accelerogram with a PGA (peak ground acceleration) of 0.23 g, while the collapse state was reached at motion with a PGA of 0.68 g. Zones of high acceleration response, such as gables, exhibited major out-of-plane damage. As a result, the study confirmed that the most vulnerable parts of such buildings under seismic action are the gable walls, while the rocking of slender piers exhibited the damage caused by the in-plane response. In 2018, Avila L. et al. [7] assessed the seismic performance of two prototypes of asymmetric masonry buildings. One of the buildings is a two-story, unreinforced building, while the other is a two-story, reinforced building. The study involved investigating the effect of geometrical configuration, the influence of reinforcement presence, and the comparison between the seismic behaviors of the two structures. It has been found that the reinforced building is capable of inputting acceleration twice the acceleration that in the unreinforced building. Shakarmi et al. (2018) [8] used the LS-DYNA software for the simulation of confined masonry walls loaded with cyclic, in-plane, lateral loads to examine the effect of aspect and reinforcement ratio on the structural behavior of the studied walls. The validity of using the micro-model has been verified by comparing it to the results of a previous test performed on a confined wall. The study showed that an aspect ratio of (height/length=1) makes the wall having better structural behavior concerning resisting mechanism, energy absorption, and deformability.

Erberik et al. (2019) [9] compared the seismic performance of URM buildings to that of CM buildings. The results demonstrated the superior, seismic performance of CM buildings over URM ones. It was found that low rise CM
buildings are suitable, even high seismic intensity exists. The confinement enhances the seismic behavior by preventing wall-to-wall action that propagates seismic damage and also to the enhancement of the structural capability of dissipating energy. The results demonstrated a high effect of masonry compressive strength on the seismic performance of URM buildings. Whereas, it is not the case for CM building models, which are notably affected by other parameters such as the reinforcement and the cross-section of confining concrete columns and diagonal shear strength of confined masonry walls. In 2019, Cazarin and Teran-Gilmore [10] discussed the relatedness of some of the new seismic provisions of the code known as “the Mexico City Building Code” released in December 2017, which increases the deformation demand of the inter-storey drift from 0.5% to 1% for CM buildings with shear walls having horizontal reinforcement. Three CM buildings of different numbers of stories (6, 8, and 10 stories) were designed according to the code requirements. Then the non-linear static analyses were performed to obtain the responses of the three buildings. The experimental evidence for the justification of the increase in lateral displacement was studied. For the three buildings, it was found that a soft story is developed in the building once its maximum shear capacity is reached. Beyond that, failure occurs if a minimal increase occurs in the lateral displacement. It was observed that a drift of 1% could not be reached before the development of the soft storey. In 2019, Dong et al. [11] presented an experimental study to investigate the effect of reinforced mortar cross strips on the structural response of unreinforced masonry walls subjected to seismic loadings. Eight walls strengthened with cross strips of reinforced mortar on one or both faces, and three URM walls were tested under the effect of a lateral cyclic load with constant pressure on the top face. It was found that the presence of reinforced mortar cross strips increased the shear strength by at least 38.2% and significantly increased the deformation capacity.

Ismail and Khattack (2019) [12] studied failure modes of the URM buildings that were damaged due to the Mw 7.5 earthquake that hit the North of Pakistan on 26 October 2015. The commonly observed failure modes encompassed toppling of minarets, local or global out-of-plane collapse of URM walls, diagonal shear cracking in piers, flexural cracking in spandrels, damage of corner, pounding damage, and damage due to ground settlement. Most fatalities were due to the collapse of URM walls and subsequent collapse of roofs. In 2019, Sorrentino et al. [13] studied the structural behavior of masonry buildings during the nine earthquakes ranging from 5 to 6 of the moment magnitude that hit Central Italy during the period between August 2016 and January 2017. The unreinforced masonry buildings represent about 75% of the constructions in the affected territory. Severe damage and complete collapse were observed in URM buildings, while better structural behavior was observed in modern buildings constructed with hollow clay blocks. This better seismic performance is attributed to the adequate quality of masonry, the relatively lightweight structures due to the presence of cavities in masonry units and the configuration redundancy.

3. Mechanical Properties of Masonry

3.1. Compressive Strength

The compressive strength of masonry can be considered its fundamental characteristic because the other mechanical properties can be estimated depending on it by proposed relationships. Masonry compressive strength depends on the compressive strength of its constituents (brick units and mortar). The difference in stiffness and Poisson’s ratio between bricks and mortar makes one of the two constituents expands laterally more than the other as masonry being compressed. Consequently, shear stresses develop at the contact surfaces between bricks and mortar initiating masonry failure [14]. If the bricks are stiffer than mortar, the mortar will be in a triaxial compression state of stress. Meanwhile, the cannon will be stretched outside if it is more inflexible. In the present study, six masonry prisms were tested, as in Figure 1, and the average compressive strength is 5.5 MPa with a standard deviation of 0.4 MPa.
3.2. Tensile Strength

The tensile strength of each of the masonry constituents is higher than the ultimate value of the bond stress exhibited perpendicular to their interaction surface. Therefore, the tensile strength of masonry is controlled by the ultimate value of this stress. In the present study, a simple method was used to test the tensile strength of masonry directly. The specimen used for the test is two bricks built together, as in Figure 2, with cement-sand mortar of 1:3 mixing proportion.

![Figure 2. Tensile strength test of masonry](image)

The lower brick of the specimen, shown in Figure 2, is loaded by the hanging weights that are put in the lower iron frame, which is free to fall when the tensile failure occurs, while the upper brick remains hanging at the top. Bricks, sand, concrete cubes, etc. are put in the suspended frame up to failure occurs. Then, all weights, including iron frame and lower brick, are summed and divided by the loaded area, which is the intersection area illustrated in Figure 3. The result of the division represents the tensile strength of the masonry specimen. Fifteen specimens were tested in this study, and the average value of the tensile strength is 0.15 MPa with a standard deviation of 0.03 MPa.

3.3. Modulus of Elasticity

The modulus of elasticity of masonry ($E_m$) can be estimated by the compressive strength value, but the challenge is that the codes have a large extent of variation in the recommended relationships as shown in Table 1.

| Code | Recommended value for $E_m$ in MPa |
|------|-----------------------------------|
| Building Code Requirements and Specifications for Masonry Structures by the Masonry Standards Joint Committee (MSJC) [15] | $700f_m$, or evaluated as the slope of the chord taken between 0.05 and 0.33 of the compressive strength of masonry in the stress-strain curve |
| Eurocode 6 [16] | $1000f_m$ |
| FEMA 356 [17] | $550f_m$ |

Where $f_m$: Compressive strength of masonry in MPa.

![Figure 3. A sketch for the top view of a specimen of masonry tensile test](image)

In the present study, a simple steel frame was prepared to measure the modulus of elasticity. Three prisms (three-brick prisms) were tested under uniaxial compression, as shown in Figure 4b. The length shortening was measured...
with a dial gauge, and the corresponding load was recorded. Only the eight screws (two from each side) touch the specimen, as in Figure 4a.

![Figure 4. (a) A Specimen with apparatus; (b) A specimen under testing](image)

The modulus of elasticity can be obtained from the stress-strain curve according to the MSJC code [15], as illustrated in Figure 5, in which the modulus of elasticity is the slope of the line segment joining the two points on the curve whose stresses are 0.33 and 0.05 \( f_m \), where \( f_m \) is the compressive strength of masonry. Consequently, the moduli of elasticity for the three specimens have been evaluated from the stress-strain curves shown in Figures 6 to 9 as in Table 2.

![Figure 5. Modulus of elasticity for masonry according to MSJC code [15]](image)

![Figure 6. Stress-Strain curve for masonry specimen No.1](image)
The average value of modulus of elasticity is 2723 MPa with a standard deviation of 777 MPa. The significant variation between the results is due to the difference between brick units, which have pretest cracks with different configurations. However, a value of 2750 MPa for the modulus of elasticity has been used in the analyses.

4. Transient Analysis

The transient analysis (also called time-history) is one of the analysis types provided by ANSYS software. It is used to determine the response of a linear or a nonlinear structural system subjected to any time-dependent load. Also, it can be used to find the response of a freely vibrating structure with or without damping effect. In this analysis type, ANSYS solves the overall equilibrium equations in the form below [18]:

![Figure 7. Stress-Strain curve for masonry specimen No.2](image1)

![Figure 8. Stress-Strain curve for masonry specimen No.3](image2)

### Table 2. Moduli of elasticity of masonry specimens

| No. of masonry specimen | Modulus of elasticity (MPa) |
|-------------------------|-----------------------------|
| 1                       | 2399                        |
| 2                       | 3610                        |
| 3                       | 2160                        |
\[
[M][\ddot{U}] + [C][\dot{U}] + [K][U] = \{F_t\}
\]

Where: \([M]\) is the global mass matrix, \([\ddot{U}]\) is the vector of nodal accelerations, \([C]\) is damping matrix, \([\dot{U}]\) is the vector of nodal velocities, \([K]\) is the global stiffness matrix, \([U]\) is the vector of nodal displacements, and \([F_t]\) is the load vector.

At any time \((t)\), the set of equations above can be considered as equations of static equilibrium, and the program utilizes the iterative approach to solve them. For the sequent time increments, an improved method (known as HHT) or Newmark integration method is used to perform the incremental dynamic analysis [20].

5. Seismic Loading for Transient Analysis

The seismic load is defined into ANSYS mechanical APDL to perform a transient analysis by applying the ground velocity and displacement that is traveled by the structure foundation during the earthquake to the nodes or areas at the level of structure base. An acceleration time-history can be converted into a displacement time-history by the double integration technique, which is nowadays carried out by professional software packages such as Seismosignal software. In the present study, seismic data files were downloaded from the site of the PEER Berkeley ground motion database. Also, the acceleration time-histories of the 7.3 Mw earthquakes that hit the Iraq-Iran border on 12 November 2017 were converted to displacement time-histories and used in the analysis. The ground acceleration files for the mentioned earthquake were downloaded from the site of the Iranian strong motion database.

6. Selection of Acceleration Time-Histories

The ground motions that chosen for the structural analysis should be as reflective as possible for the seismic characteristics of the analyzed structures site. In this study, the criteria used to select the seismic records are the magnitude (Mw), the peak ground acceleration (PGA), and the average shear wave velocity for the upper 30 m from the site soil (\(v_{s30}\)). The statistical analysis for Iraq seismicity reveals that 90.05% of events have magnitudes within the range (4-5.4), while 6.03% of the total events have magnitudes within the range (5.5-7.4). The contour map of the peak ground acceleration, according to the PSHA study introduced by Onur et al. [19], is shown in Figure 9. In the South of Iraq, the PGA map shows that its value increases from 0.1g to more than 0.5g as the site varies towards the Iraq-Iran borderline. Therefore, the selected ground accelerations have PGAs within this range.
The shear wave velocity (vs30) for an area can be estimated depending on the reported site investigations that were performed for projects erected in it. In 2017, Mohammed and Abdulrassol [20] evaluated the shear wave velocity for different sites in Iraq, depending on the geotechnical reports of the projects distributed, as in Figure 10. The main parameter used in the study is the standard penetration test (SPT), which can be used as an alternative parameter to classify sites instead of the shear wave velocity. The study evaluated the shear wave velocity ranging from 102 to 627 m/s in the South of Iraq and from 111 to 420 m/s in the Eastern South. The low values of the ranges are for soft clay soil, which is obviously observed in Basra city.

7. Modeling and Results

7.1. Model No. 1

The model is a one-story, single room with a plan shown in Figure 11 and a clear height of 3 m. It has two openings; the (1×2.1) m door and the (1×1.5) m window. The concrete slab thickness is 0.2 m. The wall thickness is 0.24 m. The lintels over openings are made of concrete. The finite element model is shown in Figure 12.

![Figure 11. plan of Model No.1](image1)

![Figure 12. Finite element model No.1](image2)

The coordinate system, shown in Figure 11 is the same as the default global coordinate system in ANSYS in which the y-axis is perpendicular to the paper (parallel to the room height). The edge length of the element was set to be 100 mm. Thus, the model is built up of 16164 solid65 elements with 22548 nodes. The characteristics of the seismic records applied to the model are as in Table 3.

| Earthquake name   | Station name       | Date       | Magnitude (Mw) | Peak ground acceleration (g) | Shear velocity (VS30) (m/s) |
|-------------------|--------------------|------------|----------------|------------------------------|-----------------------------|
| Northwest California | Ferndale city hall | 12/9/1938 | 5.5            | 0.15                         | 219.31                      |

The acceleration time-histories for the earthquake mentioned above are shown in Figures 13 to 15.

![Figure 13. H-1 component of ground acceleration of Northwest California earthquake, 1932](image3)
The horizontal H-1 components of ground velocity and displacement were applied in the z-direction, while the horizontal H-2 and vertical components were applied in the x-, and y-direction (gravity direction), respectively. The solution did not converge and terminated at a time of 0.7 seconds. The total displacement in the z-direction at roof level is shown in Figure 16.

It is so important to know that the displacement, given in ANSYS postprocessor at any node, is the total displacement \( u \) at that node. Therefore, the differential (deformation) displacement \( u \) between any two nodes (any two points within the structure) is found from subtracting ANSYS displacements for the two nodes one from the other. The total displacement \( u \) is given by Equation 2.
\[ u^f = u_g + u \]  

(2)

Where: \( u^f \) is the total displacement, \( u_g \) is the ground displacement, and \( u \) is the response (deformation). Figure 17 shows the three displacements in the sketch below:

![Displacement nomenclature](image)

Figure 17. Displacement nomenclature

The ANSYS displacement (total displacement) at the base level is the same as the ground displacement since the structure base is assumed in full integrity with the ground. Therefore, the response (displacement) in the z-direction at the roof level has been found with the use of the Excel software by subtracting the ANSYS displacement at base level in the z-direction from the ANSYS displacement at roof level in the same direction. Figures 18 and 19 show the ANSYS displacement at the base level and the response at the roof level (\( u_z \)), respectively.

![Total displacement at base level in z-direction for Model No.1 in mm](image)

Figure 18. Total displacement at base level in z-direction for Model No.1 in mm

![The response at roof level in z-direction for Model No.1](image)

Figure 19. The response at roof level in z-direction for Model No.1
Similarly, subtracting the ANSYS displacement at the base level in the x-direction from the ANSYS displacement at the roof level in the same direction by using Excel resulted in the response in x-direction shown in Figure 20.

![Figure 20](image.png)

**Figure 20. The response at roof level in x-direction for Model No.1**

The end of the solution is as shown in Figure 21, in which the diagonal cracks and horizontal cracks at the bottom courses can be clearly observed. The cracks are colored with red color, and the blue color refers to the locations where the first cracks occur which has appeared near the corners of the door and the window in Model No.1 as shown below:

![Figure 21](image.png)

**Figure 21. Cracks in walls of Model No.1 at the end of the solution**

### 7.2. Model No.2

The model is a one-story typical house with a clear height of 3 m and a plan shown in Figure 22.

![Figure 22](image.png)

**Figure 22. Plan of the typical house**

![Figure 23](image.png)

**Figure 23. Finite element model No.2**
The roof is a concrete slab having 0.2 m thickness. The finite element model is shown in Figure 23, in which the edge length of the element was set to be 200 mm, thus the model is built up of 4289 solid65 elements with 8868 nodes. The displacement-time histories used for the analysis were obtained from converting the accelerograms recorded in Ravansar station (Iranian station) during the 7.3 Mw earthquakes that hit the Iraq-Iran border on 12 November 2017. The accelerograms were converted to displacement time-histories by the use of seismosignal software. Table 4 demonstrates the characteristics of the seismic records applied to Model No.2.

| Earthquake name | Station name | Date       | Magnitude (Mw) | Peak ground acceleration (g) | Shear velocity (VS30) (m/s) |
|-----------------|--------------|------------|----------------|-------------------------------|-----------------------------|
| The 7.3 Mw, November 2017 | Ravansar | 12/11/2017 | 7.3            | 0.122                         | 267                         |

The acceleration time-histories for the earthquake mentioned above are shown in Figures 24 to 26.
The horizontal $H-1$ components of ground velocity and displacement were applied in the $z$-direction, while the second horizontal $H-2$ components were used in the $x$-direction. Of course, the vertical components $t$ were applied in gravity direction ($y$-direction). The structure responses in $z$ and $x$ directions are shown in Figures 27 and 28, respectively.

![Figure 27. Response at roof level in z-direction for Model No.2](image)

![Figure 28. Response at roof level in x-direction for Model No.2](image)

No cracks were observed in the concrete slab, as can be seen in Figure 30 which shows the crack pattern in the slab.

![Figure 29. Crack pattern in masonry walls of Model No.2 at end of solution](image)
The mesh was refined to check the acceptance of the element size, and thus the length of the element edge was set to be 150 mm. The analysis was repeated. The responses of the roof level in z-direction before and after mesh refinement are as shown in Figure 31. It can be noticed that a negligible variance occurred in the structure response. Therefore, the element size with a 200 mm edge length is acceptable.

![Figure 30. Crack pattern in concrete slab of Model No.2 at end of solution](image)

Figure 30. Crack pattern in concrete slab of Model No.2 at end of solution

![Figure 31. Responses at roof level in z-direction before and after mesh refinement for Model 2](image)

Figure 31. Responses at roof level in z-direction before and after mesh refinement for Model 2

**7.3. Model No.3**

This model is a two-story building with a repeated plan of a single room shown in Figure 32. The size of the element is 200 mm, and thus the finite element model shown in Figure 33 is built up of 5780 solid65 elements with 9261 nodes.

![Figure 32. Plan of Model No.3](image)

Figure 32. Plan of Model No.3

![Figure 33. Finite element Model No.3](image)

Figure 33. Finite element Model No.3
The seismic loading is the same loading applied to Model No.1. The responses at first and second levels are shown in Figures 34 to 37.

Figure 34. Response at first level in z-direction for Model No.3

Figure 35. Response at second level in z-direction for Model No.3

Figure 36. Response at first level in x-direction for Model No.3
Figure 37. Response at second level in x-direction for Model No.3

Figure 38 shows locations of the building where first cracks appear in masonry walls while Figure 39 shows crack pattern at the end of the solution.

Figure 38. First cracks in masonry walls of Model No.3

Figure 39. Crack pattern in masonry walls of Model No.3 at end of solution
7.4. Model No.4

The model is a confined, single-story, masonry room having the same plan and dimensions as those of Model No.1. The vertical confining components (tie-columns) have a cross-section of (240×240) mm. They are reinforced with 4 Ø12 mm longitudinal bars and Ø6 mm @200 mm ties. The mechanical properties of concrete and reinforcement steel are as in Table 5.

| Material          | Compressive Strength (MPa) | Tensile strength (MPa) | Modulus of Elasticity (MPa) | Poisson’s ratio |
|-------------------|----------------------------|------------------------|-----------------------------|-----------------|
| Concrete          | 25                         | 3.5                    | 24000                       | 0.2             |
| Reinforcement steel | ----                      | 400                    | 200,000                     | 0.3             |

The finite element model, shown in Figure 40, is composed of 32728 solid65 elements and 6637 beam elements with 39072 nodes. The finite element simulation of columns reinforcement is shown in Figure 41. The seismic loading is the same loading used in Model No.1.

The responses at roof level in z and x directions are shown in Figures 42 and 43.
Figure 43. Response at roof level in x-direction for Model No.4

Figures 44 and 45 show the crack pattern in masonry walls and concrete frame (slab and confining tie columns):

Figure 44. Crack pattern in walls of Model No.4

Figure 45. Crack pattern in the concrete frame of Model No.4

The stress in the reinforcement of the tie-columns is shown in Figure 46. The maximum stress value is 191.684 MPa which is less than one half the yield stress of the reinforcement.

Figure 46. Stress in steel reinforcement of confining columns in Model No.4
8. Results and Discussion

The solution of nonlinear equations, in which the stiffness matrix is a function of the degrees of freedom or their derivatives, is accomplished in ANSYS using the Newton-Raphson method. The Newton-Raphson equation used for the nonlinear solution can be written as in Equation 3 that follows [18]:

\[
[K^T] \{\Delta U_i\} = \{F^a\} - \{F^m\}
\] (3)

Where: \([K^T]\) is the tangential stiffness matrix, \(\{\Delta U_i\}\) is the displacement increments, \(\{F^a\}\) is the applied loads vector, and \(\{F^m\}\) is the vector of element internal loads. In transient analysis, \(\{F^m\}\) includes the effective inertia and damping forces. The present study ignored the damping effect. The set of the simultaneous equations in the form of Equation 3 are solved with an iterative process. The iterative process requires a convergence criterion to terminate when the solution satisfies the required accuracy. The nonlinear convergence criteria are used in ANSYS for the nonlinear structural solutions which are solved by the Newton-Raphson method. Force, displacement, moment, and rotation criteria are provided. In the present study, both force and displacement criteria were used.

The main criterion adopted in the study to assess the seismic performance of a studied structure is whether it resists and overcomes the applied seismic waves or not. All simulated buildings could not overcome the applied seismic loadings. Here, it should be interpreted, according to Equation 3, what it means if the convergence is not satisfied. It means that the right-hand side of the equation does not equal the left-hand side within the limited tolerance. This inequality is attributed to the reduction in the stiffness matrix, which is caused by the missing stiffness of cracked elements. Consequently, the structure no longer has the required stiffness to resist the applied forces.

The dynamic responses shown in Figures 19, 20, 27, 28 and 34 to 37 demonstrate the combined effect of in-plane and out-of-plane actions since the diaphragm (concrete slab) has two orthogonal, horizontal displacements in z and x directions. It can be observed that all studied models oscillated a few cycles, not about their equilibrium positions. The combination of responses and crack patterns arouses the inquiry of how these significant cracks occur with small deformations. The answer to this inquiry requires the determination of yield displacement of URM masonry walls in terms of the parameters governing it. In 2010, Aldemir [21] introduced a parametric study to determine the parameters affecting the structural behavior of unreinforced masonry piers subjected to lateral, in-plane loads. Then, the study has formulated the parameters of the capacity curve of URM walls. According to the mentioned study, the yield displacement of URM walls is given in Equation 4.

\[
\delta_y = 0.587 \, p^{0.543} \, e^{0.0949f_m} \, \lambda^{1.426} \, L
\] (4)

Where: \(\delta_y\), \(p\), \(e\), \(f_m\), \(\lambda\), and \(L\) are: yield displacement in mm, overburden pressure in MPa, the natural exponent, compressive strength of masonry in MPa, aspect ratio, and the length of the wall in mm, respectively. The overburden pressure on the top of the masonry wall has an essential effect on its structural behavior. Therefore, the gravity load profoundly affects the stability of URM structures subjected to lateral loads. ANSYS software applies the loads incrementally during the solution time, which is the earthquake duration in the transient analysis of seismic response. Consequently, only a part of the concrete slab is applied at the top faces of walls before the solution termination. For more accuracy, this problem must be taken into consideration to overcome. Taking Model No.1 as an example with an overburden pressure of 0.03 MPa, the yield displacement in the z-direction is 0.41 mm. Comparing this calculated value to the response shown in Figure 19 reveals that the two masonry walls in z-direction yielded with deformations less than those estimated by Equation 4. However, Equation 4 has been formulated depending on a statistical process, and is not very strict. The pressure of 0.03 MPa is the bearing stress on top faces of masonry walls parallel to the short dimension due to the weight of the concrete slab, which is the pressure in a static case. As explained above, the incremental application of loads means that the overburden pressure at the end of the solution is much less than 0.03 MPa since the solution terminated at a very early moment during the earthquake duration. Besides, Equation 4 has been formulated for a static case with an in-plane action only, which differs from the dynamic behavior. Finally, cracking of in-plane loaded URM walls with small deformations agrees with the results of previous studies. Increasing the tolerance for the nonlinear convergence criteria, which has a default value of 0.001, through the solution controls input makes the solution continue more time leading to more significant deformations in the analyzed structure. However, using high tolerances in solutions needs shaking table tests to make comparisons between the experimental results and the numerical results to verify the validation of the high values. Therefore, future studies must consider this need.

9. Conclusion

It is not strict enough to say that the studied models collapsed or not, during the applied seismic waves because the analyses stopped before the occurrence of the total collapse, which cannot be captured obviously by ANSYS simulations. However, the three URM models that studied could not overcome the applied earthquakes, and significant cracks occurred in them. Consequently, it is right to consider the unreinforced masonry buildings as unsafe structures.
under the effect of a seismic load due to their poor seismic performance. All models cracked with small deformations. Therefore, the nonlinear, dynamic analysis appears more conservative than the nonlinear, static analysis (pushover analysis). The crack patterns show that the first cracks appear near openings in masonry walls, and cracking occurs firstly on the ground floor in case of a two-story building.

To some extent, the locations of first cracks verify the accuracy of the simulation results because it is already clear that the stresses concentrate near openings, and the maximum shear force occurs at the base of the building during earthquakes if the fundamental mode governs its dynamic behavior. However, the first crack locations reveal the need for strengthening the openings of doors and windows with a suitable confinement technique. The confined masonry model also was not capable of overcoming the applied earthquake, but the minor cracks in the tie-columns compared to the significant cracks in masonry walls and unyielding of reinforcement show a good indication that the confinement can preserve the collapsed masonry walls from disintegration, which reduces losses in life and properties. Based on the study results, no guided conclusion can be presented about the structural behavior of the confined masonry building beyond the time of the end of the solution, but it is overbalanced that spreading of cracks in the concrete frame continues in progress while a detachment of brick units mainly happens in the out-of-plane direction.

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11. Conflicts of Interest

The authors declare no conflict of interest.

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Numerical Study on RC Multilayer Perforation with Application to GA-BP Neural Network Investigation

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Abstract

The finite element model of projectile penetrating multi-layered reinforced concrete target was established via LS-DYNA solver. The penetration model was validated with the test data in terms of residual velocity and deflection angle. Parametric analyses were carried out through the verified penetration model. Seven influential factors for penetration conditions, including the initial velocity of projectile, initial angle of attack of projectile, initial dip angle of projectile, the first layer thickness of concrete target, the residual layer thickness of concrete target, target distance and the layer number of concrete target, were put emphasis on further analysis. Furthermore, the influence of foregoing factors on residual velocity and deflection angle of projectile were numerically obtained and discussed. Based on genetic algorithm, the BP neural network model was trained by 263 sets of data obtained from the parametric analyses, whereby the prediction models of residual velocity and attitude angle of projectile under different penetration conditions were achieved. The error between the prediction data obtained by this model and the reserved 13 sets of test data is found to be negligible.

Keywords: Multi-layered Concrete Plates; Oblique Penetration; Deflection Angle; Neural Network Model.

1. Introduction

Since the Kosovo and Iraq wars, precision-guided ground-drilling weapons represented by the US Army's ‘Jedam’ ground-drilling missiles have developed rapidly. Researches on the damage of underground multi-story fortifications need to explore the deep mechanism of the penetration and perforation into multi-layer reinforced concrete targets [1-3]. The better understanding over projectile perforation into multi-layer RC panels may contribute to the design and construction of high-performance shelter.

At present, there is still a lack of research on multi-parameter systems for the problem of missiles penetrating multilayer reinforced concrete targets. Yue et al. [4] established a numerical calculation model of steel bullets penetrating multilayer spacer targets, and obtained the influence of the geometry, density, and mass of steel bullets on the penetration response of 5-layer spacer targets. Ji et al. [5] carried out numerical calculations on the projectile penetrating three layers of homogeneous steel plates, and obtained the velocity and acceleration change curves of the projectile, and simulated the residual velocity of the projectile perforating the three-layer target plate. Liu and Huang carried out LS-DYNA simulation research on the basis of the experiments of the projectile penetrating the three-layer

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concrete target board, and obtained a reasonable numerical calculation model [6]. Sun et al. simulated the inclination of the projectile penetrating the three-layer concrete target board, obtained the time-history change curve of the projectile velocity and acceleration, and summarized the change law [7]. Yossifon et al. studied the problem of rigid body penetrating a double-layer metal target from two aspects: theoretical analysis and simulation. It was pointed out that the theoretical analysis model can significantly save computing time compared with simulation (Autodyn2D) [8]. Booker et al. compared the penetration effects of 6 groups of equal-volume segmented concrete and monolithic concrete, showing that under the same anti-penetration effect, a method can be found to segment large monolithic concrete target into segmented concrete plates, to reduce the cost of the protective structures [9].

In this work, a finite element model of the projectile penetrating the multilayer reinforced concrete target is established with validation against the test results. Extensive simulations are conducted to analyze 7 penetration factors, such as initial velocity \( (v_0) \), initial inclination \( (\theta_0) \), initial angle of attack \( (\delta) \), first-layer target thickness \( (t_1) \), remaining Target thickness \( (t_2) \), target distance \( (s) \), number of target layers \( (n) \), etc. on the projectile's remaining velocity \( (v_f) \) and deflection angle \( (\alpha) \). Using the genetic algorithm's BP (GA-BP) neural network model for the parametric analysis results to perform machine learning training, the prediction models of the missile's residual velocity and attitude angle under different penetration conditions can be developed. The GA-BP neural network predictions agree well with the foregoing numerical modeling results.

2. Finite Element Model and Verification of Steel-multilayer Target Penetration

2.1. Introduction to Verification Test Background

The test results of the projectile penetrating the multilayer concrete target in [10] were used to verify the simulation results. The test projectile material is high-strength steel 30CrMnSiA, the projectile length is 1200 mm, the mass is 290 kg, the projectile head coefficient CRH = 3.0, and the center of gravity is 637 mm from the head. The thickness of the first layer of concrete target is 300 mm, and the thickness of the remaining targets is 180 mm. The length and width of each layer of the target plate are 4000 mm. The vertical distance between adjacent target plates is 3.5m, and the angle between the target plate and the ground normal is 17°. The uniaxial compressive strength for concrete is 40 MPa and the volume reinforcement ratio is 0.3%. The projectile was fired horizontally with an initial velocity of 688 m/s.

2.2. Establishment of Finite Element Model

In this paper, a finite element model of the projectile penetrating the multilayer reinforced concrete target is established via the LS-DYNA software. In the finite element model, the element type of the reinforcing bar is BEAM161, and the target plates are modeled with SOLID 164. Since the projectile has almost no deformation after penetration test [10-11], the projectile in simulation can be regarded as a rigid body. Considering the projectile's own weight, a weight load was applied to the body. The material model of the steel bar is MAT_PLASTIC_KINEMATIC, and the material model of the concrete is MAT_JOHNSON_HOLMQUIST_CONCRETE (referred to as HJC [12]). See Table 1 for specific material model parameters.

Table 1. Concrete and rebar material parameters

|                | Concrete                  | Rebar                  |
|----------------|---------------------------|------------------------|
| Density (ρ)/kg•m⁻³ | 2525                      | Density (ρ)/kg•m⁻³     | 7800                     |
| Shear modulus (G)/GPa | 8.76                  | Crushing pressure (P_crush)/GPa | 0.016                   |
| Normalized cohesive strength (A) | 0.79                  | Crushing volume strain (ε_crush) | 0.001                   |
| Normalized pressure hardening coefficient (B) | 1.6                  | Compaction pressure (P_comp)/GPa | 0.81                   |
| Strain rate coefficient (C) | 0.007             | Compacted volume strain (h_comp) | 0.1                   |
| Strain hardening index (N) | 0.61               | Damage constant (D₁) | 0.04                   |
| Quasi-static uniaxial compressive strength (σ_u)/GPa | 0.04            | Damage constant (D₂) | 1                      |
| Hydrostatic pressure (T)/GPa | 0.004           | Pressure constant (K₁)/GPa | 85                    |
| Reference strain rate (ε_r) | -1               | Pressure constant (K₂)/GPa | -171                  |
| Minimum plastic strain before fracture (ε_plast) | 0.01             | Pressure constant (K₃)/GPa | 208                   |

2.3. Comparative Analysis of Numerical Calculation Results and Experimental Results

Figure 1 is a comparison diagram of penetration snapshots as a projectile penetrates a four-layer target plate, taken by a high-speed photography device in the test, and penetration figures of a numerical calculation model.
It can be observed from Figure 1 (a)-(h) that the finite element model can simulate the whole process of the elastic body penetrating the four-layer reinforced concrete target. The horizontal (x-axis) residual velocity $v_r$ and the deflection angle $\alpha$ for projectile for perforating each target plate layer can be obtained through simulation results. The comparison between simulation and test data is shown in Figure 2. The experimental data are in good agreement with the simulation results, ensuring that the simulation model in this paper can be used to study the parameters of the projectile penetrating the multilayer reinforced concrete target. The attitude deflection in a medium concrete target is under the deflection mechanisms of both the initial cratering and the shear plugging sub-stages as well as the incomplete clamping mechanism of the tunneling sub-stage. In brief, Duan et al. [13] gave the explanation to the deflection mechanism claiming that the projectile tends to perforate the concrete panel in the shortest path.

![Figure 1. Comparison of field photos and numerical results of the projectile penetrating the four-layer plates](image1)

![Figure 2. Comparison of simulation and test results](image2)
Figure 3 shows the whole process of the projectile penetrating the reinforced concrete four-layer target board in the finite element model. Different from the test state in [10], it is a state where the actual simulated missile body invades the target from the top, and the direction of gravity is adjusted to the horizontal direction. The basic parameters are set as follows: the initial velocity of the projectile is $v_0 = 1000$ m/s, and the angle of attack is $0^\circ$; the thickness of the first layer of concrete target is 300 mm, and the 3 other plates' thickness is 180 mm. The angle ($\theta_0$) between the target plate and the YZ plane is $20^\circ$. The concrete and reinforcement parameters are the same as those in Table 1.

### 3. Analysis of Factors on Penetration in Multi-layer Steel Target

#### 3.1. Projectile Penetrating into Multilayer Target

Figure 3 shows the whole process of the projectile penetrating the reinforced concrete four-layer target board in the finite element model. Different from the test state in [10], it is a state where the actual simulated missile body invades the target from the top, and the direction of gravity is adjusted to the horizontal direction. The basic parameters are set as follows: the initial velocity of the projectile is $v_0 = 1000$ m/s, and the angle of attack is $0^\circ$; the thickness of the first layer of concrete target is 300 mm, and the 3 other plates' thickness is 180 mm. The angle ($\theta_0$) between the target plate and the YZ plane is $20^\circ$. The concrete and reinforcement parameters are the same as those in Table 1.
According to Figure 3, the deflection angle of the projectile during the penetration of the first layer of the target board is 0.16°, and the residual velocity of the projectile in the x-axis direction is 987.0 m/s. As the projectile passes through the fourth layer of the target board, the body deflection angle is enlarged to 1.23°, and the residual velocity of the projectile is 966.52 m/s.

The time-history curve of the projectile acceleration in Figure 4 (a) shows that the first-layer target has greatest resistance to the projectile, while the subsequent three-layer thin-target resistance peaks tend to be lower but consistent. This is because after the penetration speed is reduced, the ratio of the static resistance item becomes larger, and the penetration resistance is less affected by the reducing projectile velocity. From Figure 5, it reveals that the ballistic tunnel is approximately a circle, and the diameter of the tunnel of the first-layer target plate is slightly larger than that of the other 3 layers. For the sake of visualization, an auxiliary cross cursor at the initial impact point [14]. From the position relationship between the initial impact point of the projectile and the damage opening of each layer of target plate is added, it can be seen the projectile trajectory has a tendency to gradually shift upward.
3.2. Effect of Inclination

The initial horizontal velocity of the projectile is 1000 m/s, and the angle of attack is 0°. Since ricochet are liable to happen if the oblique angle and yaw are too large to neglect [15]. The initial inclination angles \( \theta_0 = 10^\circ, 15^\circ, 20^\circ, 25^\circ, \) and \( 30^\circ \) are selected for parametric analysis.

Figure 6 shows the change of the deflection angle of the projectile after passing through the target plate at different initial inclination angles. When the inclination angle is 10-20°, the deflection angle of the projectile is very small, and the maximum deflection angle is only 1.23°. In terms of difference, the difference between the deflection angles between different tilt angles is within 1°. When the initial inclination of the projectile is 25-30°, the deflection angle of the projectile during the penetration process is significantly enlarged, and the deflection angle of each layer is more than 60% larger than the previous layer, and the maximum deflection angle reaches 6.2°.

Figure 7 shows the velocity change of the projectile at different inclination angles. When the same inclination angle penetrates through four layers of reinforced concrete target plates, the speed in the x-axis direction changes almost linearly, and the speed decreases by approximately 7% after passing through each layer of target plates. There is little difference in the speed of the x-axis direction between different inclination angles. The difference between the final residual velocity of the inclination angle of 10° and the inclination angle of 30° is only 4.3 m/s, i.e., effect of the inclination angle on the speed drop is not very obvious.

![Figure 6. Deflection angle of the lower projectile at different inclination angles](image)

![Figure 7. Residual velocity of the projectile at different inclination angles](image)
3.3. Effect of Attack Angle

Under 1000 m/s initial horizontal velocity and no inclination angle, the initial attack angles $\delta = 1^\circ$, $2^\circ$, $3^\circ$, $4^\circ$, and $5^\circ$ are selected for parameter analyses.

![Figure 8. Deflection angle of the projectile at different angles of attack](image8.jpg)

Figure 8. Deflection angle of the projectile at different angles of attack

![Figure 9. Residual velocity of the projectile under different attack angles](image9.jpg)

Figure 9. Residual velocity of the projectile under different attack angles

It can be observed from Figure 8 that the angle of attack has a great influence on the deflection angle of the projectile penetration. When the initial angle of attack is only $1^\circ$, the projectile still produce a large deflection. When penetrating the same layer of target plate, each time the initial angle of attack increases by $1^\circ$ leading to 20% increase of projectile deflection angle.

Figure 9 suggests that as the projectile penetrates the first two layers of targets, the difference in the residual velocity of the projectile in the x-axis direction is very small whereby the maximum residual velocity difference is only 3 m/s. According to the reduction of the velocity of the projectile in the x-axis direction, the penetration attack angle can be divided into two ranges: 1-3° and 3-5°. Penetrating the same concrete target plates, the projectile velocity decreases linearly for 1-3°attack angle range, meanwhile the velocity drops more dramatically for 3-5° attack angle.

3.4. Effect of Initial Velocity, Target Thickness, and Target Distance

It is important to have a comprehensive understanding of the missile penetrating the multilayer target taking more parameters into account. Considering the effect of the angle of attack on the penetration of the multilayer target by the missile, it is necessary to study the following three factors of the initial velocity of the missile: the thickness of the target, and the distance between the targets.
3.4.1. Effect of Initial Velocity

With 1° initial projectile attack angle and no inclination angle, the initial velocity $v_0 = 600, 800, 1000$ and 1200 m/s are selected for simulation. It is observed from Figure 10, the smaller initial velocity causes greater projectile deflection angle. For larger initial velocity case, the projectile velocity decreases more dramatically after passing through the target plates, as shown in Figure 11. This is because the penetration resistance is significantly greater when penetration velocity is large [16].

![Figure 10. Deflection angle of the projectile at different initial speeds](image)

![Figure 11. Residual velocity of the projectile under different initial velocity penetration](image)

3.4.2. Effect of Target Thickness

With 1° initial attack angle and no inclination angle, the initial velocity with 1000 m/s is studied herein. The thickness of the first layer target plate $t_1 = 200$ mm, 300 mm, 400 mm (corresponding to the target thickness $t_2 = 120$ mm, 180 mm, 240 mm) are numerically investigated.

It can be seen from Figure 12 that the deflection angle of the projectile increases with the thickness of the target plate. For the same layer of target plate, the deflection angle of the projectile through the 300 mm thickness target plate is about 2 to 2.5 times the thickness of 200 mm. For the same layer, the deflection angle of the projectile through the 400 mm thickness target plate is about 300 mm. It can be seen from Figure 13 that when the bullet penetrates the first three layers of the target plate, the velocity in the x-axis direction changes linearly, and when it penetrates the fourth layer, the speed significantly decreases.

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3.4.3. Effect of Initial Velocity

With $1^\circ$ initial attack angle, $0^\circ$ inclination angle and $1000$ m/s initial velocity, and the target plate spacing $s = 2000$ mm, $3000$ mm, $4000$ mm is selected for simulation.
It can be seen from Figure 14 that the deflection angle of the projectile increases with the increase of the target plate spacing. For the same target plate spacing, the deflection angle of this layer is about twice that of the previous layer. As for the target plate, there is a linear growth relationship between the projectile deflection angle and the target distance. It can be seen from Figure 15 that under 1° attack angle, the speed change in the x-axis direction is roughly linear when the target plate spacing is between 2000 mm and 4000 mm. As the projectile penetrates the fourth-layer target board, the speed change no longer conforms to the previous linear relationship, and the speed decreases even more dramatically.

4. Establishment of GA-BP Neural Network Prediction Model

Artificial neural network is a kind of intelligent algorithm that is established by memorizing and processing information on the neural network of the brain. The BP algorithm is a multi-layer learning error back propagation algorithm, and the genetic algorithm introduces the genetic and evolutionary mechanisms of the biological world into the process of simulation calculation, and randomly searches for the global optimal solution by simulating the process of natural evolution. In recent years, BP neural network models based on genetic algorithms have been widely used in the field of nonlinear problem prediction [17-19].
4.1. Neural Network Model Design

The BP neural network model is established based on MATLAB software which structure is shown in Figure 16 [20]. Seven neural units are set in the first layer (input layer) to correspond to the seven penetration impact factors to be considered in training: the initial velocity of the projectile ($v_0$), initial angle of attack ($\theta$), initial angle of inclination ($\delta$), target thickness of the first layer ($t_1$), remaining target thickness ($t_2$), target distance ($s$), number of target layers ($n$); at the output layer of the network There are two neural units: the horizontal velocity of the projectile ($v_x$) and the deflection angle ($\alpha$). In the model, the transfer function of the second layer (hidden layer) is selected as the tansig function. It uses its own saturated nonlinearity and differentiability to enhance the ability of network model nonlinear mapping. The transfer function of the third layer (output layer) is selected as the ‘purelin’ function, which can make the output value of the network any value.

4.2. Definition of Initialization Parameters

(1) Selection of initial weight and threshold

For a general BP neural network, the initial weights and thresholds are randomly selected in the interval (-1, 1). This paper uses genetic algorithm to optimize the BP neural network [18, 21]. The initial population is defined as 50, the number of evolutions is 100, the crossover probability is 0.8, and the mutation probability is 0.09. The optimal individual obtained is decoded as the initial weight and threshold of the BP neural network.

(2) Selection of learning rate

The size of the learning rate can directly determine the magnitude of the weight changes that the network model generates in each training. Too much learning efficiency will cause network instability and even network paralysis. The lower learning efficiency will make the convergence speed of the network model during training very slow. Generally speaking, the value of learning efficiency is between 0.01-0.8, and the learning rate is chosen as 0.01 in this paper.

(3) Selection of expected error

The training stops when the error value of the network training reaches the specified limit. When the value of the expected error is too small, it is difficult to reach the standard during the network training process, and even “overfitting” may occur. When the value of the expected error is too large, the accuracy of the network model is difficult to meet the actual needs. In this work, the expected error is 0.0001.

(4) Selection of training steps

A larger number of training steps can make the training more accurate. Improper parameter setting and an increase in the number of training steps can only cause the network training model to diverge. On the premise that the above models and parameters have been determined, the maximum number of training steps is finally determined to be 10,000, and the output is defined to be displayed every 50 steps.

4.3. Selection and Processing of Training Samples

The quality of the neural network model and the strength of its prediction ability are based on the training of a large amount of accurate data, so the selection of accurate and reliable training sample data is crucial for the establishment of the neural network. The 263 sets of data obtained from the parameter analysis were extracted and divided into two groups, one of which was 250 data for training the established GA-BP neural network model, and the other was 13 data as a pair Detection of network model accuracy. The variation range of the training data of the neural network is as follows: (1) initial tilt angle ($\theta_0=10°, 15°, 20°, 25°, 30°$); (2) initial angle of attack ($\delta=1°, 2°, 3°, 4°, 5°$); (3) Initial speed ($v_0=600, 800, 1000, 1200$ m/s); (4) First layer target thickness ($t_1=200, 300, 400$ mm); (5) remaining target thickness ($t_2=120, 180, 240$ mm); (6) target distance ($s=2000, 3000, 4000$ mm); (7) number of layers ($n=1, 2, 3, 4$).

The data samples used for network testing are shown in Table 2. The 13 sets of data are not included in the training data samples, thereby ensuring that the network model has reliable accuracy.

4.4. GA-BP Neural Network Prediction and Result Analysis

Call the sim function to predict the reserved test data samples. The predicted values calculated by the network are compared with the actual test output values. The specific values are shown in Table 3. The result of comparison shows that the residual velocity error is within 5%, and the attitude angle of the projectile does not exceed 11.2%. It can be considered that the GA-BP neural network model trained in this paper is suitable for the prediction of the projectile penetrating the multilayer concrete target. It worth noting that the combined influence of initial inclination and attack angles is larger than a single factor since more complicated loading is acting on the projectile body. Moreover, it
reveals that the combined effect of initial inclination and attack angles may neutralize the deflection effect. This phenomenon has been observed by Gao and Li [22, 23] which declares that a proper negative attack angle which can minimize the trajectory turning in oblique penetration cases.

Table 2. Sample test data of the network model

| Number | \(v_0\) (m/s) | \(\delta\) (°) | \(t_1\) (mm) | \(t_2\) (mm) | \(t\) (mm) | \(\theta_b\) (°) | \(n\) | \(v_r\) (m/s) | \(\alpha\) (°) |
|--------|--------------|----------------|-------------|-------------|-----------|---------------|-----|-------------|-------------|
| 1      | 1000         | 0              | 300         | 180         | 3000      | 10            | 1   | 987.7       | 0.14        |
| 2      | 1000         | 0              | 300         | 180         | 3000      | 20            | 4   | 966.52      | 2.45        |
| 3      | 1000         | 0              | 300         | 180         | 3000      | 30            | 4   | 963.46      | 10.49       |
| 4      | 1000         | 2              | 300         | 180         | 3000      | 0             | 4   | 957.36      | 20.75       |
| 5      | 1000         | 4              | 300         | 180         | 3000      | 0             | 3   | 966.59      | 18.22       |
| 6      | 1000         | 5              | 300         | 180         | 3000      | 0             | 4   | 933.57      | 34.37       |
| 7      | 600          | 1              | 300         | 180         | 3000      | 0             | 3   | 572.68      | 11.58       |
| 8      | 1200         | 1              | 300         | 180         | 3000      | 0             | 4   | 1162.36     | 13.27       |
| 9      | 1000         | 1              | 400         | 240         | 3000      | 0             | 2   | 972.73      | 4.68        |
| 10     | 1000         | 1              | 300         | 180         | 2000      | 0             | 3   | 974.56      | 6.65        |
| 11     | 1000         | 1              | 300         | 180         | 3000      | 20            | 1   | 986.98      | 1.8         |
| 12     | 1000         | 2              | 300         | 180         | 3000      | 20            | 2   | 979.67      | 6.97        |
| 13     | 1000         | 3              | 300         | 180         | 3000      | 20            | 4   | 943.24      | 31.53       |

Table 3. Comparison of network predictions and test values

| Number | \(v_r\) (m/s) | \(\alpha\) (°) | \(\text{Forecast data}\) | \(\text{Test Data}\) | \(\text{Error (\%)}\) | \(\text{Forecast data}\) | \(\text{Test Data}\) | \(\text{Error (\%)}\) |
|--------|--------------|---------------|---------------------------|-----------------------|------------------------|---------------------------|-----------------------|------------------------|
| 1      | 987          | 0.14          | 987.7                     | -0.07                 | 0.15                   | 0.14                      | 6.25                  |
| 2      | 964.3        | 2.45          | 966.52                    | -0.22                 | 2.7                    | 2.45                      | 10.2                  |
| 3      | 964.1        | 10.49         | 963.46                    | 0.06                  | 9.8                    | 10.49                     | -6.57                 |
| 4      | 956.3        | 20.75         | 957.36                    | -0.11                 | 21.2                   | 20.75                     | 2.16                  |
| 5      | 968.3        | 18.22         | 966.59                    | 0.17                  | 17.6                   | 18.22                     | -3.4                  |
| 6      | 937.6        | 34.37         | 933.57                    | 0.43                  | 33.5                   | 34.37                     | -2.53                 |
| 7      | 571.8        | 11.58         | 572.68                    | -0.15                 | 11.3                   | 11.58                     | -2.41                 |
| 8      | 1162.2       | 13.27         | 1162.36                   | -0.01                 | 13.4                   | 13.27                     | 0.97                  |
| 9      | 973.2        | 4.68          | 972.73                    | 0.04                 | 4.4                    | 4.68                      | -5.98                 |
| 10     | 974.5        | 6.65          | 974.56                    | -0.006                | 6.7                    | 6.65                      | 0.75                  |
| 11     | 986.1        | 1.8           | 986.98                    | -0.08                 | 1.6                    | 1.8                       | -11.11                |
| 12     | 979.4        | 6.97          | 979.67                    | -0.02                 | 6.9                    | 6.97                      | -1                   |
| 13     | 941.2        | 31.53         | 943.24                    | -0.21                 | 32                    | 31.53                     | 1.49                  |

5. Conclusions

Based on the LS-DYNA numerical simulation software, a finite element model for the projectile penetrating the reinforced concrete multilayer target is established, and the model results are verified with experiments. 7 penetration factors: including the initial velocity \(v_0\), initial angle of attack \(\delta\), initial tilt angle \(\theta_b\), target thickness of the first layer \(t_1\), remaining target thickness \(t_2\), target distance \(t\), and number of target layers \(n\) are investigated to analyze their effects on the projectile residual velocity \(v_r\) and deflection angle \(\alpha\). Based on GA-BP neural network, a prediction model of projectile penetrating reinforced concrete multilayer targets is then proposed. The main conclusions are drawn as follows:

- A single parameter angle of attack has a greater effect on the deflection angle of the projectile penetration. When the attack angle is 1°, the projectile still produces a large deflection angle. When penetrating the same layer of target plate, each time the attack angle increases by 1° while the deflection angle of the projectile increases by about 20%. With a single parameter, the projectile deflection angle is negligible when the inclination of the projectile is 10-20°. When the initial inclination of the projectile is 25-30°, the deflection
angle of the projectile during the penetration process is significantly enlarged, and the inclination angle is highly related to the velocity. The effect of projectile falling down is not obvious.

- Under 1° initial attack angle, the projectile velocity changes linearly in the x-axis direction as it passes through the first three layers of target plates under the combined influence of different parameters such as target plate thickness and target plate spacing. During penetration the fourth concrete layer, the projectile velocity decreased significantly.

- The GA-BP neural network model established in this paper has good prediction ability for residual velocity and deflection angle of the projectile penetration in reinforced concrete multilayer target plates.

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7. Conflicts of Interest

The authors declare no conflict of interest.

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Study of a Highly Effective and Affordable Highway Interchange - ITL Interchange

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Abstract

In this paper we present a new solution for the highway interchange, which represents the best compromise between the traffic capacity, the land area used and construction cost. The difference between the known and the new design solution is in the implementation of the opposite directional ramps which are widely separated in the area of the interchange. In the middle, between the directional ramps, some space is created for the left directional ramps. Interchange should be used for four-way highway interchanges or other heavy traffic roads junction in order to increase the capacity and traffic safety at the crossing point. It has no conflict points. ITL Interchange left directional ramps is much shorter than all other known solutions for interchanges. The interchange is built in two levels. These two facts significantly lower the cost of construction. The study compares different types of interchanges. We made a geometric comparison and performance measures. In geometric comparison, the greatest advantages of the ITL interchange are the shortest overall roadway length and the shortest overpasses length. Therefore, such an interchange is advantageous in terms of construction and maintenance costs. When measuring performance, ITL Interchange achieves the best results regardless of the number of vehicles.

Keywords: Highway; ITL Interchange; Left Directional Ramp; Traffic Capacity.

1. Introduction

Modern highway interchanges and other heavy traffic roads interchanges have to ensure the highest possible traffic safety and capacity. As with intersections, left-turning traffic movements are the most challenging to accommodate at interchanges. At interchanges between freeways, or other full-access control facilities, a directional interchange offers the highest level of service by directly serving all movements with minimal or no reductions in speed.

1.1. Types of Interchanges

The most common interchange type is the diamond interchange, named for its diamond shape when viewed from above \cite{4}. The diamond interchange is common because of its economical design and construction, but is limited in capacity. A cloverleaf interchange is typically a two-level, four-way interchange where all turns across opposing traffic are handled by non-directional loop ramps. Assuming right-handed traffic, to go left vehicles first cross over or under the target route, then bear right onto a sharply curved ramp that turns roughly 270 degrees, merging onto the target route from the right, and crossing the route just departed. These loop ramps produce the namesake cloverleaf.
shape. Two major advantages of cloverleaves are that they require only one bridge which makes such junctions inexpensive as long as land is plentiful. The cloverleaf involves weaving maneuvers. When the weaving volume in a particular weaving section exceeds 1,000 veh/h, the quality of service on the main facility deteriorates rapidly, thus generating a need to transfer the weaving section from the through lanes to a collector-distributor road [6].

In the increasingly dense population areas, interchanges must network two major highways, rather than a major highway and a lesser surface street. The Stack interchange accommodates lesser conceptual. The stack is a massive complex of two pairs of left-turning ramps stacked at an imposing height in a network configuration above, below or even between the two interchanging highways. A stack interchange can be far more expensive to construct and take up considerably more space than conventional interchanges, but it can be far safer [5].

Turbine interchange design circles all left-turning traffic around a central bridge in a counterclockwise direction, like a whirlpool, allowing a high volume of traffic to travel between two interstates at highway speed. Since it features smaller bridges with smaller supports and lower roadway profiles than a traditional interchange, a turbine interchange has less impact to traffic during construction, and costs less to build and maintain than other types of conventional interchanges.

A new two-level interchange of a unique design called Pinavia is the latest generation of interchanges. Pinavia is functionally like a conventional four-level stacked interchange: transport flows do not intersect, the driving speed in all directions can be equal to the speeds of the intersecting roads, and the design allows arbitrary capacity in any direction. The Pinavia design makes it possible to utilize the center area of the junction making it unique in its class [2].

1.2. New, Effective and Affordable Highway Interchange

An interchange is the most costly type of intersection. The combined cost of the structure, ramps, through roadways, grading and landscaping of large areas, and possible adjustments in existing roadways and utilities generally exceeds the cost of an at-grade intersection [7]. We present a new solution for the highway interchange, which in most comparisons achieves very good and, in many things, the best results. The characteristic of this interchange is that in the area of the interchange the opposite carriageways of a single highway (roads) are separated to the extent that in the middle there is space for left directional ramps. That's where the name comes from: Inside Turning Left Interchange (ITL Interchange).

Figure 1. ITL Interchange with driving directions

2. Basic Characteristics of Design ITL Interchange

2.1. Purpose

ITL Interchange should be used for four-way interchanges or other heavy traffic roads junction in order to increase the capacity and traffic safety at the crossing point. ITL Interchange is suitable for interchanges where traffic is approximately evenly distributed in all traffic directions.
ITL Interchange has no conflict points. It is less suitable for roads where most vehicles drive straight ahead and only a few vehicles turn right or left.

ITL Interchange left turning ramps is much shorter than all other known solutions for interchanges. The interchange is built in two levels. These two facts significantly lower the cost of construction.

2.2. Innovation

Innovation is shown in the fact that in the area of the interchange the opposite carriageways of a single highway (roads) are separated to the extent that in the middle there is space left for directional ramps.

![Figure 2. Area for left turning ramps](image)

In the known solutions, the left directional ramp in the first part of the turn is to the right. Then, the longer turn to the left, as the turn angle is at least 140° or more. In the final part, there is again a turn to the right. ITL Interchange has a left directional ramp with only one turn left. The entire horizontal angle of the ramp is 90°. Therefore, the length of the left directional ramp in this case is significantly shorter.

![Figure 3. Comparison of the length of the left directional ramps](image)

2.3. Designing the ITL Interchange

2.3.1. Vehicles Sorting Before the Interchange

At a sufficient distance before the interchange on the highway (at least 1500 m), it is necessary to limit the speed and inform the drivers with the vertical and horizontal signalling which lane leads to which traffic direction. This also helps avoid unnecessary weaving within the interchange and prepare drivers for timely sorting.
The ITL Interchange is suitable where traffic is approximately evenly distributed in all directions. The inner lanes lead to left directional ramps. Vehicles that turn to the left do not change the lane. Vehicles driving straight or turning to the right, move to the right-hand lanes before the interchange.

2.3.2. Level Change of the Slip Road for Turning to the Left

Left directional ramp has to remain on the unchanged level until it crosses both of the left directional ramps at the opposite level. This length is about 2/3 of the entire length of the directional ramp. Therefore, there is a very short distance to pass to come to the opposite altitude level. Sharp vertical convex and concave curves allow significantly lower speeds than allowed by a horizontal turn. In order to mitigate vertical curves, the first part of the left directional ramp at the upper level is additionally raised. On the lower level, the situation is reversed. In the first part, the left directional ramp is additionally deepened.

Thus, at the upper level, the highest point is reached at 1/3 of the total length of the left directional ramp. From this point onward, the ramp can be steadily lowered to reach the opposite level. On the lower level, the situation is reversed. The schemes below show the solutions.

![Figure 4. Directional lanes](image)

![Figure 5. Left directional ramp – Ride downhill](image)

![Figure 6. Left directional ramp – Ride uphill](image)
3. Geometry Comparison of Interchanges

Comparison is made for interchanges which allow higher speeds also on the left directional ramps and thus ensure greater traffic capacity. These interchanges also have no conflict points. This group includes: Stack Interchange, Turbine and Pinavia.

There are also other types of interchanges. However, at these interchanges, a crucial speed reduction is required when turning to the left. These interchanges are: Cloverleaf, Contraflow Left, Diverging Windmill ... Due to the low cost of construction, the Cloverleaf is included in the comparison. However, for the same area of the entire interchange as ITL Interchange, the Cloverleaf has a much lower speed limit for turning to the left. The Cloverleaf also has conflicting points, while other interchanges do not.

Comparison is made for interchanges with horizontal radius for the left directional ramp R=250 m. This radius allows driving at a speed of 80 km/h. In case of the Cloverleaf on the same area, horizontal radius is R=100 m for turning to the left.

Parameters:
- Radius of the horizontal circular curve for left directional ramps R=250 m (Cloverleaf R=100 m).
- Maximum transverse inclination 7%.
- Vertical rounding with a convex radius of 2000 m and a concave radius of 1500 m.
- Maximum longitudinal inclination 6%.
- Altitude difference between individual levels 6 m.
- Speed limits 80 km/h.

![Figure 7. Schemes of interchanges](image)

3.1. Area

The smallest area is needed for the Stack Interchange, 18.5 ha. On the other hand, the largest area is needed for the Turbine. This interchange extends at 58 ha. The area for other interchanges is 33.5 ha.

![Figure 8. Area comparison](image)
3.2. Lengths of Ramps and Overpasses

Stack Interchange, Turbine and Cloverleaf have a completely straight line when driving through. ITL Interchange has a slightly longer distance due to the separation of carriageways. Pinavia has an even longer distance because lanes run along the circle.

Construction for right directional ramps is similar in all cases. ITL Interchange and Stack Interchange have the shortest length of ramps. The Cloverleaf and Pinavia have an approximately double length, and Turbine, due to its size, has about a triple length according to the most favourable variants. However, construction for left directional ramps totally differs. There are the greatest differences between compared interchanges. Ramps mostly lead over the overpasses. ITL Interchange has an extremely short length of ramps. A little longer distance is in the Cloverleaf, but due to the small radius, there is a lower speed limit. The distance is greater by factor 2 on Stack Interchange and more than by factor 3 on Pinavia and Turbine.

Cloverleaf has the shortest length of overpasses. However, it has lower speed limits for turning to the left and some conflict points. At other compared interchanges, ITL Interchange has the shortest length of overpasses. The distance of overpasses is greater approximately by factor 2.5 on Stack Interchange and Turbine. Pinavia has by far the highest length of overpasses. Compared with ITL Interchange, the factor is more than 5. More technical data for each interchange and comparison with horizontal radius $R=250$ m. This radius allows driving at a speed of 80 km/h.

| Characteristics of interchange | ITL Interchange | Stack Interchange | Turbine | Pinavia | Cloverleaf (*A) |
|-------------------------------|----------------|------------------|---------|---------|----------------|
| Arc through (m)               | 250            | 0                | 0       | 250     | 0              |
| Arc turn right (m)            | 250            | 250              | 250     | 250     | 250            |
| Arc turn left (m)             | 250            | 250              | 250     | 250     | 100            |
| Area of interchange (ha)      | 33.5           | 18.5             | 58      | 33.5    | 33.5           |
| Number of levels              | 2              | 4                | 2       | 2       | 2              |
| Road distance                 |                |                  |         |         |                |
| Road distance straight (m)    | 1.360          | 1.300            | 1.300   | 1.420   | 1.300          |
| Road distance right (m)       | 330            | 390              | 1.070   | 680     | 590            |
| Road distance left (m)        | 395            | 805              | 1.295   | 1.415   | 460            |
| Road distance total (m)       | 8.340          | 9.980            | 14.660  | 14.060  | 9.400          |
| Overpasses distance           |                |                  |         |         |                |
| Overpasses dist. straight (m) | 620 /200*(C)   | 100              | 100     | 3.060   | 100            |
| Overpasses dist. right (m)    | 0              | 0                | 0       | 0       | 0              |
| Overpasses dist. left (m)     | 790            | 3.220            | 4.140   | 4.600   | 0              |
| Overpasses dist. total (m)    | 1.410 /990 *(C) | 3.320           | 4.240   | 7.660   | 100            |

(A) The cloverleaf in traffic characteristics is not comparable with the other interchanges. The calculation is added as the simplest version of the interchange.

(B) The outer edge of the road is considered.

(C) The road straight on the upper level can also be carried out mostly after the embankments instead of the overpasses. In this case, we have overpasses in the length of 200 m and the embankments in the length of 420 m.

3.3. Summary

The characteristics of interchanges which stand out with their positive or negative characteristics from other intersections.

Advantages:
- Stack Interchange: the smallest area.
- Pinavia: using the area inside the interchange for other purposes.
- ITL Interchange: the shortest length of ramps.
• ITL Interchange: the shortest length of overpasses.
• ITL Interchange: the lowest cost of construction and maintenance.

Disadvantages:
• Turbine: the largest area.
• Pinavia: very large length of ramps and overpasses.
• Stack Interchange: four-level construction.

4. Performance Measures of ITL Interchange and Comparison with other Types

Traffic simulation techniques have been used since early development of traffic theory. Therefore, delay analysis of ITL interchange has been done by microsimulation software, which we usually use for the analysis of complex traffic problems at intersections and interchanges.

Microsimulation software tool is the ideal for setting up a clear and conclusive knowledge basis for decisions for all kinds of traffic engineering questions and can provide the analyst with valuable information on the performance. The microsimulation has been designed for analysing and modelling transport networks of any size, and traffic systems of all types, from individual intersections right up to entire conurbations. PTV Vissim link-connector structure of the network topology allows for highest versatility and – in combination with detailed movement models – extremely precise traffic flow modelling.

Table 2. O/D Matric – origin/destination matrix of traffic flows in percentage terms

| O/D Matric |   |   |   |
|------------|---|---|---|
| 0.33       |   |   |   |
| 0.33       |   |   |   |
| 0.33       |   |   |   |
| 0.33       |   |   |   |
| 0.33       |   |   |   |
| 0.33       |   |   |   |

Transportation analysis performance measures (outputs of microscopic model) estimate the performance of different interchange designs; including the ITL. Performance measures in analysis was driven by a goal to determine the capacity of ITL interchange and to estimate the comparison between some of the most common used highway interchanges including some new types like Pinavia.

In this paper we focused on Delay, Average Speed and Distance Travelled. We analysed one traffic distribution test matrices (Table 2): \( \rho_1 \) (1/3 of entry traffic crossed the intersection, 1/3 turned left and 1/3 turned right). Performance measures should be sensitive enough to differentiate between analysis scenarios and therefore we used three different load scenarios (2500 veh/h, 3500 veh/h and 4500 veh/h). The fleet composition included in the highway network reflects most common composition on the Highways including passenger cars (90%) and heavy good vehicles (10%). The following assumptions are used:

• Since the ITL interchange presented in this paper only exists on the study stage, no real situation can be observed to calibrate and validate the model according to validation standards (DMRB 12, GEH statistics),
• The vehicle speed at the interchange was modelled according the previous research and recommendations presented in User Manual of Vissim.
• Car Following psycho-physical perception model developed by Wiedemann (1974) was used for all the analysed scenarios,
• The topology of the modelled area used is used with limitation (no additional influence due to acceleration/deceleration),
• The performance of chosen geometry was evaluated according to several measures such as: delay, queue, travel time, distance travelled,
• The Level of service was not calculated, but it can be determined from Average delay.

There is no one-size-fits-all performance measure that can address all the objectives of a design many performance
measures focus only one dimension of a problem while ignoring the other. Too many performance measures for a given design may create conflicts and/or confusion during the evaluation process.

4.1. Results

The results of traffic simulation are shown in Table 3. At lower volumes (2500 veh/h) the performance is almost identical for all interchange designs. For middle volume (3500 veh/h) Cloverleaf and Turbine interchange designs are already over congested with Average Delays higher than 140 s/veh. The Average speed drops below 40 km/h in Cloverleaf and 46 km/h in Turbine design. For highest volume traffic scenario (4500 veh/h) only ITL and Pinavia Interchange can throughput the demand with slightly lower delay of ITL; 10.2 s/veh than Pinavia: 13.6 s/veh. Total Delay time of ITL is 25% lower than Pinavia (51 hours vs 68 hours) and the travel distance of ITL is 3.6% less than Pinavia.

Some measures may not be clearly understandable to the reader of this paper and therefore additional explanation is provided. If we compare Dist. Total (km) in Table 3 for the ITL and Turbine design, there is much less distance travelled for Turbine design, which can lead to misunderstanding that this design has much better performance. In the sum of this measure there are all vehicles that are in the network or have already left it. For Turbine, volume scenario 4500 veh/h, the performance of Average Delay is very high (295.8 s/veh) and therefor many demands are not served and as result much less Total kilometres travelled.
Figure 11. Comparison of Average Speed

Figure 12. Comparison of Total Distance Travelled

Table 3. ITL Interchange vs. Conventional Interchanges – traffic scenarios and performance results

|                  | ITL INTERCHANGE | CLOVERLEAF | PINAVIA | STACK | TURBINE |
|------------------|-----------------|------------|---------|-------|---------|
| (Veh/h)          | 2500            | 3500       | 4500    | 2500  | 3500    | 4500    | 2500  | 3500 | 4500    | 2500  | 3500 | 4500    |
| Delay Avg. (s)   | 3.6             | 5.9        | 10.2    | 5.1   | 193.3   | 859     | 4.6   | 6.8  | 13.6    | 4.4   | 12.9 | 243.2   | 7.6   | 147  | 295.8   |
| Speed Avg (km/h) | 85              | 84         | 82      | 84    | 36      | 11      | 84    | 83   | 80      | 84    | 80   | 33      | 83    | 46   | 30      |
| Dist. Total (km)| 39906           | 55663      | 71506   | 41691 | 46541   | 29304   | 41273 | 57732| 74143   | 39468 | 54989| 56486   | 42260 | 51430| 46844   |
| Travel Total (km)| 471            | 667        | 879     | 496   | 1289    | 2760    | 490   | 695  | 927     | 469   | 687  | 1698    | 510   | 1129 | 1545    |
| Delay Total (h)  | 10              | 23         | 51      | 14    | 751     | 2421    | 13    | 27   | 68      | 12    | 50   | 1045    | 21    | 534  | 1003    |
| Delay Total (h)  | 10              | 23         | 51      | 14    | 751     | 2421    | 13    | 27   | 68      | 12    | 50   | 1045    | 21    | 534  | 1003    |
5. Conclusions

In this paper we analysed new type of ITL Interchange and compared with conventional designs Cloverleaf, Pinavia, Stack, Turbine. ITL Interchange has proven to be a very good or the best choice in all benchmarks.

The geometry comparison concludes:

- The lengths of all ramps at other interchanges are 20-75 % longer than in the ITL Interchange;
- The lengths of all overpasses at other interchanges are from two to five times longer than in the ITL Interchange. In Stack-Interchange, the length of the overpasses is longer by the factor of 2.5, but it has a four-level construction;
- Overpasses incur the highest construction costs. In particular, the ITL Interchange is cheaper to build because it has a significantly lower length of overpasses than other interchanges. Maintenance is much cheaper.

The following conclusions can be made from the Performance analysis:

- For higher traffic volumes (4500 veh/h), the ITL Interchange has better performance and offers much lower delays than conventional types like Clover, Stack and Turbine. Total Delay time of ITL is 25 % lower than Pinavia;
- For lower traffic volumes (2500 veh/h), the ITL Interchange has almost the same Average Delay (3.6 s/veh) than others (from 4.6 s/veh till 7.6 s/veh);
- Average Speed and Total Distance Travelled are much higher for ITL Interchange and it is slightly higher than Pinavia Interchange.

6. Recommendation for Future Research

The safety aspects of the ITL Interchange design need to be studied in detail. A Surrogate safety assessment model (FHWA) is widely used for analysis. The proposed safety model aims at extracting the safety features from VISSIM traffic simulation model by analysing the trajectory of vehicles and estimating their proximity. Another recommendation would be to compare the different load matrix scenario.

7. Conflicts of Interest

The authors declare no conflict of interest.

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Fibers, Geopolymers, Nano and Alkali-Activated Materials for Deep Soil Mix Binders

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Abstract

Ordinary Portland Cement (OPC) and Lime (CaO) have traditionally been used as binder materials for Deep Soil Mix (DSM) ground improvement. Research has been conducted into possible alternatives such as pozzolans to reduce reliance on either cement or lime. However, pozzolans still undergo similar calcium-based reactions in the strengthening process. In this review, further alternative binder materials for soil strength development are explored. These recent developments include fiber reinforcement materials, alkali activation methods, nanomaterials and geopolymers, which can potentially achieve equal or improved performance. Research to date has shown that alkali-activated materials and geopolymers can be equivalent or superior alternatives to pozzolanic supplemented cement binders. The case is made for GP cements which potentially produces 80% less CO\textsubscript{2} than conventional portland cement during manufacture. One-part AAM and GP cements are a promising substitute for portland cement in DSM. A combined approach which incorporates both Ca and alkali activated/geopolymer types of materials and hence reactions is proposed.

Keywords: Reinforcement Fibers; Nanomaterials; Alkali-Activated Materials; Geopolymers; Deep Soil Mix.

1. Introduction

The Deep Soil Mix (DSM) method applies soil stabilization principles, which comprises inserting binder materials with other fillers and mixing together with the soil to form strengthened columns of treated soil below ground. The manufacture of the predominant binder materials, cement and lime, impose significant CO\textsubscript{2} emission and high energy demands. Although studied as a potential supplement and/or partial replacement to reduce the usage of OPC and lime, pozzolanic materials still rely primarily on similar calcium (Ca) reaction processes to produce the same calcium silicate hydrate (C-S-H) and calcium aluminate hydrate (C-A-H) gel products for treated soil compressive strength improvement. In addition, pozzolanic binders react incompletely and require a longer time to realize improvements in the treated soil.

This paper reviews several alternatives to Ca type reactions to improve soil properties for DSM, which offer different pathways for strength / soil properties improvement. The primary soil properties of interest for improvement are 1) shear strength ($S_u$); 2) Compressive strength ($q_u$); 3) Stiffness (Young’s Modulus, $E$); 4) Dynamic properties ($G$, $D$) and 5) Permeability ($k$).

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Reinforcement fibres (natural or synthetic), by mechanical means, improves the stability, increase tensile strength and reduce settlement / lateral deformation of soil [1].

Nanomaterial binders enhance the reaction efficiency of their macro scale counterparts due to the extremely high specific surface areas and surface charges on the binder nano particle [2].

Alkali-activated binder materials utilize a different chemical reaction pathway altogether which does not rely on calcium to develop strength gain [3]. They can be mixed in slurry, utilized in the wet mixed method of DSM as a medium to reach lower soil strata [4].

Finally, Geopolymers are a class of synthetic inorganic alkali aluminosilicate materials with its 3D network polymeric structure which overcomes possible long-term stability shortcomings of alkali-activated materials.

2. Reinforcement Fiber Materials

Adding /mixing of reinforcement fibers offers a mechanical process as opposed to the chemical process of cementitious / pozzolanic binders to improve the properties of soil. The reinforcement binders can be either natural or synthetic in origin.

- Natural fibers are derived from plant-based or cellulosic materials – e.g. barley straw, jute, palm, sisal, bamboo, coconut fibers etc.;
- Synthetic fibers can be any form of man-made plastic, mineral or metal-based material. Examples researched and applied have included polyvinyl alcohol (PVA), polypropylene (PP), polyester (PET), polyethylene (PE), nylon (NL), steel (ST) etc. some of which, can also be derived from waste industrial materials.

Research and studies have been conducted on the contribution of fibers (with varying fiber length (L) and diameter (d), either applied solely or in conjunction with chemical process binders for soil stabilization. Comprehensive reviews were recently conducted for natural and synthetic fibers describing the history, development and applicability to soil stabilization [1, 5]. However, the long-term / permanent requirements of DSM columns may preclude the usage of natural fibers due to their organic and bio-degradable nature. If fibers are applied with DSM methods, it would need to be pre-mixed with a binding agent (typically cement with water) to form in a slurry for injection under pressure into the soil.

Conventionally, polypropylene fibers have been used for control of thermal and shrinkage induced cracks with dosage ranges from 0.6 to 0.9 kg/m3 when added to concrete mixes for crack control [6,7].

Laboratory studies on soil stabilization using OPC as a binding agent and polypropylene fibers on peat soils showed a clear trend that addition of fiber also increased unconfined compressive strength (UCS) in comparison with soil–cement mix alone [6].

Research study on rapid stabilization of weak soils for road and airfield applications compared PP, PET and PVA fibers either alone or with chemical stabilizers in clay. Increased soil strength and toughness was encountered up to a maximum dosage of ~ 1% dry weight. Thereafter, mixing became difficult with soil. Longer fibers increased strength, but the addition of fibers alone was insufficient to meet strength requirements. When combined with other stabilizers (e.g. cement / lime) and in secondary role, the shorter fibers contributed to increased toughness whereas improved
compressive strength was determined by the primary chemical stabilizer. Dispersion of fibers influenced UCS as it may have introduced pockets of weakness/failure planes [8].

Arasan et al. (2015) studied the feasibility of utilizing polymers as a binder for rapid stabilization of sandy soils with DSM by conducting UCS tests on different ratios of polyester-soil mix. UCS was observed to increase with increasing polyester ratio, effective diameter, relative density and curing period. The highest UCS achieved was with 0.6-1.18 mm grain size, 30% polyester ratio and 40% relative density respectively [9].

Laboratory studies testing on fiber reinforced soil cement (FRSC) samples of clay soils in Bangkok, Thailand were conducted to investigate effect on flexural performance (bending strength @ L/15 deflection, \( f_{150} \)) improvement [10]. It was observed that PP fiber performed better than steel fibers – the fully crimped shape of PP fibers achieved greater bond strength than straighter steel fibers. Hence, brittleness in cement-based binders in deep soil mix columns could be improved with fiber reinforcement which increases toughness. Some recent research is listed below:

| Research          | Soil (USCS)                  | Reinf. Fiber / Sec. Binder | Effect AS % Nano Material Increases | Opt. Mix / Max. UCS / Other Improvements |
|-------------------|------------------------------|-----------------------------|------------------------------------|------------------------------------------|
| John Paul & Sneha (2016) [11] | Black Cotton Soil \( q=6.9 \) kPa | **Bamboo**
  \( L=25 \) mm; \( d=0.45 \) mm;
  0.25–1 \% wt. FA
| Bamboo            | Bamboo                      | UCS                         | OMC                              | 1\% fiber + 20\% FA                    |
|                   | Fly Ash (FA) (class F)     | 15–25 \% wt. soil          | MDD                              | ~ 100\% improvement                    |
| Sharma et al. (2017) [12] | Sand                        | **Jute**
  \( L=20 \) mm; \( d=0.3-0.45 \) mm;
  0.5–2 \% wt. soil | UCS                         | OMC                              | 1.5\% fiber                           |
| Cai et al. (2006) [13] | Clayey soil \( q=90 \) kPa  | **Polypropylene**
  \( L=12 \) mm; \( d=0.034 \) mm;
  0.05–0.25 \% wt. soil | UCS                         | Shrinkage (%)                    | 0.25\% fiber + 5\% lime                |
|                   | c = 90 \% kPa; \( \varphi = 19.1\)° | Lime (CaO)                  | c                               | 880 kPa (28 d)                        |
|                   |                             | 2–8 \% wt. soil            | Φ                               | 292.7 kPa; \( \varphi = 45\)°         |
| Estabragh et al. (2011) [14] | Silty Clay (CL) \( q=131 \) kPa @ 13.5\% strain \( \varphi = 27\)° | **Nylon**
  \( L=4 \) mm; \( d=0.44 \) mm;
  10–30 \% wt. | UCS                         | Swelling (%)                    | 30\% fiber                            |
|                   |                             | Cement (OPC)                | Cc                              | 241 kPa @ \( \varepsilon=20.2\)\%      |
|                   |                             | 15–30 \% wt. soil          | Φ                               | \( \varphi = 44\)°                     |
| Kalantari and Huat (2008) [6] | Peat \( q=28.5 \) kPa CBR=0.78\% | **Polyprop. (PFSC)**
  \( L=58 \) mm (L) | UCS                         | –                             | 15-50\% OPC                           |
|                   |                             | **Steel fiber. (SSFSC)**
  \( L=60 \) mm (L) | Flexural strength           | –                             | 77–400 kPa (28 d)                      |
|                   |                             | \( \varnothing = 5.0,75 \) & 1 \% vol. | PP better than steel | CBR=19–35\% (90 d)                    |
|                   |                             | Cement (OPC)                | Short fiber better than long fiber| –                                             |
|                   |                             | 10–20 \% wt. soil          | \( f_{150}^D = 0.14 \) MPa (SSFSC-S1.0) |                                                 |
| Sukontasukkul and Jamsawang (2012) [10] | Clay (Bangkok) Su=15.6 kPa \( q=31.2 \) kPa | **Polyprop. PP6 | 1.25 MPa (28 d) |
|                   |                             | PP12                       | @ MC=70\%                        | \( f_{150}^D = 0.20 \) MPa (PFSC-L1.0) |
|                   |                             | L=6 mm | 12 mm | \( f_{150}^D = 0.11 \) MPa (SSFSC-L1.0) |
|                   |                             | Polyvinyl alcohol PVA6 | 1494 kPa (PVA6) | \( f_{150}^D = 0.14 \) MPa (SSFSC-S1.0) |
|                   |                             | PVA12                      | 1240 kPA (PPL6)                   | –                                             |
|                   |                             | L=6 mm | 12 mm | \( f_{150}^D = 0.07 \) MPa (SSFSC-L1.0) |
|                   |                             | 0–0.32 \% vol. soil       | 1445 kPA (PVA12)                  | –                                             |
|                   |                             | Cement (OPC)                | 1354 kPA (PPL12)                  | –                                             |
|                   |                             | 20–30 \% wt. soil          | –                               | –                                             |

3. Nanomaterials (nM)

3.1. Reaction Mechanism

Nanomaterials are defined as physical substances with at least one dimension from 1 to 150 nm (1 nm = 1 × 10^-9 m) [16]. Nanomaterials can be produced through the following approaches:
• “Top Down” approach whereby larger particles are scaled down in size to nano range of dimensions whilst maintaining original properties without resorting to “atomic scale level of control or manipulation (e.g. electronics industry miniaturization of computer chips). Nano scale versions of pozzolans can be produced mechanically with pulverizing techniques using high energy ball milling [17];
• “Bottom Up” approach (known also as molecular nanotechnology) whereby materials are assembled from singular atoms or molecules.

Nanomaterials have been proven to enhance the performance of concrete [18, 19] – e.g. with the addition of nano-silica (nS), concrete compressive strength can increase by up to 30% [20]. Improvements in the flexural strength and elasticity (Young’s modulus, E) can be achieved by introducing Carbon nanotubes (CNT) [21].

The application of nano materials has been considered as a potential binder material in soil improvement [2, 22]. The primary characteristics from nanomaterials that induce soil improvement can be described below [23]:
• Particle size – As the particle size approaches or decreases to less than light wave wavelength (De Broglie wave), the periodic boundary condition of the particle is destroyed, and surface atomic density decreases, leading to different physical properties from that at the micro or macro scale;
• Microstructure – which can be categorized into 2D structured nano tubes and 3D structured nano particles. The two categories induce different improvement effects on the soil;
• Particle surface area – likewise, the specific surface area of the particle increases, which leads to greater ion exchange capacity and increase interaction with other particles.

Furthermore, since the nanomaterial will need to be mixed in some form of solution prior to injection into the soil, the rheological suspension properties in solution will have also an influence on dispersion and enhancement effect into the soil. Nanomaterials applications and understanding of it is still in its infancy – it has only been recently researched as a potential additive for concrete and many developments would still be under commercial consideration [21]. Some examples of recent research are compiled in Tables 2 to 4.

3.2. Carbon Nanotubes (CNT)

Carbon nanotubes (CNT) are tube-shaped carbon materials where the diameter of the tube is measured in the nanometer scale [16]. CNTs can be up to several millimeters in length and can be arranged in one-layer walls (known as Single-wall carbon nanotubes – SWCNT) or multi-wall structures (known as Multi wall carbon nanotubes – MWCNT). In general, CNTs have 5 x Young’s modulus (E) and 8 x the strength of steel at 1/6 the density of steel. This strength is due to the covalent sp² bonds formed between the individual carbon atoms. Thus, there can be potential gains in increased flexural strength and improved control of crack propagation with CNT enhanced concrete and by extension, to soil treated with a combination of a primary binder (e.g. cement) and CNT.

![Figure 2. Schematic Structure of SWCNT and MWCNT [24]](image)

Due to the size and fineness of CNTs, it is possible to distribute/disperse on a finer scale within concrete than for micro reinforcement fibers, thus CNT infused composites can achieve greater compressive and flexural strengths. A comparison on flexural and compressive strengths achieved from the research by Kahidan and Shirmohammadian [25] showed up to 19% compressive and 25% flexural improvement. This is supported by Sáez de Ibarra et al. [26] who reported 80-90% increase in E_{concrete} with the addition of only 0.10-0.20% MWCNT/SWCNT by cement weight and Cwirzen et al. [27] reporting 50% improvement in compressive strength with 0.045 – 0.15% MWCNT by cement weight.

Direct addition of nanocarbon filaments to sandy soil mixed with bentonite in proportions ranging from 0.05 to 0.2% of total dry weight of soil resulted in dry density increase and subsequent decrease in soil shrinkage / expansive strains [28, 29]. This is compared with fiber reinforcement addition to soil which also reduced soil cracks but increased hydraulic conductivity. It is suggested by Taha et al. [30] that the better dispersion of the CNT additives
would provide the potential to overcome these desiccation cracks in soil associated when using fiber reinforcement and binder.

The potential for utilizing CNT together with binder material as deep soil mixing supplement has not been explored at depth. The present high expense of carbon nanotubes may have a deterring effect from the application in this field [21]. In addition, challenges faced with consistent dispersion of the CNT needs to be overcome when applied to soil stabilization [30]. Correia and Rasteiro [31] reported adding a surfactant to the blended solution of MWCNT/OPC in improving the dispersion and achieving higher UCS and Youngs Modulus (E).

3.3. Nano Titania (nTiO2R) / Nano Fly Ash (nFA)

Nano Fly Ash enhances the activation of pozzolanic reaction and further densifies concrete like its non-nano counterpart [32]. Babu and Joseph [33] conducted research to study the effect of Nano Titanium Dioxide (nTiO2) and Nano Fly Ash (nFA) on properties of soft soil (Silty clay of USCS classification CH-MH). With increasing nano material additive (from 0% to 2%), the following improvements were observed:

- Atterberg limits – decreased LL;
- Compaction – increased MDD and decreased OMC;
- Strength – increased shear strength (and consequently, UCS);
- CBR and Settlement – improved CBR values and reduced settlement.

3.4. Nano Clay (nC)

Nano Clays (nC) can be defined as nanoparticles of layered mineral silicates also commonly known as phyllosilicates. Some Nano Clays are:

- Montmorillonite Nano Clays – this is the most common Nano Clay, consisting of ~ 1 nm thick alumino silicate layers with lateral dimensions ranging from few hundred nM to ~ 10 μm, combined into large stacks;

![Figure 3. Schematic Structure of Montmorillonite Nano Clay [34]](image)

- Halloysite Nano Clays – naturally occurring aluminosilicate nanotube with a wall thickness of 10-15 atomic aluminosilicate sheets, an outer diameter averaging 50 nM, an inner diameter of 12–15 nM, and length of 0.5–1 μm.

![Figure 4. Halloysite Nano Clay nanotube structure](image)
Ali et al. [35] studied the potential use of nC (montmorillonite) to increase the strength of contaminated soil. Soil contaminated with kerosene experienced reduction in UCS down to 61% of original UCS depending on kerosene %. However, the addition of nC up to 2% for contaminated soil and 1% for uncontaminated soil increased the bearing capacity of the soil. Increase in LL, PL and shear strength of silty soils was observed by Bahari et al. [36] with the addition of up to 2% by weight nC (montmorillonite) to silt. A linear correlation for shear strength was observed from direct shear tests conducted.

### Table 2. Research on nano materials – CNT, NanoClay

| Research                      | Soil Type (USCS) | Nanomaterial / Secondary Binder | Effect AS % Nanomaterial Increases | Opt. Mix / Max. UCS / other improvements |
|-------------------------------|-----------------|---------------------------------|-----------------------------------|------------------------------------------|
| Correia and Rasteiro (2016)   | Silt            | • CNT (MWCNT) 1% dry wt. OPC    | • Greater dispersion of MWCNT→ stronger and stiffer soil skeleton matrix formed OPC | • 175 kg/m² OPC + 0.001% CNT 237.5 kPa E_0 =38.7 MPa |
|                               | q=143 kPa       | • Cement (OPC) @ 175 kg/m³ + surfactant 1. Amber 4001 2. Glycerox |                                    |                                          |
|                               | E50 =15.8 MPa   | • Distilled water               |                                    |                                          |
| Alsharif et al. (2016)        | Residual / clayey sand (SC) | • CNT (MWCNT); CNF 0.05–0.2 % CNT 0.1, 0.2 % CNF Distilled water | • MDD* | • Specific gravity OMC porosity Soil permeability (k) |
| Taha (2018)[22]               | Clay (CL/CH)    | • CNT; CNF 0.05–0.2 % dry wt. soil • Bentonite 10 & 20 % dry wt. soil + ultrasonication | • PI MDD | • Soil shrinkage/ expansive strains Desiccation cracks are suppressed |
| Ali et al. (2016) [35]        | Clay (CL)       | • Nano-Clay (nC) 1–2 % dry wt. soil | • UCS | • Linear shrinkage of soil 0.2% nC 159 / 325 kPa (OL/CH) 0.3% nMgO 101 / 188 kPa (OL/CH) |
|                               | q=40.9 kPa      | – | • Empirical function developed to model curing time (D, day) vs UCS | – | 1% nC 194 kPa |
| Bahari et al. (2013) [36]     | Silt (ML/MH)    | • Nano-Clay (nC) 0.5–2 % dry wt. soil | • MDD* PL; LL Su; ϕ | – | – |
|                               | q=50 kPa        | – | • UCS | – | – |
| Majeed et al. (2014) [37]     | Org. Clay (OL) | • Nano-Copper (nCuO) 0–1 % dry wt. soil | • UCS* | • LL, PL, PI Linear shrinkage of soil 0.07% nCuO 150 / 330 kPa (OL/CH) |
|                               | q=90 kPa        | • Nano-Clay (nC) 0–0.3 % dry wt. soil | • MDD* | – | – |
|                               | Silt Clay (CH)  | • Nano-Magnesium (nMgO) 0–0.4 % dry wt. soil | • UCS* | – | – |
|                               | q=42.6 kPa      | – | – | – | – |
| Mohammad and Niazzian (2013)  | Clay            | • Nano-Clay (nC) 0.5–2 % dry wt. soil | • CBR* PL; LL | – | – |
| Vol. 6, No. 4, April 2020     | q=-50 kPa       | – | • CBR* PL; LL | – | – |

* Until optimum % thereafter decreases

### 3.4. Nano Silica (nSi)

Nano Silica (nSi) is silicon dioxide in nano particle size form. It can directly be produced from bio waste e.g. rice husk ash (RHA) aerosol-gel method, electric arc method, precipitation method etc. [39].

Chemically, nSi particles would react with calcium hydroxide (Ca (OH)₂) to develop more of the strength contributing C-S-H material in concrete. In addition, concrete workability, increased resistance to water penetration and reduced leaching of calcium has also been encountered with nSi. The effective surface area plays a large part in influencing the improvement and nSi was reported to be more effective than micron-sized silica e.g. Silica Fume due to the exposed surface area to the pozzolanic reaction [18]. Improvement from nSi addition is affected by water/binder ratios [40].
Table 3. Research of nano materials – nano Fly Ash, nano Silica

| Research | Soil Type (USCS) | Nanomaterial / Sec. Binder | Effect AS % Nanomaterial Increases | Opt. Mix / Max. UCS / other improvements |
|----------|-----------------|---------------------------|-----------------------------------|----------------------------------------|
| Babu and Joseph (2016) [33] | Silty Clay (CH-MH) | Nano Titania (nTiO2) | Increase | Decrease |
| | | Nano Fly Ash (nFA) | Su* | PL; LL; SL |
| | | 0.5–2% dry wt. soil | MDD | OMC |
| Prabhu et al. (2017) [41] | Clay (CH) | Nano Fly Ash (nFA) | OMC | LL |
| | | Fly Ash (FA) | UMS | MDD |
| | | 10–30% dry wt. nCem | UCS | UCS |
| | | Nano Alumina (nFA) | Soil permeability (k) | Soil permeability (k) |
| | | Cement (Cem) | Nano particle equivalent achieves 1.2 times UCS than non-nano particles | |
| Khalid et al. (2015) [42] | Clay (CI) | Nano Soil (nSoil) | UCS | PI |
| | | 0–4% dry wt. soil | PI | PI |
| Bahmani et al. (2016, 2014) [43,44] | Residual Soil (CH) | Nano Silica (nSi) | UCS* | – |
| | | 15, 80 nm particle size | – | 0.4% nS + 6% OPC |
| | | 0–1% dry wt. soil | – | 1287 kPa (28 d) |
| | | Cement (OPC) | – | 0.4% nS + 8% OPC |
| | | 6, 8% dry wt. soil | – | 2000 kPa (28 d) |
| | | Higher UCS achieved with smaller particle size nanomaterial. | – | 6% OPC |
| | | SEM analysis shows formation of secondary C–S–H gel in reactions between hydration products and SiO2 nanoparticles. | – | 534 kPa (28 d) |
| Changizi and Haddad (2017, 2016) [45,46] | Clay (CL) | Nano Silica (nSi) | UCS* | 0.7% nS |
| | | 760 kPa @ | C = 36.6 kPa | 1.18 MPa @ e=7.8% |
| | | e=11% | | C=42.3 kPa; q=28° |
| | | C=36.6 kPa | | E50=14.5 MPa |
| | | q=14.3° | – | 1% nS |
| | | E50=10.3 MPa | | 1.16 MPa @ e=6.15% |
| | | 11–13 nm particle size | – | C=45 kPa; q=29.5° |
| | | 0.5–1% dry wt. soil | Peak UCS occurs at lower strain than for untreated soil treated soil is more brittle, and failure triggered by tension cracks | E50=19 MPa |
| Choobasti and Kutanai (2017) [47] | Sand | Nano Silica (nSi) | UCS* | 4% nS + 6% OPC |
| | | 0–12% dry wt. soil | – | 0.98 MPa (28 d) |
| | | Cement (OPC) | Adding nanoparticles (up to optimal %) promotes hydration process especially at early curing times and changes the unhydrated CH crystal needles into C-S-H gel. | 8% nS + 6% OPC |
| | | 6% dry wt. soil | Beyond optimal %, increasing further nS % prevents suitable CH crystal growth. This leads to increased micro-cracks and reduced UCS. | 1.12 MPa (28 d) |
| | | Distilled water | UCS increases as curing time increases | 12% nS + 6% OPC |
| Lin et al. (2016) [48] | Clay (CL) | Nano Silica (nSi) | UCS | 15% OPC |
| | | 32.5 kPa | – | 1:1 SSA/OPC |
| | | PI=8.8 | – | 364 kPa (28 d) |
| | | 2% dry wt. soil | 1% SSA/OPC | PI=0 (28 d) |
| | | Sewage sludge ash (SSA) | 15% OPC | 410 kPa (28 d) |
| | | SSA/OPC = 1:1, 2:1, 3:1, 4:1 | Soil permeability (k) | PI=0 (28 d) |
| | | Cement (OPC) | Volumetric swelling | |

* Until optimum % thereafter decreases [A decreases until optimum % thereafter increases again.

### 3.5. Nano Alumina (nA)

Nano Alumina (nA) may come in the form of nearly spherical nanoparticles or as oriented / undirected fibers. As nano fibers, manufacture can be by [49]:

- Selective oxidation of aluminum on the surface of the molten Ga-Al in a humid atmosphere at a temperature of 20 to 70 °C (Method of IPCE RAS);
- Synthesis of nano structural aerogel AIOOH from molten Ga-Bi and Al-Al (Inst. of RF IPPE);
- Growing fiber nano oxide of aluminium on the surface of the aluminium melts (ANF Technology).
When blended with concrete, it results in higher tensile and flexural strength (up to 2% replacement of cement with typical particle sizes of 15 nM) [50]. León et al. (2014) achieved increased abrasion and fracture resistance in cement mortars blended with nA [51].

Pozzolanic binders (CaO and CaO-MK binder mix) when combined with of nSi and nA, have been reported with enhanced properties such as increased compressive strength in conjunction with reduced porosity values [52]. This is due to denser microstructure, decreased carbonation and water absorption. nA did not contribute to the development of C-S-H compounds which are the main contributors to strength. Decreased carbonation was encountered, due to nA which had a negative effect on compressive strength, porosity and water absorption. However, this is on a smaller scale compared to the nSi reaction.

Naval and Chandan (2017) researched the effect of nano MgO (nMg) and nA when added to kaolinite clay and demonstrated improvements in soil properties such as Atterberg limits (e.g. reduced LL, PL and PI of soil), swelling potential decrease and maximum dry density increase [53].

Both Luo et al. (2012) and Lin et al. (2016) investigated using nA from sewage sludge ash/cement mix to stabilize clay soil. The optimum 1% nA achieved UCS 4.2 times higher than untreated soil after 7 days. Improved CBR values and reduced volumetric swelling was also observed [48, 54].

### 3.6. Nano Lime (nCaO)

Nano-sized lime particles (nCaO) have recently been considered to overcome some limitations of traditional lime binders, e.g. difficulties in achieving complete carbonation. This may be addressed by the much smaller particle size and greater surface area for reaction of nCaO.

Improvements were reported in Atterberg limit properties (e.g. decreases in liquid limit and plasticity index), maximum dry density/increase in OMC as well as compressive strength increase by using nCaO / nSi when compared to conventional particle size lime and silica binder in silty clay [55]. Permeability was also recorded to be reduced by a factor of 10 in comparison to non-nano sized additives of silica and lime. In addition to greater reactivity because of surface area, it is proposed that nano particles can effectively fill in the pores of soil particles due to greater fineness.

The strength contribution of nCaO becomes more apparent with increasing curing time [56]. The effect of nCaO exhibits both positive (aggregation and pozzolanic reaction increasing C-S-H content and creating alkaline environment with more OH-/Si ratio) and negative effects (cement hydration is impeded when Ca (OH)₂ concentration becomes too high and excessive Ca (OH)₂ crystallization leads to strength decrease). Wang et al. (2016) therefore concluded that there was insufficient justification to utilize nCaO in lieu of common CaO. Comparison is made with other nanomaterials whereby nSi is considered more effective, nCaO being comparable to nA but better than nTiO₂ which exhibited negative effects [56].

| Research | Soil Type (USCS) | Nanomaterial / Sec. Binder | Effect AS % Nanomaterial Increases | Opt. Mix / Max. UCS (q) / other improvements |
|----------|-----------------|--------------------------|---------------------------------|---------------------------------------------|
| Luo et al. (2012) [54] | Clay (CL) q=40 kPA pH=6 | Nano Alumina (nA) 0–3 % dry wt. soil | pH | Max. Unit weight 1:1 SSA/OPC; 185 kPa (28 d) |
| Naval and Chandan (2017) [53] | Clay-Kaolinite (CH) | Nano Alumina (nA) Nano Magnesium (nMgO) 0–2 % dry wt. soil | OMC; MDD | LL; PL; PI 235 kPa (90 d) |
| Eswaramoorthy et al. (2017) [55] | Clay (CH) q=254 kPA | Nano Lime (nCaO) 2–10 % dry wt. soil | UCS; OM; MDD | LL; PL; PI 493 kPa (7 d) |
| | | Nano Silica (nSi) 5–15 % dry wt. soil | | Soil permeability (k) 5% nSi + 10% nCaO 589 kPa (7 d) |
| | | Silica (SiO2) 5–15 % dry wt. soil | | Nano particle equivalent achieves 1.2 times UCS than non-nano particles |
| | | | | Nano particle equivalent achieves greater effects than non-nano particles |
| | | | | Optimum % for nS at 5% |

### Table 4. Research on nano materials – nano Alumina, nano Lime, nano Magnesium
4. Alkali-Activated Materials (AAM)

The development of alkali-activated binder materials has been claimed to have commenced from ancient binders used for the pyramids to recent applications utilizing Palm Fuel Oil ash (POFA) precursors with NaOH / KOH alkali [5, 58, 59 and 60]. AAM has also been utilized to produce alkali-activated cements with lower CO₂ / energy requirements compared to conventional cement types (OPC) [61].

Alkali-activated material (AAM) binders react with any amorphous mineral aluminosilicates source either in the soil or introduced with alkali (Na or K base) or alkali earth metals (typically Ca). The process mechanism requires a source material for the Si-Al raw material, namely the prime material or precursor together with corresponding alkali activators (which can be a liquid or solid, but which requires water to dissolve – e.g. NaOH, KOH etc.) [58]. The AAM binder is formed from the Si-Al raw material that has dissolved in a solution of alkali activators to form a mixture of gels and crystalline compounds which then hardens to a new, strong matrix amorphous condensed structure. It involves [58, 62]:

- Dissolution (breakdown) and hydrolysis (consuming water) of the mineral aluminosilicates in a strong alkaline solution – leading to breaking of covalent bonds between the Si, Al and O atoms ;
- Transport, orientation and creation of oligomer species [SiO₄]⁻⁴ and [AlO₄]⁻⁵ comprising polymeric bonds of Si-O-Si and /or Si-O-Al precursor ions into monomers;
- Condensation and stabilization phase whereby these Al and Si components form extensively into cross-linked networks eventually hardening into a 3-D, amorphous Si-O-Al and Si-O-Si mineral structures.

![Figure 5. Composition of various alkali activated materials [64]](https://example.com/figure5.png)

Škvára (2007) [64] defined alkali-activation materials as a whole range alumino-silicate binder types activated by stronger alkali agents with progressive replacement of C-S-H / C-A-H phase with Mn[−(Si−O)z−Al−O]n·wH₂O phase (where M is alkali cation e.g. K, Na or Ca; z is 1, 2 or 3 and n is degree of geopolymerization) [3]. Two (2) alkali-activation models are established [61, 65]:

- Where, Ca is significant, activation with Si + Ca precursor (e.g. GGBS, OPC, lime etc.) in mild alkaline solution, yields C-A-S-H / C-S-H as the main reaction products;
Where Ca is insignificant or absent, Si + Al precursors (MK, FA etc.) may react with a medium to highly alkaline solution (either NaOH or KOH). Activation produces a polymeric structured material. It is noted that the requirement for calcium in any part of the alkali-activated structure is bypassed in the second model (in the case of A-S-H) [4].

Where Al is prevalent, the reaction is as follows:

$$Al_2O_3 + 3H_2O + 2(OH)^- \rightarrow 2[Al(OH)_4]^-$$(1)

Where Si is prevalent, the following reactions are included:

$$SiO_2 + H_2O + OH^- \rightarrow [Si(OH)_3]^-$$(2)

$$SiO_2 + 2OH^- \rightarrow [SiO_2(OH)_2]^{2-}$$ (3)

In the case of alkali activation using Si + Al rich precursors; for metakaolin (MK), a suggested optimum ratio to achieve strength was reported at Si/Al and Na/Al in the range of 3.5-3.8 for the former and 1.2 for the latter respectively [66]. For Fly Ash (FA) precursors, Si/Al at 3.9 and Na/Al at 1 are the observed optimum ratios [67].

Studies also indicated that by increasing the amount of silicon, it results in more Si–O–Si bonds, which are stronger than Al–O–Al and Al–O–Si bonds [62, 63]. Hence, the strength of the alkali-activated binder would increase with the Si/Al ratio since Si–O–Si bonds density increases as the Si/Al ratio increases.

The stabilization of organic peat soil with sodium silicate system grout with a combination of sodium silicate with calcium chloride/aluminium sulphate acting as a reactor/accelerator was studied by Moayedi et al. (2012) whereby UCS of stabilized soil increased to 270% untreated organic soil [68].

The effect of alkaline activation using Fly Ash with Portland cement as a binder was researched using sodium silicate / sodium hydroxide as the alkaline activator solution [4, 69]. Fly Ash as a binder was utilized to achieve long-term strength gain in stabilized soil. Optimum levels of sodium hydroxide concentration were established together with the influence of solution/ash ratio. Fly ash was selected as more cost effective than metakaolin (MK).

Work done similarly on fly ash with sodium silicate + sodium hydroxide on silty sand achieved up to 2.8 MPa @ 28 days and 5.2 MPa @ 90 days UCS [70, 71]. Sargent et al. (2013) experimented with sodium silicate / sodium hydroxide precursors and FA / GGBS / red gypsum binder on soft alluvial soil. The stabilized soil exhibited higher UCS but higher brittleness over untreated soil. Highest strength gains were gained, using alkali activated GGBS binders [72].

Pourakbar et al. [60] experimented with sodium hydroxide and potassium hydroxide together with Palm Oil Fuel Ash binder material and revealed the main factors for determining the strength of stabilized soil being 1) quantity of source binder 2) type of alkali activator 3) water content of soil 4) curing conditions.

Alkali-activation reactivity depends on the amorphous content of silica and aluminium [58, 59]. The reactivity is linked to the material structure, being higher for higher amorphous content. Provis (2018) has recently discussed the utilization potential of AAM as a replacement for OPC in construction practices [73]. The disadvantage and hazards associated with difficult to handle concentrated alkali activator solutions may be resolved with recently developed one-part alkali-activated materials. One-part AAM which involves a dry mix of the solid aluminosilicate precursor, solid alkali source and other admixtures would only require water added.

![Figure 6. Production of one-part AAM [74]](image)

Similar end-products (N-A-S-H and K-A-S-H gels) are produced from one-part AAM reactions. These include instantaneous dissolution of the solid alkali activators and slower reactions involving aluminosilicates like two-part AAM [74]. Some examples of recent research (mainly focused on strength) are as follows:
### Table 5. Research on alkali-activated materials

| Research            | Soil                  | Alkali Activator (AA) Mol/L(M) | Main Stabilizer/Precursor | Effect AS AA Concentration (M) And/ Or Precursor % Increases | Opt. Mix / Max. UCS / other improvements |
|---------------------|-----------------------|--------------------------------|---------------------------|---------------------------------------------------------------|------------------------------------------|
| Pourakbar et al.    | Clay (CH)             | • KOH (5–15 M)                 |                           | • UCS                                                         | • 10 Mol KOH / 20% POFA 1.2 MPa (28 d)   |
| (2016) [60]         |                       | • NaOH                         |                           | • Scale laboratory model of treated column groups (diam = 23mm / length = 200mm) tested for UCS – replacement area ratios of 9.9, 11.9 and 15.82% |                                          |
|                     |                       | • Palm Oil Fuel Ash (POFA)     |                           | • Curing time at 7, 14 and 28 days – higher strength gain at later stages observed |                                          |
| Moayedi et al.      | Organic Soil          | • Hydrous Na2SiO3 – (3 M); CaCl2/Al(SO4)2 – (0.1 M); Kaolinite found in soil |                           | • UCS                                                         | • 3 M Na2SiO3 22 kPa (14 d)             |
| (2012) [68]         |                       |                                |                           | • Improved UCS (up to 270%) with increasing Na2SiO3 up to 3 mol/L Al2(SO4)3 | • 3 M Na2SiO3 + 0.1 M CaCl2 27 kPa (14 d) |
| Cristelo et al.     | Sandy Clay            | • Na2SiO3 + NaOH (Na2SiO3: NaOH = 2:1) (10M, 12.5M, 15M) (AA/Binder material = 0.4 to 0.45) | • Cement (OPC) 0.5–1 W/C 20–40 % wt. | • UCS                                                         | • 3 M Na2SiO3 +0.1 M Al2(SO4)3 25 kPa (14 d) |
| (2011,2013) [4,69]  |                       | • Fly Ash (class F) (20–40 % wt.) |                           | • AA + FA stabilization requires a longer curing period to achieve same UCS as cement. | • 12.5 M AA + 40% FA 7.1 MPa (28 d)     |
|                     |                       |                                |                           | • Strong dependency between the AA / FA ratio and mechanical strength. A lower ratio leads to higher strength | • 17 MPa (90 d) 44 MPa (1 yr.)           |
|                     |                       |                                |                           | • NaOH concentration is important – practical limit of 12.5 due to difficulties in mixing beyond that. | • 30%, 1 W/C OPC 11.6 MPa (28 d)        |
|                     |                       |                                |                           | • Beyond 90 days curing, AA / FA ratio more critical than AA concentration. | • 12.5 M AA + 30% FA 5.2 MPa (28 d)     |
| Rios et al.         | Silty Sand            | • Na2SiO3 + NaOH (Na2SiO3: NaOH = 1:2) (7.5 M) (AA/Binder = 0.781) | • Fly Ash 15, 20, 25 % wt. total wt., soil + binder mix | • UCS                                                         | • 11.7% AA + 15% FA (M1) 2.3 MPa (28 d) |
| (2016, 2017)[70,71] |                       |                                |                           | • Compaction is more important than FA quantity / activator type. | • 4.8 MPa (90 d) c = 287 kPa; $\varphi = 65^\circ$ |
|                     |                       |                                |                           | • The strength of soil-cement tapers off after 28 days whereas strength for AA stabilized soil continues to improve | • 11.7% AA + 15% FA (M1) 2.3 MPa (28 d) |
|                     |                       |                                |                           | • Very high internal angle of friction and cohesion intercept values also achieved from triaxial tests. | • 4.8 MPa (90 d) c = 287 kPa; $\varphi = 65^\circ$ |
|                     |                       |                                |                           | • Scale laboratory model of treated column groups (diam = 23mm / length = 200mm) tested for UCS – replacement area ratios of 9.9, 11.9 and 15.82% | • 11.7% AA + 15% FA (M1) 2.3 MPa (28 d) |
|                     |                       |                                |                           | • Curing time at 7, 14 and 28 days – higher strength gain at later stages observed |                                          |
| Vitale et al.       | Clay (Kaolin)         | • Na2SiO3 (AA/Binder = 0.5)    | • Cement (OPC) 20–40 % wt. | • Yield stress                                                | • Soil compressibility –                |
| (2017) [75]         |                       | • Fly Ash 20–40 % wt.          |                           |                                                              |                                          |

### 5. Geopolymers (GP)

Geopolymers are a class of synthetic inorganic alkali aluminosilicate materials. They are be produced by the reaction of a solid alumino silicate with a highly concentrated alkali hydroxide/alkali silicate solution. The resultant geopolymer product from reaction is a generally amorphous, polymeric Si-O-Al framework binder material with potential in soil stabilization [76]. Feng et al. (2004) defined a geopolymer as basically a 3D aluminosilicicate mineral polymer formed by several amorphous to semi-crystalline phases [77]. Geopolymers are formed by dissolution of aluminosilicate solids in a solution of alkali or alkali salts producing a mixture of aluminosilicates, aluminates and silicates in solution. With sufficient concentration, the solution solidifies through several gel phases and undergoes polymerization that hardens into a 3D aluminosilicate framework.
Like AAM, geopolymer materials have advantages over traditional cement binders in that the production process imposes less demands on energy consumption and produces less greenhouse gases (CO₂) [3]. Raw materials for polymers can be sourced from a wide range of industrial waste materials which contain silicate and/or alumina – e.g., natural pozzolans such as fly ash, ground granulated blast furnace slag, agricultural/construction waste materials with high silica/alumina content such as RHA, palm oil fuel ash (POFA), red clay brick waste and metakaolin [78].

Improved sulphate resistance properties of geopolymer concrete (prepared from blended Waste Fuels Ash precursor and sodium silicate alkali activator) was observed [79].

Du et al. (2017) investigated the physical, hydraulic and mechanical properties of clayey soil stabilized by geopolymer composed of a GGBS precursor and sodium silicate/calcium carbide residue alkali activator [80]. The lightweight geopolymer stabilized soil (LGSS) developing greater water absorption, permeability (k of LGSS being 10 x k of LCSS) and material strength (qᵤ LGSS = 2-3.5 qᵤ LCSS) when compared to benchmark lightweight cement stabilized soil (LCSS). C-S-H content in LGSS was ~ 2 times found in LCSS.

The effectiveness of soil–geopolymer stabilization and comparison between Fly Ash and GGBS based geopolymer types were made by Singhi et al. (2016) [81]. Alkali activator solution used selected was sodium hydroxide and sodium silicate. The unconfined Compressive strength from slag based geopolymer stabilized soil (~11 MPa @ 20%) was found to be much higher than that with Fly Ash-based (~0.3Mpa @ 20%). The difference in UCS between the two geopolymer base types starts to increase beyond 8% content of source geopolymer stabilization material in the soil.

Study by Zhang et al. (2013) on the effectiveness of metakaolin based geopolymer (MKG) soil stabilization on clay soils showed UCS values of MKG stabilized soils being much higher than for original soil as well as 5% cement stabilized soil at MKG contents > 11%. There was also an improvement in shrinkage strains at MKG concentrations > 8%. UCS values of MKG is not significant between 7 and 28-day strengths indicating predominantly fast reactions leading to early strength gain – this may be due to the precursor completing geopolymerization and strength development within 7 days [82]. Improvements in soil Young’s Module were also recorded, but still, less than 5% cement stabilized soil.

![Geopolymer systems](image)

**Figure 7. Geopolymer systems – adapted from Al Bakri Abdullah et al. [83]. Geopolymers with Si:Al = 2 have low CO₂ emissions and energy demand during manufacture (e.g. geopolymer cements and concretes) [84]. Cement curing requires only room temperatures [85].**

However, Davidovits (1994) [84] asserts that geopolymers (GP) should be separated from AAM in definition, as both belong to different chemistry systems. Although conceptually following a similar reaction mechanism for creation, Davidovits [3, 84] differentiates GP from AAM by restricting geopolymer definition to only those obtained by pure metakaolin precursors and with end products derived, namely, through polycondensation to a 3D K-poly(sialate-siloxy) polymer excluding N-A-S-H / K-A-S-H previously included by earlier research [84]. The interchangeable interpretation of AAM and geopolymers are due to similarities between alkali-activation and first step of geopolymerization. For geopolymers, the first step should instead be termed alkalinization instead of alkali-activation.

AAM type cements (e.g. Alkali-activated Slag cement) have a disadvantage to geopolymers due to the generation of leachates leading to potential long-term stability problems although AAM type cements generally achieve higher initial strengths over geopolymer cements. Geopolymer (GP) cements are now being developed in the form of 1) slag-
based; 2) rock-based 3) fly ash-based and 4) ferro-sialate-based types. The manufacture of GP type cement can generate up to 80% less CO₂ and requires far less energy than portland cement [86].

### Table 6. Research on geopolymer materials

| Research          | Soil                  | Activator % Mol/L(M)/ Geopolymer (Gp) | Effect AS Geopolymer % Increases | Opt. Mix / Max. UCS / other improvements |
|-------------------|-----------------------|----------------------------------------|----------------------------------|-----------------------------------------|
| Zhang et al.      | Clay (CL) qe=780 kPA   | Na₂SiO₃ + NaOH                          | UCS E                            | MK 11%                                  |
|                   |                       | Meta kaolin geopolymer (MKG)            | Volumetric strain Britteness     | 2.9 MPA (28 d)                          |
|                   |                       | 3–15 % dry wt. soil                    | Shrinkage strain                | MK 15%                                  |
|                   |                       | Cement (OPC) 5 % wt. dry wt. soil       |                                  | 3.8 MPA (28 d)                          |
| Du et al.         | Clay (CL)             | Na₂SiO₃ + Calcium Carbide Residue (CCR)| Higher density mixes achieve higher UCS | OPC 5%                                  |
|                   |                       | Cement (OPC)                            | LGSS permeability (k) is 10x higher than LCSS | 3.35 MPA (28 d)                       |
|                   |                       | GGBS                                   |                                  |                                         |
|                   |                       | LGSS                                   |                                  |                                         |
|                   |                       | CCR: Na₂SiO₃: GGBS = 1:1:8              |                                  |                                         |
|                   |                       | LCSS                                   |                                  |                                         |
|                   |                       | CCR: Na₂SiO₃: GGBS = 1:1:8              |                                  |                                         |
|                   |                       | Mixed with 385, 430.475.520 kg/m² soil |                                  |                                         |
|                   |                       | to achieve 900, 1000, 1100, 1200 kg/m² density stabilized soil mix |                                  |                                         |

### 6. Discussion

Being a mechanical process of improvement to the soil, reinforcement fiber materials have an immediate effect without curing in comparison to other binders which require curing time due to the hydraulic / chemical reaction process. Review of laboratory research results on reinforcement fiber materials demonstrated improvements in treated soil shear strength and axial strain to failure. However, if acting by itself, the level of compressive / shear strength improvement was still inferior to other binder materials. A higher tensile strength which defines the brittle to ductile transition in the improved soil due to the embedded fibers was clearly observed [5]. This can be important in the case of soils subjected to cyclic / dynamic loading.

The mixing of reinforcement fibers in soil also encountered difficulties in compaction and subsequent maximum density reduction with increasing dosage. Consistent and effective mixing of the fibers (possibly affecting viscosity in the slurry and hence limited to WDSM approach), application and distribution in soil may be difficult to achieve for DSM in the field. It may be more practical to pair with chemical based binder – e.g. cementitious, pozzolanic, alkali-activated types etc. This could lead to a synergistic combination of improved compressive and tensile strength.

Due to smaller dimensions, nanoparticles increase rate of improvement compared to their micron / macro sized counterparts. With a different order of magnitude on the specific surface, reaction of the same materials, albeit on a nano vs micro scale, is more rapid and effective. Moreover, lesser amounts of nanomaterials can produce significant enhancements in soil improvement. Different nanomaterials lead to different effects – e.g. CNT potentially increases flexural strength and control crack propagation whereas nano-versions of lime and silica increased compressive strength. The use of nanomaterials for ground improvement is presently hindered by high cost and the requirement to install via a slurry media (hence by the wet method) to ensure effective dispersion into the soil. The challenges of effective field mixing and dispersion into soil again needs to be resolved in DSM ground improvement.

Whilst cementitious and pozzolanic binders rely on Ca based reactions, AAM and GP binders undergo a different reaction pathway (Si/Al-based) without reliance on calcium, to improve soil properties. Research to date has shown the potential of alkali-activated binders to match or surpass the compressive strength gain compared to traditional cementitious binders. However, the strength gain comes at the cost of increased curing period (beyond 28 to 90 days) compared to short curing period of soil-cement mixtures (7 to 28 days). This is due to the faster dissolution rate of the calcium-type glassy material, forming the C-S-H gel that can be found in cement hydration [70]. However, this is compensated by greater benefits in environment reduction in CO₂ emissions (due to reduced usage of cementitious binder materials) and better resistance to aggressive soil environments, due to sulphate, chloride and acid exposure.

The difficulties and hazards associated to on-site handling of highly alkaline aqueous solutions can be largely avoided with development of one-part alkali activated materials which already comes pre-mixed in dry powder form like cement, requiring only addition of water. This allows the possibility of dry method DSM in high moisture content soils.
A recent development is the potential application of geopolymers to ground improvement. Research conducted on geopolymers produced from fly ash and metakaolin source materials have demonstrated the clear advantages of geopolymers over other binders in toughness and durability whilst further improving mechanical strength. Geopolymers are also more stable than AAM as they are not subject to potential leachate generation in AAM binders in the long-term.

High early strength for type 1 alkali -activated Fly Ash geopolymers (Si: Al ratio of 1 to 2) can be achieved with curing at optimum temperature range of 40 °C to 90 °C [85, 87]. It may be possible to achieve this from exothermic reaction with sufficient dosage of lime. Another possibility would be a combined approach, when both Ca and alkali activated types of reactions are allowed to take place – calcium-based reactions leading to C-S-H / C-A-H phase and through activation of suitable silica/ alumina rich materials by strong alkali agents to produce aluminosilicate geopolymers (UCS potentially reach up to 160 MPa [64]). In the combined approach, it is noted that cementitious calcium-based reactions are also exothermic. A combined mix incorporating primary calcium-based reactions supplemented by pozzolanic secondary and alkali-activated/geopolymer tertiary reactions is also recommended for further research. In addition, type 2 slag / fly ash-based GP cements (Si: Al ratio of 2) which may harden at room temperatures and which do not require toxic solvents can also be applied.

7. Conclusions

The background and reaction mechanism behind alternatives to cementitious and pozzolanic binders and its application to DSM ground improvement have been covered in this review. Of these alternatives, both alkali-activated materials (AAM) and Geopolymer materials (GP) present an effective alternative chemical process pathway to soil improvement. Hazards associated with handling of alkali activator chemicals on site - e.g. Na₂SiO₃, NaOH, KOH may be largely avoided by using one-part pre-blended AAM or GP cements. This leads to research opportunities on the applicability of this hybrid implementation in real geotechnical solutions such as:

- A systematic investigation using various combinations of calcium-based (which may include both cementitious and pozzolanic materials) and alkali activated alumino-silicate based binders and the effectiveness and specific improved properties for different soil conditions. The optimum proportions for combined binder types which can work synergistically for application to DSM can be determined;
- Methods in mixing of these combined binder materials and effective dispersion into the soil;
- Deriving a predictive constitutive improved soil model of 1) calcium based 2) alkali-activated / geopolymer as well as 3) hybrid combination in deep soil mix methods design for various soil types;
- Application geopolymer cement as a binder;
- As strength of the improved soil in DSM columns increase to higher compressive strengths approaching conventional concrete, the geotechnical model now transitions from improved ground to that of ground with rigid inclusions like unreinforced piles. Research is needed to establish the crossover point.

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9. Conflicts of Interest

The authors declare no conflict of interest.

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