Analysis distribution sulfur dioxide and nitrogen dioxide concentration from PLTU Pangkalan susu with callpuff method

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Abstract - Coal-fired power plants will emit several types of pollutants into the ambient air such as particulates and gases. One way to estimate the extent of the impact distribution of these pollutants is by using air quality modeling. The model used in this study is Calpuff , where this model is a non-steady state model and is influenced by variations in meteorological factors. The research location is PLTU Pangkalan Susu (2x200 MW) with SO_2 and NO_2 parameters. The purpose of this study was to calculate the concentrations of SO_2 and NO_2 with Calpuff , to validate modeling with field observations and to simulate the distribution of impacts. The results showed that the concentration of SO_2 model obtained was 0.32 - 3.57 µg/m3 and NO_2 was 0.51 - 5.15 µg/m3. Meanwhile, the observation results showed that the SO_2 concentration was 27 - 39.88 µg/m3 and NO_2 was 19.77 - 29.73 µg/m3. The simulation results of the distribution of SO_2 and NO_2 concentrations with the Calpuff model show that the impact distribution area is in the direction of the wind in the windrose and the affected area is in the southwest of the PLTU Pangkalan Susu. The results of model validation for the values of d = 0.97, r = 0.616 - 0.665 and FB = -1.719 - -1.849, which means that the Calpuff model is quite valid and can be applied to predict the impact distribution area at PLTU Pangkalan Susu.

Keywords: Calpuff, Distribution, Electric Steam Power Plant, NO_2, and SO_2

I. INTRODUCTION

The existence of fossil fuel power plants, especially coal, will have an impact in the form of a decrease in ambient air quality. This occurs because of the specific emissions resulting from the coal-fired steam power plant (PLTU) process such as particulates, SO_2, NO_x, Opacity and Hg which enter the ambient air, thus affecting the function of the air (Pemerintah Republik Indonesia 1999).

The PLTU chimney is a point source category pollutant emission source. Each PLTU chimney is equipped with an air pollution control device that aims to reduce the emission load resulting from plant operations. Emissions emitted from the PLTU chimney will be dispersed into the ambient air so it is necessary

to estimate the concentration level of these pollutants. One way to estimate the ambient air concentration from a point source is by air quality modeling. The use of computer model simulations can be done at low cost and can also perform calculations under various combined conditions (Khosro Ashrafi, Ali Ahmadi Orkomi 2017).

One of the steps in choosing air pollution control technology is knowing the pollutant distribution pattern. Pollutant distribution patterns provide information on the direction and concentration of scattered pollutants, so that it becomes a reference for analyzing the controls that must be carried out so that the impact of hazardous pollutants can be controlled. There are several methods in modeling the spread of pollutants, such as

gaussian models, eulerian models, lagrangian models (Gusrianti, Tarigan, and Suryati 2017).

Dispersion is a process by which contaminants move through the air and spread over a large area and the concentration of pollutants contained in them is reduced. The smoke spreads horizontally and vertically. If the smoke is poisonous, then the movement of the smoke molecules will follow the rules of gas diffusion (Jenned and Dewi 2017).

The release of toxic gases into the air carried by the wind has the characteristics of a plume (smoke that comes out continuously) or a puff (the smoke that comes out is not continuous) (Rasdiana Rahma Nur 2015). According to (Crowl 2011), there are two types of dispersion modeling that are commonly used, namely the model for the plume and the model for the puff. Plume modeling describes a steady-state concentration for a continuously dispersed material. Meanwhile, puff modeling depicts the changing concentration for each distribution. The Calpuff dispersion model is designed to model the dispersion of particles and gases using space and time with varying meteorologies (N.S. Holmes 2006).

In particular, the Calpuff model has been used to simulate the concentration distribution, and health impacts of gaseous and particulate pollutants from various pollution sources and regions. (K. Ghannam 2013). Concluded that the Calpuff model shows the smallest variance, highest correlation, and highest number of predictions in a factor of two compared to the steady state model (Aermod and ISC2) (Rood 2014). Using Calpuff and Aermod to evaluate the spread of odors from industrial estates in the Seobu industrial complex in Korea. The results of his study concluded that Calpuff predicted a concentration that was more suitable to the observations compared to Aermod (Jeong 2011).

Gaseous pollutants that will be modeled for distribution with the Calpuff model in this study are Sulfur Dioxide (SO_2) and Nitrogen Oxide (NO_x). These two parameters include the specific parameters of the coal fired power plant emission. SO_2 is a gas that comes from burning fossil fuels in power plants, industrial facilities, as well as burning fuel at mobile sources such as locomotives, ships, vehicles, other equipment and household combustion (Gusti Ayu Khrisna Saraswati Maharini, 2017).

Sulfur in coal exists in inorganic and organic forms. Pyrite ($FeS2$) is inorganic sulfur other than headquarters ($FeS2$) and sulfate found in coal. Coal sulfur is said to be high if it is greater than 0.8% and the maximum permissible ash content is 26.30%. (Amsya and Rahmalina 2020). The high sulfur content in coal when burned will produce Sulfur Dioxide (SO_2) gas. SO_2 is a colorless gas with a very strong and irritating odor. The impact of SO_2 exposure to humans can cause irritation and sunburn and when it comes into contact with the eyes it can cause damage to the visual system (Wijiarti, Darundiati, and Dewanti 2016).

Another important parameter of PLTU gas emission is Nitrogen Oxide (NO_x). Nitrogen oxides (NO_x) are a group of nitrogen gas present in the atmosphere consisting of nitrogen monoxide (NO) and nitrogen dioxide (NO_2). Nitrogen dioxide can be a liquid and a yellowish brown gas. If the NO_2 concentration is higher than 100 ppm it is lethal to most animals, and 90% of these deaths are due to symptoms of pulmonary edema. NO_2 concentrations of 800 ppm or more resulted in 100% mortality in the tested animals in 29 minutes or less. If a person is exposed to 5 ppm NO_2 for 10 minutes it causes little difficulty breathing (Fardiaz 1992).

Wardhana (2004) added that acid rain occurs because the high levels of SO_2 and NO_2 gases diffuse into the atmosphere and react with water to form sulfuric acid and nitric acid then fall with rainwater. Acid rain will damage ecosystems and materials that are exposed to acid rain. The long-term impact of SO_2 and NO_2 in the ambient air around the PLTU location will have a negative impact on the environment, especially human health. One way to estimate the extent of the impact distribution is modeling so that air quality monitoring can be planned. Based on these problems, this study was conducted to calculate the concentrations of SO2 and NO2 using the Calpuff model, validate the concentration of the model with field observations and simulate the distribution of SO2 and NO2 impacts from PLTU Pangkalan Susu with the Calpuff model.

II. METHODS

The process of estimating and analyzing the distribution of SO_2 and NO_2 in this study is divided into several stages of activity. These stages include primary and secondary data

collection, model application, model simulation, and model validation.

A. Research location

This research was conducted at PT PLN (Persero) Pangkalan Susu Units 3 and 4, located in Tanjung Pasir Village, Pangkalan Susu District, Langkat Regency, North Sumatra Province. The location is ± 7.5 Km from the capital city of Pangkalan Susu ± 107 Km to the northwest of Medan City. PLTU Pangkalan Susu units 3 & 4 with a capacity of 2x200 MW has coordinates LU: 04 ° 06'59.31 ", BT: 098 ° 15'31.58" with an altitude of ± 1 meter above sea level. The total area of the Pangkalan Susu PLTU is 105 Ha. The research location can be seen in Figure 1.

Figure 1. Research Location (source: https://www.google.com/maps/)

B. Data collection
1. Primary Data

Primary data collected in this study were ambient SO_2 and NO_2 concentration data at several sampling points where this concentration data was used to test the model validation. Because PLTU Pangkalan Susu has carried out monitoring of ambient air quality every semester (2 times in 1 year), the sampling points in this study are adjusted to the monitoring points that have been carried out. The sampling points can be seen in Table 1.

Ambient air SO_2 and NO_2 samples were taken using an impinger and analyzed in the laboratory according to SNI according to SNI 19-7119.2-2005 on how to test NO_2 levels with the Griess Saltzman method using a spectrophotometer (Standar Nasional Indonesia 2005a) and SNI 19-7119.7-2005 on how to test SO_2 levels with the pararosanillin method using

a spectrophotometer (Standar Nasional Indonesia 2005b)

Table 1. Sampling Points for SO_2 and NO_2 Concentrations at PLTU Pangkalan Susu

No	Lokasi	Koordinat	
		LU	BT
1	Pulau Sembilan	04°11'11.0"	098°14'59.4"
2	Desa Pintu Air	04°6'25.9"	098°16'8.7"
3	Desa Sungai Siur Dusun IV	04°6'17.6"	098°14'22.1"
4	Desa Tanjung Pasir Dusun V	04°6'0.3"	098°15'7.6"
5	Desa Beras Basah Dusun VI	04°6'34.6"	098°13'48.5"
6	Lokasi PLTU	04°7'3.8"	098°15'38.5"

Source: PLTU Pangkalan Susu, 2020

2. Secondary Data

Secondary data required in modeling SO_2 and NO_2 concentrations using Calpuff are:

a. NCEP-FNL data with a resolution of 1° x 1° as input for the WRF model http://rda.ucar.edu/datasets/ds083.2/
b. Topographic data from Shuttle Radar Topography Mission Version 3 (SRTM3) with high resolution (~ 90 meters or 3 arc sec). (https://dds.cr.usgs.gov/srtm/version2_1/SRTM3/)
c. Land cover data uses the Modis Land Cover which is a product of the U.S Geological Survey (USGS). This Modis Data has a resolution of 0.5 km and can be downloaded at http://landcover.usgs.gov/global_climatology.php
d. CEMS SO_2 and NO_2 parameter data for the period July 2019 to March 2020.
e. Chimney characteristics such as coordinate points, stack height (meters), chimney diameter (meters), emission velocity (m/s), stack temperature (K), height from sea level (meters) and average emissions in wet and dry months (g/s).

C. Application and simulation of the calpuff model

Calpuff is a model that uses a non-steady state approach that takes into account the effects of spatial changes from meteorological components and surface characteristics. Calpuff is able to model the accumulation of pollutants for hours, recirculation and causality effects that the steady state model cannot model (Barclay & Scire, 2011) in (Pratama 2015). The Calpuff modeling system consists of 3 main components, namely:

a. Calmet, is a meteorological model that generates a diagnostic wind field that takes into account the objective analysis and parameterization of tilt flow, topographic kinematic effects, topographic drag effects, minimizes divergence and is a micrometeorological model that can be used up to the boundary layer.
b. Calpuff ,
c. is a Lagrangian Gaussian model that takes into account various parameters, namely complex topographic effects, displacement over water, coastal interaction effects, downwash effects and chemical transformation.
d. Calpost, is a post-processing program capable of calculating the average concentration and prediction of flux deposition from the results of the CALPUFF model. The results of CALPOST can be visualized using Calview.

Basically, the Calpuff model can simulate the distribution of emissions from various sources, such as point, line, area and volume sources. The basic equation used in the Calpuff model is as in the following equation.

$$C = \frac{Q}{2\pi\sigma_x\sigma_y} \, g \, exp\left[-\frac{d_a^2}{2\sigma_x^2}\right] exp\left[-\frac{d_c^2}{2\sigma_y^2}\right]$$

$$g = \frac{2}{(2\pi)^{1/2}\sigma_z} \sum_{n=-\infty}^{\infty} exp[-(H_e + 2nh)^2 / (2\sigma_z^2)]$$

Information:

C: Soil surface concentration (g/m^3),
Q: Mass of pollutant (g) in puff

σ_x : Standard deviation (m) of the Gaussian distribution parallel to the wind direction,
σ_y : Standard deviation (m) of the Gaussian distribution perpendicular to the wind direction,
σ_z : Standard deviation (m) of the Gaussian distribution along the vertical axis,
d_a : Distance (m) from the center of the plume to the receptor parallel to the wind direction,
d_c : Distance (m) from the center of the puff to the receptors perpendicular to the wind direction,
G : Vertical Gaussian equation (m),
H : Effective height above ground level from the center of the plume (m)

D. Model validation

Validation is used to determine the suitability and performance of the model used in predicting a condition. Validation is often used to compare model data with field observations, especially air quality modeling, including Wilmott's Index of Agreement (d), Normalized Mean Square Error (NMSE), Root Mean Square Error (RMSE), correlation (r) and Fractional Bias (FB) (Tarigan, Suryati, and Gusrianti 2018). In this study to test the model validation the following approach was used:

a. *Wilmott's Index of Agreement* (d)
$$d = 1 - \frac{(Cpred - Cobs)^2}{((Cpred - Cobs) + (Cobs - Cobs))^2}$$
b. *Correlation (r)*
$$r = \frac{\sum_{i=1}^{N}(C_{pred,i} - \overline{C_{pred}})(C_{obs,i} - \overline{C_{obs}})}{\sqrt{\sum_{i=1}^{N}(C_{pred,i} - \overline{C_{pred}})^2 \sum_{i=1}^{N}(C_{obs,i} - \overline{C_{obs}})^2}}$$
c. *Fractional Bias (FB)*
$$FB = \frac{2\,(\overline{C_{pred}} - \overline{C_{obs}})}{C_{pred} + C_{obs}}$$

Information:

C_{pred} : Concentration model ($\mu g/m^3$)
C_{obs} : Concentration of observations in the field ($\mu g/m^3$)
$\overline{C_{pred}}$: Model concentration mean ($\mu g/m^3$)
$\overline{C_{obs}}$: Average concentration of observations in the field ($\mu g/m^3$)

According to (Willmott, Robeson, and Matsuura 2012) The level of suitability between the model and measurement is high if the index of agreement (d) value obtained is close to 1. The correlation coefficient values range from -1 to +1. A value of +1 indicates a strong linear relationship which is directly proportional, while a negative value indicates the model result is inversely proportional to observation. The closer to +1, it means that the two variables show an increasingly similar pattern. The correlation coefficient of 0 indicates that there is no linear relationship between the two variables.

According to (Ganguly, Broderick, and O'Donoghue 2009), if the Fractional Bias (FB) value is close to 2, it indicates that the condition between the model and measurement is below the prediction, while if the value is close to -2 it indicates that the conditions between the model and measurement exceed the prediction.

III.   RESULTS

1. Windrose

Windrose is a description of the dominant wind direction and speed in a location. In the analysis of pollutant disperse modeling, wind direction and speed is an important parameter. The results of windrose around the Pangkalan Susu PLTU can be seen in Figure 2.
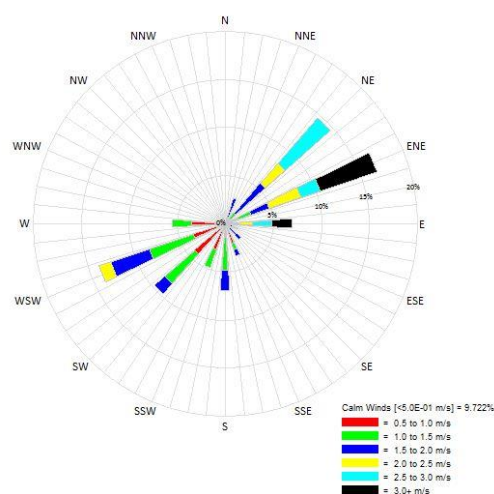

Figure 2. The results of windrose around the Pangkalan Susu PLTU

Based on Figure 2, it can be seen that the dominant wind direction comes from TTL (Northeast East) to BBD (Southwest Southwest) with speeds ranging from 1 m / s -

3 m/s. Apart from the BBD (Southwest Southwest), the wind direction is also dominant from the Northeast Sea to the Southwest. When viewed from the dominant wind direction, the areas that will be exposed to the impact of SO_2 and NO_2 emissions from the Pangkalan Susu PLTU are areas in the Southwest and BBD (Southwest Southwest). In addition, the position of the Pangkalan Susu PLTU is on the edge of the Malacca Strait so that the dispersion of pollutants is greatly influenced by sea breezes during the day and land winds at night.

2. SO_2 and NO_2 Concentrations CALPUFF vs Field Observation Modeling

Calpuff modeling requires input data as shown in Table 1.

Table 1. Calpuff   data input

No	Type of Data	Value	Unit
1	Coordinate	04°06'59.31" LU dan 098°15'31.58" BT	
2	Chimney height	185	m
3	Base chimney elevation	1	m
4	Chimney diameter	4.5	m
	Dry Month		
5	SO_2 density	170.09 – 217.32	mg/m^3
6	SO_2 Flowrate	151.41 - 179.09	m^3/s
7	SO_2 Emission Load	30.46 – 32.90	g/s
8	NO_2 density	263.25 – 313.16	mg/m^3
9	NO_2 Flowrate	151.41 - 179.09	m^3/s
10	NO_2 Emission Load	42.31 – 47.42	g/s
11	Flow speed	9.52 - 11.27	m/s
12	Temperature	391.37 – 391.63	Kelvin
	Wet Moon		
13	SO_2 density	279.84 – 361.24	mg/m^3
14	Flowrate SO_2	206.15 – 267.42	m^3/s
15	SO_2 Emission Load	74.47 – 74.83	g/s
16	NO_2 density	310.10 – 404.42	mg/m^3
17	NO_2 flowrate	206.15 – 267.42	m^3/s
18	NO_2 Emission Load	0.41 – 3.76	g/s
19	Flow speed	12.97 – 16.82	m/s
20	Temperature	390.55 – 395.94	Kelvin

Source: PLTU Pangkalan Susu, 2020

After all the data required for modeling is entered, the Calpuff   program is executed so that the SO_2 and NO_2 concentrations of Calpuff modeling are obtained and for the validation of the modeling results, sampling is carried out at the same coordinate points as the modeling so that the observation concentration is obtained as in Figures 3 and 4.
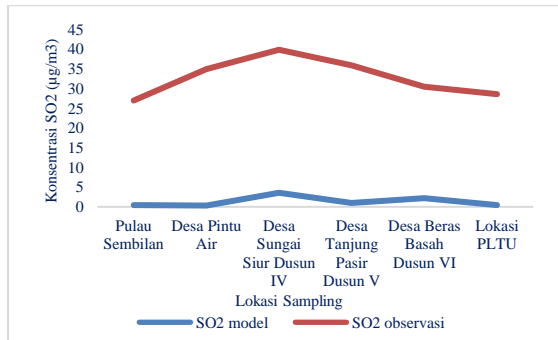
Figure 3. SO_2 Model Concentration and Observation SO_2 Concentration at PLTU Pangkalan Susu

Figure 3 shows the SO_2 concentration using the Calpuff model and the results of field observations. In Figure 3 it can be seen, the point that has a high concentration for observation and modeling is at point 3 (Sungai Siur Village) of $\pm$ 39.88 µg / m3 for observation and $\pm$ 3.57 µg / m3 for modeling. When viewed as a whole from the graph in Figure 3, the pattern / trend of the concentration values with models and measurements tends to be the same. The results of this study are in line with research conducted by (Shubbar et al. 2019).

The point that is not in accordance with the modeling pattern is point 2 (Pintu Air Village) where the model results show a decrease but the observation results have increased. While at point 5 (Beras Basah Village), the SO_2 model concentration value shows an increase and the sampling value shows a decrease. In addition, the results of both observation and modeling concentrations are still below the ambient air quality standard for SO_2 (1 hour) of 900 µg / m^3. (Kementerian Lingkungan Hidup dan Kehutanan 2019).
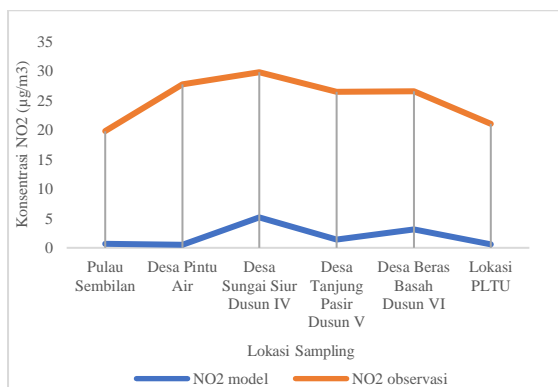

Figure 4. Model NO_2 Concentration and Observation NO_2 Concentration at PLTU Pangkalan Susu

Based on Figure 4, it can be seen that the trend pattern of NO_2 concentration modeling with observation has the same trend. This can be seen in the modeling of the point that has a high concentration is point 3 (Sungai Siur Village) of $\pm$ 5.15 µg / m3 and the results of observations in the field show that point 3 also has the highest concentration of $\pm$ 29.73 µg / m3. The unequal pattern between the model and observation is seen only at point 2 (Pintu Air Village) where the observation has increased while the modeling has decreased. Overall the results of modeling and field observations show that the NO_2 concentration is still below the ambient air quality standard NO_2 (1 hour) of 400 µg / m^3 (Kementerian Lingkungan Hidup dan Kehutanan 2019)

3. Simulation of the distribution of SO_2 and NO_2 from PLTU Pangkalan Susu with Calpuff

Calpuff modeling is carried out using wind modeling output from Calmet. The pattern of concentration distribution with Calpuff can be made an average per hour, a average per day and a mean total period. The distribution results that will be presented in this study are the total period average. The map of the distribution of SO_2 and NO_2 with the source of emissions from PLTU Pangkalan Susu is shown in Figures 5 and 6.
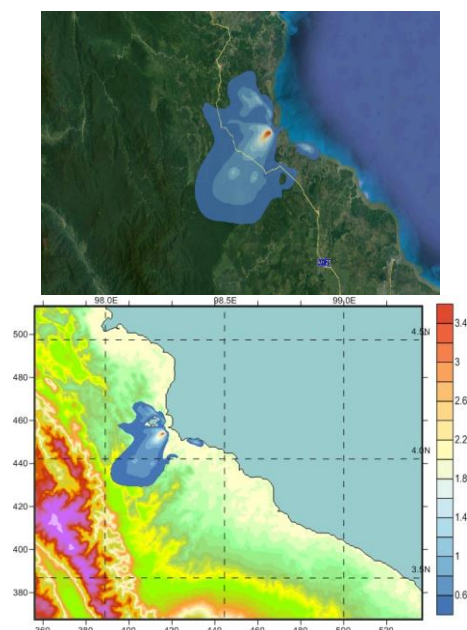

Figure 5. Simulation Results of SO_2 Distribution Patterns (Total Period Average) around PLTU Pangkalan Susu

Based on Figure 5, it can be seen that the distribution of SO_2 pollutants to the Southwest and Southwest with the highest concentration according to the Calpuff modeling is 3.57 µg / m3 at a maximum distance of 2,205.79 m from the source (PLTU Pangkalan Susu). When seen from Figure 2 (windrose), the dominant wind direction comes from the Northeast to the Southwest, so it can be concluded that the SO_2 distribution modeling with Calpuff follows the wind movement pattern. PLTU Pangkalan Susu is a seafront area so it is greatly influenced by sea breezes during the day and land winds at night. Sea winds are strong enough to bring pollutant dispersions ashore during the day.
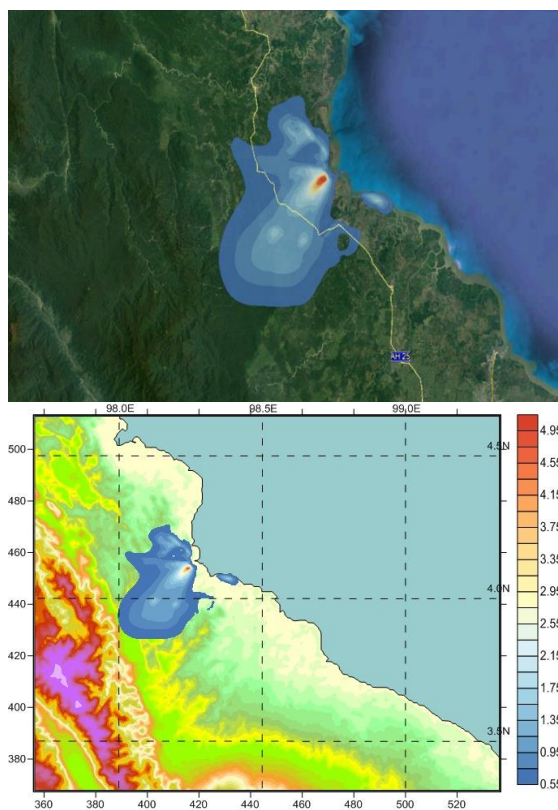

Figure 6. Simulation Results of NO_2 Distribution Patterns Around PLTU Pangkalan Susu

Research result (Pratama 2015) For modeling the distribution of SO_2 from the chimney of PT Semen Padang also tends to be in the direction of the wind. The area of the PT Semen Padang area which is on a hill causes the distribution of SO_2 at night to be higher during the day due to the blocking effect of the hills in the southern part, resulting in a buildup in the valley.

According to (Abdul-Wahab, Sappurd, and Al-Damkhi 2011), The use of the Calpuff model to determine the distribution of SO_2 pollutants from oil refinery activities in Oman is also in the direction of the wind and Calpuff also has better performance than ISCST. This statement is also corroborated by the results of research conducted by (Rood 2014) which compared the performance of using the Aermod, ISC2, Calpuff and Ratchet models.

In Figure 6, you can see the distribution of NO_2 concentrations originating from the Pangkalan Susu PLTU activities spreading to the Southwest and Southwestern directions. This is consistent with the dominant wind direction from the windrose (figure 2) coming from the Northeast. The maximum distance for the distribution of NO_2 pollutants is 2,224 m with a maximum concentration of 5.15 µg / m3.

The Calpuff model is a non-steady state model so that the pollutant distribution pattern is strongly influenced by meteorological conditions, especially wind direction and wind speed. Research result (Prueksakorn, Kim, and Vongmahadlek 2014) shows that the Calpuff model can reliably predict the distribution of odors in various weather parameters such as temperature, wind speed and wind direction which vary over time, complex terrain with the bottom topography of the basin, surrounded by mountains of the city of Changwon, South Korea. (Abdul-Wahab et al. 2011) obtained the simulation results of the Calpuff case study showing that winter NO_x concentration levels exceed US EPA allowable concentrations of emissions from a steel mill in Muscat, Oman.

IV. DISCUSSION

The results of the model validation with field observations for the d, r and FB values can be seen in Table 2.

Table 2. Model validation results

No	Parameter	d	r	FB
1	SO_2	0.972	0.616	-1.849
2	NO_2	0.972	0.665	-1.719

The index of agreement (d) value obtained from Calpuff modeling at PLTU Pangkalan Susu is 0.972 or it can be interpreted that 97.2% of the data obtained is valid and 2.8% error. This value can be classified into the criteria for the index of agreement (d) where the level of

suitability between the model and measurement is high if the index of agreement (d) value obtained is close to 1.

The correlation values (r) of the modeling for the concentrations of SO_2 and NO_2 were 0.616 and 0.665, which means a positive sign indicates a linear relationship between the model and observation. The numbers 0.616 and 0.665 show that it is getting closer to +1, meaning that the two variables show an increasingly similar pattern. The Fractional Bias (FB) values obtained for SO_2 and NO_2 are -1.719 and -1.849 which indicates that these values fall into the Fractional Bias (FB) criteria, which is in the range -2 to 2 which means the value is close to -2 indicating that the intermediate conditions models and measurements exceed predictions.

V. CONCLUSION

Based on the results of the research that has been done, it can be concluded as follows:

1. The SO_2 concentration results from the Calpuff model ranged from 0.32 - 3.57 µg / m3 with the exposure distance at the maximum concentration of 2,205.79 m, meanwhile for the NO_2 concentration the Calpuff model results ranged from 0.51 - 5.15 µg / m3 with the exposure distance at the maximum concentration as far 2,224 m.
2. SO_2 concentrations from field observations ranged from 27 - 39.88 µg / m3 and NO_2 observations were 19.77 - 29.73 µg / m$_3$.
3. The concentrations of SO_2 and NO_2 from modeling and observation are still below the ambient air quality standard PP No. 41 of 1999.
4. The simulation results of the distribution of SO_2 and NO_2 in the direction of windrose where the affected area is the area in the southwest of the Pangkalan Susu PLTU.
5. The results of model validation by observation show the value of d = 0.972, r = 0.616 - 0.665 and the value of FB = -1.719 - - 1.849. These results indicate that the Calpuff model is quite valid and can be applied to predict the distribution of pollutants from PLTU Pangkalan Susu.

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