Optimization of thermal conductivity lightweight brick type AAC (Autoclaved Aerated Concrete) effect of Si & Ca composition by using Artificial Neural Network (ANN)

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Abstract. Lightweight brick is the most important component of building construction, therefore it is necessary to have lightweight thermal, mechanical and acoustic thermal properties that meet the standard, in this paper which is discussed is the domain of light brick thermal conductivity properties. The advantage of lightweight brick has a low density (500-650 kg/m\textsuperscript{3}), more economical, can reduce the load 30-40\% compared to conventional brick (clay brick). In this research, Artificial Neural Network (ANN) is used to predict the thermal conductivity of lightweight brick type Autoclaved Aerated Concrete (AAC). Based on the training and evaluation that have been done on 10 model of ANN with number of hidden node 1 to 10, obtained that ANN with 3 hidden node have the best performance. It is known from the mean value of MSE (Mean Square Error) validation for three training times of 0.003269. This ANN was further used to predict the thermal conductivity of four light brick samples. The predicted results for each of the AAC\textsubscript{1}, AAC\textsubscript{2}, AAC\textsubscript{3} and AAC\textsubscript{4} light brick samples were 0.243 W/m$\cdot$K, respectively; 0.29 W/m$\cdot$K; 0.32 W/m$\cdot$K; and 0.32 W/m$\cdot$K. Furthermore, ANN is used to determine the effect of silicon composition (Si), Calcium (Ca), to light brick thermal conductivity. ANN simulation results show that the thermal conductivity increases with increasing Si composition. Si content is allowed maximum of 26.57\%, while the Ca content in the range 20.32\% - 30.35\%.

1. Introduction
Energy consumption of a building is influenced by various factors, one of which relates to the thermal insulation capability of the material used in the construction of the building. Use of materials with good thermal insulation capability can reduce energy consumption for indoor cooling requirements. One material that is currently widely used because it has good thermal insulation capability is a lightweight brick. The lightweight brick has a porous structure so it has lower density and better thermal insulation ability than conventional brick. The material's thermal insulation capability, including the lightweight brick is determined by its thermal conductivity where the smaller the thermal conductivity value, the better its thermal insulation capacity. In the case of light bricks, factors affecting thermal conductivity include: density, moisture content, temperature, porosity, and lightweight brick mineral composition [1-5]. Research conducted by Stuharova (2016) shows that there is a nonlinear relationship between thermal conductivity, density and the content of light brick vapor. This relationship is expressed in terms of mathematical equations, developed from the
experimental data. In some cases, experimental data are not possible to be used in modeling the relationship between the properties of a material and the factors that influence it in terms of mathematical equations. This can be accomplished by modeling artificial neural networks. Artificial Neural Network (ANN) is an information processing system with the ability to learn, remember, and solve problems based on the learning process (training). ANN has been widely used in various studies to predict material properties including thermal properties and mechanical properties [4-7]. In this study, using Backpropagation Neural Networks to predict lightweight brick thermal conductivity based on Si and Ca composition variations.

2. Methodology

2.1 Materials and Methods

The first step in this research is data collection. In this research, there are two types of data that is secondary data for training of ANN and primary data used for testing. Based on the results of the literature study, 18 pairs of data were composed of Si, Ca, Al, O and density from three research papers [8-10]. This data is collected in a database as input for the training needs of ANN. Meanwhile, the next variable is the thermal conductivity paired with each of the above variables collected as the target data. The summary of input and target data can be shown in table 1 and table 2 below:

| Table 1. Input Training Data. |
|-----------------------------|
| Variables | *N | Maximum Composition (wt.%) | Minimum Composition (wt.%) | Mean Composition (wt.%) | Standard Deviation |
| Si | 18 | 32.56 | 12.18 | 20.67 | 6.93 |
| Ca | 18 | 31.96 | 18.3 | 23.69 | 3.51 |
| Al | 18 | 6.67 | 1.11 | 4.09 | 2.22 |
| O | 18 | 46.28 | 38.87 | 41.66 | 1.86 |
| ρ | 18 | 1210 | 504 | 712 | 180.13 |

* ρ – density (kg/m³) ; * N - the amount of data

| Table 2. Targeted Training Data. |
|-----------------------------|
| Variables | *N | Maximum Composition (wt.%) | Minimum Composition (wt.%) | Mean Composition (wt.%) | Standard Deviation |
| ρ | 18 | 0.376 | 0.123 | 0.23 | 0.09 |

* ρ – density (kg/m³) ; * N - the amount of data

Primary data for the purposes of ANN testing were obtained from thermal conductivity testing on four light brick samples with each AAC1, AAC2, AAC3 and AAC4 samples.

![Four light brick sample models](image-url)
In the four light brick samples, density measurements, composition tests with EDX shown in figure (2), and thermal conductivity tests were performed. The summary of test input and target data is shown in table 3 below.

![Figure 2. EDX composition test results of sample AAC1.](image)

| Variables | *N | Maximum Composition | Minimum Composition | Mean Composition | Standard Deviation |
|-----------|----|----------------------|---------------------|------------------|---------------------|
| Si        | 4  | 5.56                 | 27.37               | 17.24            | 11.02              |
| Ca        | 4  | 29.62                | 51.5                | 40.43            | 11.87              |
| Al        | 4  | 0                    | 1.69                | 0.84             | 0.97               |
| O         | 4  | 38.71                | 41.8                | 40.12            | 1.61               |
| *ρ        | 4  | 509                  | 632                 | 585              | 53.33              |

*ρ – density (kg/m³); *N - the amount of data

### 2.2. Making Artificial Neural Networks (ANN)

The making of ANN program is done by using Matlab R2015a software. Neural Network Toolbox in Matlab provides various functions that support the creation and development of ANN. Making Artificial Neural Networks is done through the following stages:

- Loading training data (input and target)
- Normalization of input and target data into ranges 1 and -1.
- Function equations of data normalization used are as follows:

$$y = \frac{2(x - x_{\text{min}})}{x_{\text{max}} - x_{\text{min}}} - 1$$  \hspace{1cm} (1)
Where: $x$ is initial value, $y$ is values after normalization, $x_{\text{max}}$ is maximum value in the data, $x_{\text{min}}$ is the minimum value in the data

1. Initialization of Artificial Neural Networks. The activation function used is tanh and purelin
2. Training parameter determination (three important parameters specified are epochs = 100, training goal = 1e-5; validation checks = 10, while other parameters are left to default)
3. Initiate training and display the weight of training outcomes and validation.
4. Save on the network.

In making this Artificial Neural Network conducted variations of hidden node is 1-10. For each variation of hidden node, do the training 3 times with different initial weight. In this study, 85% of the total 18 data were used for training purposes, while the remaining 15% were used for validation purposes. Artificial Neural Network Architecture Backpropagation used as in figure (3) below:

![Figure 3. Backpropagation ANN architecture.](image)

2.3 Artificial Neural Network (ANN) Selection

To determine the best ANN model of 10 different hidden node types depends on the mean value of MSE (Mean Squared Error) validation of each ANN. MSE is calculated by the following equation (2):

$$\text{MSE} = \frac{1}{N} \sum_{i=1}^{N} (T_i - Y_i)^2$$

Where: $N$ is amount of training or validation data, $T_i$ is target value of ANN, $Y_i$ is the output value of ANN

2.4 Artificial Neural Network (ANN) Test

At this stage, ANN testing is performed by looking at network output (prediction) if new input data is fed to the network. The first step that needs to be done before testing is to call the data and load it into the Matlab workspace. The network used in the testing phase is the network selected from the
evaluation results [11]. Next will be compared the value of target and output of ANN which are both lightweight thermal conductivity

### 2.5 Analysis of the Effect of Composition on Thermal Brick Thermal Conductivity

Si and Ca, and is the main composition that affects the formation of dominant phase contained in the light brick of calcium silicate hydrate. The effect of such composition variation on thermal conductivity can be known by simulating using ANN, where one of the composition values is varied while the other composition is kept constant. The boundary value of the composition of an element found in the light brick can be found using the equation below:

\[
V_f = \frac{\lambda_f (\lambda_m - \lambda)}{\lambda (\lambda_m - \lambda_f)}
\]  

(3)

Where : \(V_f\) is fraction volume, \(\lambda\) is thermal conductivity of simulation, \(\lambda_f\) is thermal Conductivity at atmosfer pressure and \(T = 300\) K (0.026 W/m.K), \(\lambda_m\) is thermal conductivity of tobermorite (0.2 W/m.K).

### 3. Result and Discussion

#### 3.1 Lightweight Brick Composition

Table 4 below shows the composition contained in lightweight bricks (four samples AAC1, AAC2, AAC3 and AAC4). The high concentrations of calcium and oxygen and the presence of sulfur in all light brick samples indicate that the area on the surface of the test sample has been carbonated due to environmental influences. Carbonation of one type of light brick degradation that occurs when Ca(OH)$_2$ and C-S-H phase found in lightweight brick react with CO$_2$ in the air to form CaCO$_3$, and degradation can also occur when carbonated CaCO$_3$ reacts with sulfuric acid in the air and produces gypsum. This mechanism leads to the emergence of sulfur content in the four light brick samples [12].

| Sample Lightweight brick | The composition (wt%) is average |
|--------------------------|---------------------------------|
|                          | Si   | Ca   | Al  | O    | Mg   | S    |
| AAC1                     | 27.37 | 30.74 | 1.67 | 38.79 | 0.61 | 0.83 |
| AAC2                     | 23.89 | 29.62 | 1.69 | 41.19 | 0.61 | 1.00 |
| AAC3                     | 5.56  | 51.50 | 0    | 41.80 | 0    | 1.14 |
| AAC4                     | 1.26  | 49.88 | 0    | 38.71 | 0    | 1.26 |

#### 3.2 Results of Training and Evaluation of Artificial Neural Network (ANN)

The training of ten models of ANN with variations of the number of hidden nodes gives the results as shown in Table 5 below. The ANN with 3 hidden nodes yields the MSE average validation of the smallest value of 0.003269.
Table 5. Comparison of MSE training and validation scores ANN with hidden.

| Amount hidden node | MSE (Average) Training | MSE (Average) Validation |
|--------------------|------------------------|-------------------------|
| 1                  | 0.002855               | 0.005908                |
| 2                  | 0.002668               | 0.005516                |
| 3                  | **0.002434**          | **0.003269**            |
| 4                  | 0.004751               | 0.003833                |
| 5                  | 0.002383               | 0.006464                |
| 6                  | 0.002625               | 0.007059                |
| 7                  | 0.002716               | 0.008955                |
| 8                  | 0.002250               | 0.003891                |
| 9                  | 0.002897               | 0.008206                |
| 10                 | 0.002974               | 0.004768                |

Table 6 below shows a comparison of MSE training and validation between 3 ANNs with 3 hidden nodes trained with different initial weights. ANN2 resulted in MSE validation of the smallest value of 0.002252.

Table 6. MSE Value Validation of ANN with one hidden node for three training.

| Filename of ANN | MSE Training | MSE Validation |
|----------------|--------------|----------------|
| ANN1           | 0.002694     | 0.003716       |
| **ANN2**       | **0.002764** | **0.002252**   |
| ANN3           | 0.001845     | 0.003840       |

The comparison between MSE training and ANN2 validation is shown in Figure 4 below. The results show the best validation performance or MSE validation reaches the minimum value in the 11th epoch. In the next epoch, it shows that MSE validation has increased until training ends at the 21st epoch.

Based on the training function with the Levenberg-Marquardt (trainlm) method, training will cease during one of the following six conditions: Epoch, Performance Goal, Gradient, Mu, Validation Checks, and Time are reached. In MSE validation reaches a minimum, training is still on going to find out whether the value of MSE can still be reduced or not. If, in this case, in the next ten epoch fails to decrease the MSE and the five cessation conditions (Epoch, Performance Goal, Gradient, Mu, Time) have not been reached, the training will cease with a termination condition of validation checks or max_fail achieved, as shown in figure (5). The stored network weight refers to the weights when the MSE validation is of minimum value or when the training reaches the 11th epoch, then the weighting of the ANN used refers to the value of the validated MSE, Figure 5 below:
The next step taken to evaluate the artificial neural network linearity is with the regression curve. The regression curve shows the relationship between the output of network (output), regression of training result and validation of ANN2 obtained value of training correlation coefficient and validation reach 0.99. This value of 0.99 shows the optimal correlation between the target value and the output of the ANN2 training results, shown in figure (6) below:

3.3 Artificial Neural Network Testing

The ANN test with composition input data from the EDX test results, and light brick density yields the output value (prediction) as shown in Table 7 below. Based on the training MSE curve and the validation of the ANN as shown in Figure (4), it appears that the validation and training curves are almost coincidental. This indicates that ANN has a good generalization. This generalization is related to the prediction ability of ANN if given new input data that is not part of the training data.

| Sample Lightweight brick | Thermal conductivity (W/m.K) Target | Thermal conductivity (W/m.K) Prediction |
|--------------------------|------------------------------------|---------------------------------------|
| AAC1                     | 0.214                              | 0.243                                 |
| AAC2                     | 0.212                              | 0.29                                  |
| AAC3                     | 0.214                              | 0.32                                  |
| AAC4                     | 0.214                              | 0.32                                  |
3.4. Effect of Silicon Variation (Si) and Ca Calcium

Si, and Ca, is the main composition that affects the formation of dominant phase found in light brick of Calcium Silicate Hydrate (C-S-H). In addition, the density also affects the lightweight thermal brick conductivities. Simulation of ANN using ANN2 is done by varying the composition to its thermal conductivity.

3.4.1 Effect of Silicon (Si) variation on thermal conductivity

Figure 7 below shows the relationship between thermal conductivity and the variation of Si composition. The result shows that the larger the Si composition on the lighter brick the higher the thermal conductivity, this is due to the quartz-SiO$_2$ content in the lightweight brick one of the constituent elements is Si. The matrix phase in the AAC light brick dominated by the Calcium Silicate Hydrate phase (C-S-H) is the tobermorite phase. When the autoclave process takes place most SiO$_2$ does not react to produce quartz residue (SiO$_2$).

![Figure 7. Thermal conductivity curves with variations of Si composition.](image)

| Mineral                 | Thermal conductivity (W/mK) |
|-------------------------|----------------------------|
| Quartz (kristal tunggal)| 7.2 – 13.6                 |
| Tobermorite             | 0.18 – 0.2                 |

Table 8 above shows the thermal conductivity value of quartz and tobermorite. It appears that quartz has a thermal conductivity that is worth 35 times higher than the lightest thermal brick conductivity in general. Therefore, to produce lightweight bricks with low thermal conductivity values, one of the things to note is to try to keep the quartz residue present in the matrix phase much lower. This can be done with regard to the ratio of cement and sand composition to sufficient mineral minerals to be reacted with silica. Another thing that can be done to reduce the quartz residue contained in the lightweight brick matrix is to use a more reactive silica source so it can more easily react when the autoclave process takes place. To determine the maximum limit of Si content in light brick, calculated the value of $V_f$ using equation (3). $V_f$ denotes the fraction of air volume in the lightweight brick. Based on this simulation result, the limit of Si content in light brick is 26.57%, where there is composition of Si worth more than 26.57%, $V_f$ will be negative value.

3.4.2. Effect of Ca variation on thermal conductivity

Ca composition is related to the content of CaO which is one of the main minerals of light brick minerals that is calcium silicate hydrate. Based on the result of simulation of Ca variation shown in figure (8) and calculation of $V_f$ value using equation (3), it is known that the limitation of Ca
composition in light brick is 22.32% - 30.35%. Beyond this limitation, \( V_f \) is negatively negative which is not allowed.

![Figure 8. Thermal conductivity curves with variations of Ca composition.](image)

4. Conclusion

From the results of this study can be drawn conclusion as follows: (1) Based on ANN simulation having performance with MSE validation of 0.002252; (2) A light brick ANN simulation found that the maximum allowable composition for Silicon (Si) is 26.57%, while the composition of Calcium (Ca) is 20.32% - 30.35%; and (3) ANN tests performed for the prediction of thermal conductivity in four light brick samples were obtained: AAC1 = 0.243 W/m.K, AAC2 = 0.29 W/m.K, AAC3 = 0.32 W/m.K, AAC4 = 0.32 W/m.K, or thermal conductivity average is 0.2933 W/m.K.

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