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Dear Dr. Nur Hamzah,

Hope this e-mail finds you well.

I am contacting you based on your expertise.

Currently, we are in the process of editing the manuscript with the title "Evaluation of Kinetic Mechanism for Modelling Di-methyl Ether Jet Diffusion Flame" to be published by Faculty of Engineering and Technology, Sampoerna University. In order to strengthen the overall quality of this important publication, I would like to kindly invite you to assist me in the review process of this publication. We do believe that your review process can make a significant contribution for this coming publication (October 2022).

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Evaluation of Kinetic Mechanism for Modelling Dimethyl Ether Jet Diffusion Flame

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ABSTRACT

Many countries use liquefied petroleum gas (LPG) for various purposes, such as cooking and heating. As the population and the need for energy grow, demand for LPG steadily increases. This situation causes the rise in LPG imports for countries with an insufficient local supply, including Indonesia. To overcome this problem, the Indonesian Government plans to substitute LPG fuel with dimethyl ether (DME). However, stoves and household burners widely used in Indonesia are designed for LPG. Thus it is necessary to study the fuel flexibility of the burners. Many experimental studies on the substitution of LPG with DME are reported in the literature, but few models have been developed to simulate it. This paper aims to evaluate the performance of reaction mechanisms developed to model DME diffusion flames with various burner temperatures ranging from 300 to 1500 K. It was found that existing models could simulate the chemical structure of the flame but could not predict the formation of enthalpy of combustion reactions.

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1. INTRODUCTION

Since the implementation of the kerosene to LPG conversion policy in 2007, the need for LPG in Indonesia has continued to increase. The LPG supply in 2019 reached more than 7 million tons, of which around 2 million tons (26%) came from domestic refinery production, and around 5.7 million tons (74%) were obtained from imports. The most significant LPG consumption was in the household sector, which reached 95.9%, followed by the commercial sector with

2.66% and the industrial sector with 1.45% (ESDM, 2019). From the results of modeling the needs and supply of LPG in 2015 - 2050 (Setkab, 2017), it can be seen that the number of LPG imports will be suppressed through the use of other types of fuel, namely Dimethyl Ether (DME) and municipal gas networks (jargas).

DME is a simple ether compound produced from various raw materials such as natural gas, coal, and biomass. It has a high cetane number and properties similar to LPG, such as viscosity, boiling point, and pressure. In addition to being used in industry, transportation, and power generation as a substitute for fossil fuels, DME also offers the option to replace LPG as a household, trade, and industrial fuel currently still being imported (Kang et al., 2015; Zhang et al., 2022).

Previously, an experimental study was performed by Anggarani et al. (2014) to identify the physical, chemical, thermal, and flame stability characteristics of DME and LPG blends up to 50% concentration. It was found that the introduction of DME to LPG did not affect the flame stability in various stoves. However, DME lowered the stove's fuel efficiency and heat input due to the lower calorific value than LPG. The study recommended further study on burner design optimization for DME.

Arya et al. (2016) reviewed studies on DME as a cooking fuel alternative for Indian households. This study discusses the DME production method, fuel, and combustion characteristics of DME. The review study recommended further study on the basic combustion behavior of DME/LPG blends, developing a compact LPG-DME mechanism, and more studies on DME diffusion flames. Furthermore, burner design should enable an efficient combustion process to minimize emissions that are harmful to the environment (Jusli et al., 2021).

Fundamental studies on DME combustion enable the development of precise reaction mechanisms. Many fundamental studies on DME combustion have been reported on jet-stirred reactors, flow reactors, laminar burning velocity, and shock tubes (Huang et al., 2021). Apart from the accuracy of the mechanism, the improvement of the mechanism also considers the size of the reaction mechanisms to minimize the computational cost of running the combustion simulation. Previously, the reduced mechanisms have been proposed by Prince et al. (2015) and Pan et al. (2015).

Reducing the size of the combustion mechanism may cost the model's accuracy (Pan et al., 2015). Moreover, the mechanisms are mostly validated against the fundamental experimental data such as shock tubes, jet-stirred reactor(JSR), and many more. More experimental data is required to validate the accuracy of the combustion mechanism. It is interesting to know the mechanism's performance in a Computational Fluid Dynamic (CFD) model, such as a jet flame simulation.

DME jet diffusion flame simulation has been performed previously by Kang et al. (2015). The study investigated the effect of hydrogen addition on DME combustion characteristics using experimental and numerical methods. The experiment used identical geometry as used in the 2D CFD model. The model could predict the chemical structure of DME jet diffusion flame validated with their experimental data. However, the study did not vary the wall and unburnt gas temperature.

The utilisation of alternative fuels requires fuel flexibility of the burners. The availability of an accurate combustion model reduces the dependency on the experimental work, which is costly and time-consuming to evaluate the performance of burner designs when running on alternative fuels. Also, combution models can

optimize the design of burners before the prototype is manufactured. With the advancement of the DME combustion mechanism, this study aims to model DME jet diffusion flame, which can add more insight into experimental data reported previously in the literature. It emphasizes the effect of temperature on the prediction of DME flames.

2. RESEARCH METHODOLOGY

This study used ANSYS R2.1 for simulating the DME jet diffusion flame. **Figure 1** illustrates the geometry of the model. The geometry of the model was designed symmetrically to minimize the computational cost. The geometry is a rectangular shape with a width of 240 mm and a length of 1900 mm. Also, at the bottom-right of the geometry, there is an inlet with a diameter varied up to 10 mm. The top, left, and right boundaries are pressure outlets. The bottom boundary is a velocity inlet that supplies the airflow. The air was defined as theoretical air consisting of nitrogen and oxygen at 79 and 21 percent, respectively. Meanwhile, the pressure was set to atmospheric condition.

After building the geometry, the meshing process was performed. It resulted in more than 90,000 elements, which is sufficient compared to the work of (Kang et al., 2015). Moreover, the mesh integrity test was performed to know the effect of grid refinement on the results. The test indicated that adding elements to the mesh did not shift the results enormously.

The reaction mechanism was taken from Zhao et al. (2008). It is a detailed DME reaction mechanism with 55 species and 290 reversible reactions. The reaction mechanism has been tested against experimental data, such as shock tube, counterflow diffusion flame, burner-stabilized premixed flame, and spherical bombs from previous studies. The prediction from the reaction mechanisms reproduces these experimental data reasonably well. Furthermore, the setup of FLUENT was defined to run a steady state simulation with energy equations activated and *a k*-epsilon turbulence model. All simulations were executed until convergence is reached. The results were exported and analyzed using Tecplot software.

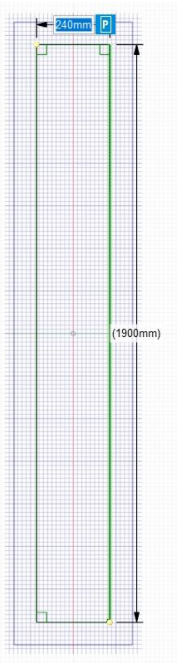

Figure 1. The geometry of the CFD model

3. RESULTS AND DISCUSSION

The initial simulation shows that the results were sensitive to the unburnt gas and wall temperature. Thus, this study created several scenarios of various walls, and unburnt gas temperatures ranging from 300 to 1500 K. **Figure 2** shows the typical results of DME jet flame temperature prediction. This scenario uses wall and unburnt gas temperatures of 300 K and 900 K (right) and 900 K and 300 K (left), respectively. It can be observed that the highest temperature of the flame occurs directly at the fuel inlet. This location of the highest temperature should not happen because it indicates that the reaction happens very close to the inlet,

where there is no oxygen concentration to oxidize the fuel. Alternatively, the temperature was changed to 900 K of nozzle wall and 300 K of unburnt gas. This scenario indicated that there is no ignition in all regions.

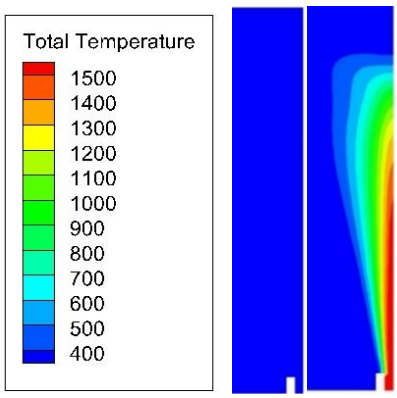

Figure 2. Prediction of the total temperature of DME flames in Kelvin

Compared to the work from Kang et al. (2015), which also used a similar range of wall and gas temperature, this work could not predict the flame's dark zone, which is the region where the fuel is unburnt because it is not introduced to oxygen yet. In this work, the highest temperature of the flame occurs in the expected dark zone instead.

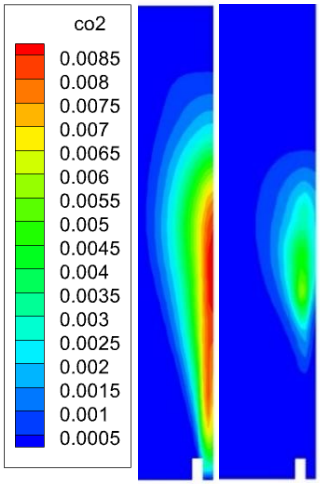

Figure 3. Prediction of CO_2 concentration of DME flames

Despite having issues with temperature prediction, the model was able to provide a prediction for the flame chemical structure. **Figure 3** presents the carbon dioxide concentration prediction in DME flames. The left image is the scenario for 1500 K nozzle and unburnt gas temperature, while the right image is the scenario for 900 K nozzle and unburnt temperature. It can be seen that increasing the wall and unburnt gas temperature enhances the production of CO_2.

The peak of CO_2 concentration was predicted at the middle of the flame at 0.85%. This value is relatively low compared to the expected CO_2 concentration at complete combustion reaction. Ideally, the peak of CO_2 concentration for a jet diffusion flame should occur in the region close to the interaction with ambient air.

Figure 4 indicates the concentration of DME from the inlet nozzle to the ambient air. The left image is the scenario for 1500 K nozzle and unburnt gas temperature, while the right image is that for 900 K. It indicates that at the inlet point, both scenarios have nearly 100 percent of DME concentration, which is as expected. At the same time, the change in the gas and nozzle wall temperature affects the conversion of DME to other species. At high temperatures, DME molecules were converted faster. Thus the area with high DME content is concentrated close to the inlet nozzle. At a lower temperature, the conversion of DME becomes slower, thus dispersed wider from the inlet nozzle. In the combustion kinetic model, the temperature is essential in determining the reaction rate. Considering that the concentration of CO_2 is low, DME might undergo thermal decomposition and partial oxidation.

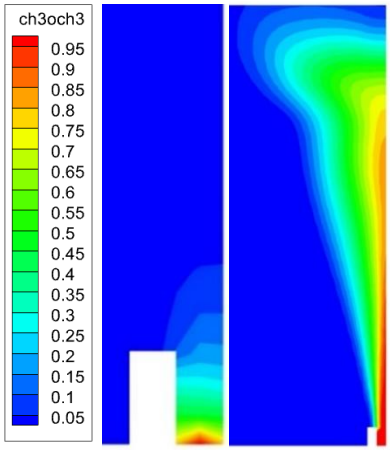

Figure 4. Prediction of DME concentration of DME flames.

Figure 5 illustrates the oxygen concentration around the expected flame zone. It visualizes oxygen diffusion from ambient air consumed by the combustion reaction. It indicates diffusion flame by showing low oxygen concentration (blue region) at the inlet nozzle. The oxygen concentration gradually increases at higher locations due to natural diffusion, which attracts oxygen to the reaction zone.

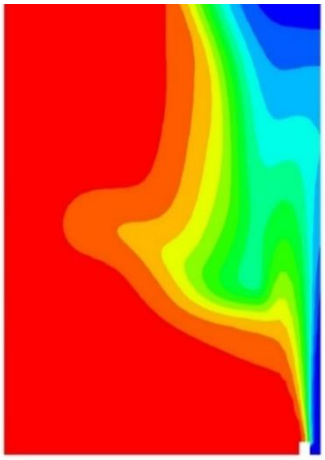

Figure 5. The typical result of oxygen concentration of DME flames.

Figure 6 shows the OH concentration near the flame zone. OH is a radical active that is abundant in combustion reactions. It initiates a chain reaction in the combustion mechanism. OH radicals also indicate a reactive zone in the flame. The oxygen atom in the OH radical can be formed from the ambient oxygen or oxygen in the decomposed DME molecule. From **Figure 6**, higher OH concentration occurs at higher flame positions. This observation is reasonable since, at a higher position, the unburnt gas receives higher oxygen concentration, yielding OH production. The higher temperature shows more OH concentration, while lower OH concentration was found in the lower temperature. The higher temperature provides more energy for the bond breaking of the molecules for forming the radicals.

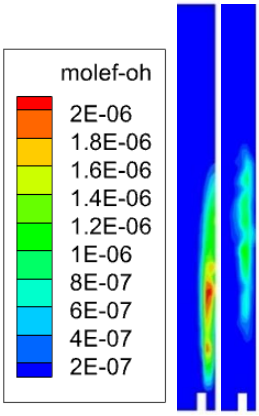

Figure 6. The typical result of OH concentration of DME flames.

The data shows that the maximum temperature obtained never exceeds the temperature entered for the wall temperature. Based on this finding, an investigation was performed for a methane simulation with a different reaction mechanism, namely GRI mech 3.0. (Smith et al., 1999). This simulation was carried out with the same boundary condition setup and calculation method. The comparison to Zhao mechanism is presented in **Figure 7.** It is clear that using Zhao mechanism; the model could not predict the ignition process. Thus, the gas temperature did not increase from 300 K since there was no enthalpy production at the expected flame zone. Meanwhile, the

GRI mechanism could simulate the ignition process. Thus, it results in a higher temperature at the flame zone, which exceeds 1000 K despite having a 300 K wall and unburnt gas temperature due to the enthalpy production.

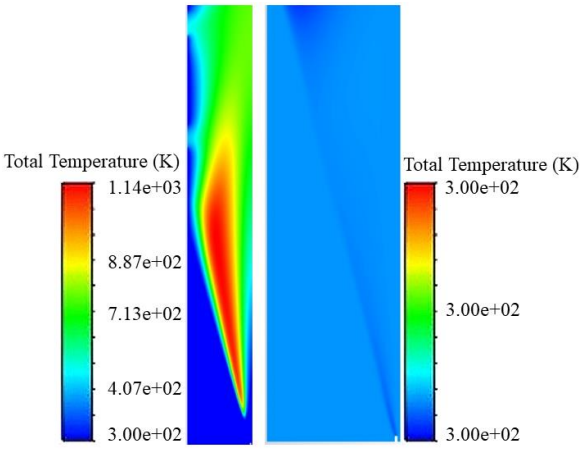

Figure 7. Comparison of methane jet diffusion flame simulation using GRI mech 3.0 (Smith et al., 1999) (left) and Zhao mech (right)

The temperature of auto-ignition of the methane-air mixture at atmospheric pressure is between 793 K and 923 K (Norman, 2008). However, in the current simulation, auto-ignition is observed at room temperature. Thus, further study must be conducted to investigate the cause of methane flame ignition in the model.

4. CONCLUSION

The advancement of fundamental DME combustion studies enables the prediction of DME flames through a CFD simulation. This paper investigates the effect of the wall and unburnt gas temperature on the structure of DME jet diffusion flames.

At low and high temperatures, the temperature variation shows different concentration distributions of major species, such as carbon dioxide, OH radical, DME, and oxygen.

Several observations made in the current simulations are:

1. The amount of CO_2 rises with the increase in the temperature of the wall and unburnt gas.
2. The spread of DME is inversely proportional to temperature. At a higher temperature, DME content is mainly near the nozzle.
3. The amount of O_2 increases as the air inlet and nozzle temperature decreases.
4. The amount of OH produced is proportional to the temperature of the air inlet and nozzle.

There is still a room for improvement for the current model to achieve a better accuracy. Other researchers can use the current simulation model as a base model to test various chemical reaction mechanisms and boundary conditions. This will significantly reduce the duration of the research.

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