Investigation of air pollution dispersion from kiln stacks based on seasonal using multi-model integration (WRF/CALPUFF)

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Abstract. Air pollution is one of the environmental problems that have a bad impact on human life. Air pollution sources come from various sources such as industry, mining, transportation activities, etc. This study aims to identify the seasonal dispersion of Sulfur Dioxide produced by kiln stacks in PT Semen Padang, Tbk. The Dispersion model used in this study is CALPUFF (For air pollution model) integrated with WRF (Weather Research Forecasting) (For meteorological model). CALPUFF requires the wind field generated by the CALMET model and the WRF model. From the simulation, the direction of SO2 dispersion on the wet season and the dry season is influenced by meteorological phenomena such as sea breeze and land breeze. The dispersion of Sulfur Dioxide in the dry season passes the urban area more than in the wet season, with the highest concentration is 122 µg/m³. On the other hand, in the wet season, the highest concentration is 120 µg/m³. These results are below of national quality standard in Indonesia (365 µg/m³). The statistic also shows that the correlation and error (RMSE) between the model and observed data are 0.63 and 5.49 in the wet season, whereas the correlation and error (RMSE) in the dry season are 0.74 and 2.89.

1. Introduction
Air pollution is one of the environmental problems that have an important impact on human life. Air pollution comes from various sources such as burning coal, transportation, combustion materials in the cement industry, domestic waste processing, and chemicals emitted directly into the air by human activities. The contaminants can be in the form of NO2 (Nitrogen Dioxide), SO2 (Sulfur Dioxide), Particulate Matter, etc. Fundamentally, pollution occurs when the number of pollutants generated from the activity exceeds a predetermined threshold [1]. If this happens, it will directly impact human health, the fertility of agricultural and plantation areas, and even affect the infrastructure damage for a longer period [2].

One of the industries that produces a large number of pollutants is the cement industry. The activity that has significant emissions is the combustion process in the kiln. Incomplete combustion of coal and the grinding process in the crusher causes the production of pollutants in particles and gases such as PM10, SO2, NO2, CO, HC, and Pb. At the PT Semen Padang Tbk, pollutants in the form of particles undergo a filtering process using an electrostatic precipitator. In contrast, pollutants in the form of gases are directly released into the atmosphere. Based on data from emissions monitoring reports in the first semester of 2014, Sulfur Dioxide is one of the pollutants with a large number of emissions from the combustion process.
Air pollution models have proven useful for determining the Spatio-temporal distribution of air pollutants and developing emission control policies that allocate air pollutant emissions threshold [3]. The CALPUFF model is a multi-layer non-steady-state puff dispersion model designed to model particles and gases' dispersion using space-time varying meteorology [4]. This model is also applicable to the stagnant condition. In Indonesia, one of the problems when running air quality models is the limited hourly meteorological data. Therefore, in this research, the air quality model (CALPUFF) is combined with the meteorological model (WRF). Lee et al. (2014) used the CALPUFF model to simulate the dispersion of PM$_{10}$ and SO$_2$ in Ulsan, South Korea. They found that pollutant dispersion using that model showed a good agreement (typically, it values for PM$_{10}$: 0.850 and SO$_2$: 0.895) against 14 monitoring stations [3]. Amnauylawjarun et al. (2010) used the Fifth-Generation NCAR/Penn State Mesoscale Model (MM5) and CALPUFF modeling system to investigate the meteorological variables affecting the dispersion of PM$_{10}$ released from forest fires in Chiang Mai province, Thailand [5]. They found that the dispersion of PM$_{10}$ depended on atmospheric features such as stability, wind direction, velocity, and topography.

This research aims to investigate the dispersion of air pollution produced by the burning process in the kiln stacks in the PT. Semen Padang, Tbk. This simulation uses a combination of air pollution model (CALPUFF – California Mesoscale Puff) and meteorological model (WRF – Weather Research and Forecasting) based on the different seasons, namely the wet season and the dry season. PT Semen Padang has a complex topography and is directly adjacent to the Indian Ocean and Barisan hills [6]. Research on the meteorological model (WRF) as an alternative to meteorological data for air pollution is scarce in Indonesia.

Overall, this study's result could be useful to evaluate the WRF model as an alternative to meteorological data when the hourly data is limited. It could also help the industry design the appropriate seasonal regulation to reduce the ambient concentration of air pollution and assist environmental administrators in controlling the sources that contribute the most to the degradation of air quality.

2. Methodology

2.1 Study location

This research was conducted at PT. Semen Padang Tbk, located in Indarung, Padang City, West Sumatra. The study location is about 15 km east of Padang City with an altitude of 200 meters above sea level. The image below is a map of the study area.

![Figure 1. Study location.](image-url)
Simulations were carried out in the wet and dry seasons in 2015 using the SO\textsubscript{2} (Sulfur Dioxide) parameter. The main sources of emissions come from 5 kiln stacks with the location coordinates as follows.

- Burner (kiln-raw mill Indarung II) with coordinates 0.951\textdegree S dan 100.471\textdegree E
- Burner (kiln-raw mill Indarung III) with coordinates 0.9507\textdegree S dan 100.471\textdegree E
- Burner (kiln-raw mill Indarung IV B) with coordinates 0.949\textdegree S dan 100.471\textdegree E
- Burner (kiln-raw mill Indarung IV C) with coordinates 0.949\textdegree S dan 100.471\textdegree E
- Burner (kiln-raw mill Indarung V) dengan koordinat 0.945\textdegree S dan 100.472\textdegree E

2.2 Data sources
Sulfur Dioxide dispersion using the CALPUFF model requires several primary data, namely (1) NCEP-FNL data with a resolution of 10 x 10 as input for the WRF model; (2) Topographic data from SRTM3 (Shuttle Radar Topography Mission Version 3) with the resolution of ~ 90 meters or 3 arcsec; (3) Land cover data from Modis Land Cover with a resolution of 500 meters; (4) Sulfur Dioxide observation data at 10 locations; and (5) Stack characteristics data such as geographic coordinates, stack height (meters), stack diameter (meters), emission velocity (m/s), stack temperature (K), height from sea level (meters) and pollutant emission rate (g/s). Data on points 4 and 5 are obtained from the annual report of PT. Semen Padang, Tbk in 2014. The emission rate is calculated using equation 1.

\[\text{Emission rate (g/s) = volume rate (m}^3/\text{s) x emission total (g/m}^3)\] (1)

2.3 Meteorological model
In the WRF model, four nested domains are used for the WRF model with the ratio of 1: 3: 3: 3, where the parent domain has a spatial resolution of 27 km, and the smallest domain has a resolution of 1 km. The parameterization used in the WRF model refers to the research conducted by Putriningrum et al. (2014) regarding the effect of atmospheric boundary layer parameterization on the generation of gravity waves over West Sumatra [7].

The WRF model's output is converted to 3D.dat data and used as an initial guess for generating a diagnostic wind field in the CALMET model. This wind field is generated by considering several aspects, such as (1) kinematic effects; (2) slope flow; (3) barriers effect; and (4) minimize divergence [4]. The output of this process is called "The step 1 Windfield" [4]. After that, an objective analysis of the observational data is carried out by calculating the interpolation, smoothing, controlling O’Brien, and reducing the divergence. The output of this process is called "The step 2 Windfield" [4]. In this step, meteorology data from WRF is interpolated in the CALMET model to the resolution of 250 meters by considering geographical conditions, meteorological parameterizations, and meteorological data. The output of the CALMET model is a .dat file. This output will be an input to the CALPUFF model together with the emission and stack characteristics data to produce the SO\textsubscript{2} dispersion.

2.4 CALPUFF model
The CALPUFF is an advanced non-steady-state meteorological and air quality modeling system developed by atmospheric Studies Group (ASG) scientists at TRC companies [5]. CALPUFF has been adopted by the U.S Environmental Protection Agency (U.S. EPA) in its Guideline on Air Quality Models as the preferred model for assessing long-range transport of pollutants [4]. The modeling system's main components are the CALMET, CALPUFF, and CALPOST (a post-processing package) [4]. In the CALPUFF model, the calculation of the dispersion of SO\textsubscript{2} is carried out by considering several aspects, such as downwash building effects, plume rise transitions, partial puff movement, topographic interactions, and broader effects such as pollutant removal (wet and dry deposition), chemical transformation, vertical wind shear, the effect of movement over the water surface and the effect of interaction with the coast [4]. The CALPUFF model primarily able to simulate the distribution of pollutants from various sources, such as point, line, area, and volume sources.
The output of the SO₂ dispersion produced by the CALPUFF model is used as input for the CALPOST model. The aims of CALPOST are to see the spread of pollutants in the range of 1 hour, 3 hours, and 24 hours. Before testing the CALPUFF model's ability to simulate the dispersion of SO₂, it is necessary to verify the concentration data in the environment. The verification method is done by calculating the correlation value (r) and root mean square error (RMSE). The correlation value shows the linear correlation between the model output and observation data. Meanwhile, RMSE is used to calculate the difference or error between the model's calculation output and the observed value. The greater the RMSE value, the model's error will be large, and vice versa. The smaller the RMSE value, the error will be smaller.

3. Results and discussion

3.1 Simulation output
CALPUFF modeling is carried out by using wind fields generated from the CALMET and WRF models. The outputs of the distribution of pollutants are plotted at an altitude of 10 meters, assuming that the concentration of SO₂ can affect human activities within that altitude. The following are the outputs of the dispersion of SO₂ for 24 hours during the wet and dry seasons.

Figure 2. Overlaying of the average SO₂ concentration during 24 hours (ug/m³) in the dry season with land cover. The red box shows the highest concentration in the location.

Figure 3. Plotting of windrose during the dry season. The color shows wind speed, and the length of color shows the probability of wind direction.
From the above figures, it can be seen that the distribution of SO$_2$ is divided into two directions. In the wet seasons, the SO$_2$ is dominantly spread to the east and southwest (figures 4 and 5), while in the dry season, it tends to spread to the northeast and west following the dominant wind direction (figure 2 and 3). The distribution of SO$_2$ in the dry season is more spread across residential areas with the highest concentration of 122 ug/m$^3$, which is at a distance of 500 meters from the emission center. While in the other residential locations, the concentration of SO$_2$ ranges from 10 – 47 ug/m$^3$. In the wet season, residential areas affected by the spread of SO$_2$ are only around the emission source, which is at a distance of 600 meters with the highest concentration of 120 ug/m$^3$.

There is an accumulation of concentration in the valley in the wet season with a distance of 3.5 km from the emission source, which values within 220 ug/m$^3$. Even though the area is not residential, this condition can negatively affect the area's ecosystem if it is not anticipated. The occurrence of pollutant accumulation in the valley is often referred to as “plume trapping” [8]. The accumulation of SO$_2$ is caused by the “blocking effect” in the valley and the lowering of the bottom of the inversion, bringing SO$_2$ to the ground. Also, the valley's wind flow is not too dominant, causing SO$_2$ to become stuck on the earth's surface.

3.2 Model verification
Verification is done by comparing the model output with the sample point at 10 locations. This verification aims to test the model's performance in simulating the spread of SO$_2$ in the environment.

The correlation between the observational data and the model output has a value of 0.74 in the dry season and 0.63 in the wet season. It shows that the CALPUFF model can predict the distribution pattern of SO$_2$ well even though the resulting error is quite large, namely 2.89 for the dry season and 5.49 for the wet season. The error value is because the model does not consider the SO$_2$ from other sources such as vehicles, domestic, etc. while the SO$_2$ concentration data in the field is a combination of various sources. The Indarung area is one of the intercity crossings areas where many public vehicles such as trucks and buses, carry passengers and logistics, such as cement raw materials.

3.3 Discussion
Basically, Padang city has unique characteristics, especially from geographic factors. It is bordered by the Indian Ocean in the west, and in the east, it is directly adjacent to the Barisan hill [6]. This characteristic causes wind patterns in the city of Padang and its surroundings to be influenced by local
phenomena such as land winds and sea breezes [6]. From the simulation output of the CALMET wind field (windrose output), it can be seen that the local phenomenon in the study area looks very strong. It is indicated by the presence of 2 dominant wind directions both in the wet and dry season. The difference in wind direction is caused by differences in heat capacity between the Indian Ocean in the west and the Bukit Barisan hill in the east (mainland). During the day, the oceans absorb more heat from the sun than the land. It is because the heat capacity of the oceans is greater than that of land [8]. This large heat capacity causes the absorbed radiation to be greater than the reflection by the surface so that the temperature of the oceans during the day is cooler than the land [8]. Land that has a small capacity can only absorb a small amount of radiation and reflects more surface radiation so that the land temperature during the day is greater. Fundamentally, the wind moves from the area of high pressure (low temperature) to the area of low pressure (high temperature) [8]. It causes the wind to blow more dominantly from the ocean towards the land during the day. The opposite happens at night; the ocean can store a large amount of heat radiation during the day, causing the ocean's temperature to be warmer than the land so that the air pressure is horizontally lower at night. It causes the wind to blow from the colder land towards the ocean. However, the influence of the dry season and wet season on local phenomena in the study area has an impact on the deflection of the dominant wind direction. During the dry season, where the dominant wind comes from the southeast, the wind movement, especially the land breeze, is slightly deflected. During the dry season, the land breeze tends to be in the same direction as the Australian monsoon wind, namely from the southeast, while the sea breeze comes from the southwest and south. Meanwhile, during the wet season where the monsoon winds originate from the north and northeast, it can be seen that the land breeze is slightly deflected when compared to the dry season, namely blowing from the northeast (following the Asian monsoon winds) while the sea breeze comes from the west.

From the concentration level in the environment, it can be seen that the highest concentration produced is still below the threshold set by the government. In Indonesia, the regulation regarding the threshold for a pollutant is in Government Regulation No. 41 of 1999, where the threshold of SO$_2$ for 24 hours has a value of 365 ug/m$^3$. On the other hand, the simulation outputs show that the highest concentration that occurs is 122 ug/m$^3$ in the dry season and 220 ug/m$^3$ in the wet season. The highest concentration in the wet season is caused by the "Plume trapping" phenomenon, where the concentration of SO$_2$ is accumulated in the hilly valleys. The driving force of pollutants, especially the wind speed, is not sufficient to pass through hills [8].

To see the model's ability to perform simulations, model verification needed to be done. It is done by using correlation and error calculations using RMSE. The model is able to simulate the pollutant distribution pattern. It is indicated by a good correlation value (>0.5) even though the error is relatively high. For further research, especially to reduce the model's error value, the researcher suggests that other significant pollutant sources in the study area be included in the CALPUFF model simulation, such as transportation and domestic sources.

4. Conclusion
Based on the simulation results of the dispersion of SO$_2$ using the integration of the CALPUFF and WRF models, it can be concluded that the distribution pattern of SO$_2$ in the study area is strongly influenced by local phenomena, namely land and sea breezes. However, the monsoon effect in wet and dry season causes a deflection of the wind direction. In the wet season, SO$_2$ tends to spread to the southwest and east. Meanwhile, during the dry season, the dominance is spread to the northeast and west. Distribution of SO$_2$ in the dry season is more spread across residential areas than in the wet season. The highest concentration from the simulation results obtained 122 ug/m$^3$ for the dry season and 120 ug/m$^3$ for the wet season. This value is below the Indonesian government's threshold in Government Regulation Number 41 of 1999, which is 365 ug/m$^3$ (24 hours).

The CALPUFF model is able to simulate the dispersion pattern of SO$_2$ well, which is shown by the correlation value of 0.74 (dry season) and 0.63 (wet season) even though the error value is large, namely 2.89 in the dry season and 5.49 in the wet season.
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