Jurnal Teknologi

COMPUTATIONAL STUDY ON COMBUSTION AND EMISSION CHARACTERISTIC OF PILOTED FLAMES BY VARYING COMPOSITION CO_2 OF SIMULATED BIOGAS

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> This study investigates the performance of flamelet model technique in predicting the behavior of piloted flame. A non-premixed methane flame of a piloted burner is simulated in OpenFOAM. A detailed chemistry of methane oxidation is integrated with the flamelet combustion model using probability density function (pdf) approach. The turbulence modelling adopts Reynolds Average Navier Stokes (RANS) framework with standard k-E model. A comparison with experimental data demonstrates good agreement between the predicted and the measured temperature profiles in axial and radial directions. Recently, one of major concern with combustion system is the emission of pollution specially NOx emission. Reduction of the pollutions can be achieved by varying the composition of CO2 in biogas. In addition, the effect of the composition of biogas on NO_x emission of piloted burner is still not understood. Therefore, understanding the behavior composition of CO2 in biogas is important that could affect the emission of pollution. In the present study, the use of biogas with composition of 10 to 30 percent of CO2 is simulated to study the effects of biogas composition on NO_x emission. The comparison between biogas and pure methane are done based on the distribution of NO_x, CO₂, CH₄, and temperature at different height above the burner. At varying composition of CO2 in biogas, the NOx emission for biogas with 30 percent CO2 is greatly reduced compared to that of 10 percent CO₂. This is due to the reduction of the post flame temperature that is produced by the dilution effect at high CO2 concentration.

Keywords: CFD, combustion, biogas, flamelet, methane

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1.0 INTRODUCTION

Biogas can be utilized directly as heat source to generate power in gas turbines and internal

combustion engines. The heating value of biogas is generally 600-800 Btu/fts [1,2]. Biogas that is derived from decomposition of organic waste is considered to be renewable energy source [3, 4] and the fuel offers advantages over conventional fuels in terms of



Radial distance (m)

Article history

Received 18 April 2017 Received in revised form 30 April 2017 Accepted 15 August 2017

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Full Paper

combustion efficiency and emission. Natural gas is used widely in automobile industry due to the high performance and low emissions. However, resource of natural gas has dramatically decreased in certain region due to the high demand. Alternatively, biogas can be used as energy source in domestic and industrial application to support the shortage conventional fuel. Biogas that is produced by the anaerobic fermentation of biomass has been proven to produce low level of emission. Biogas has similar characteristics with the natural gas in terms of the composition of methane (50-75 %) and carbon dioxide (20-50%). The biogas derived from agricultural waste may be classified as carbon neutral fuels that have minimal greenhouse effects to the environment [5, 6]. The combustion characteristic of simulated biogas that is diluted with CO₂ has been studied due to the positive effects on emission. The simulated biogas reduces flame temperature and NO_x emission due to reduction of the reactive species concentration [7, 8]. Previously, NO_x emission in a diesel engine is decreased significantly using biogas fuel blend. The effects of CO2 dilution in fuel or oxidiser stream was investigated by several studies [9-20]. Numerical investigation on the effects of dilution was performed on flame structure of methane diffusion flame has been studied. Other studies investigated the effects of CO2 dilution on the blow off [12] and extinction characteristics [13]. Even though few studies have been done on the effects of CO2 dilution on the flame characteristics, a more detailed analysis is needed to understand the mechanism of NOx reduction via dilution. The present study will analyse and compare the effects of the CO₂ dilution in biogas on flame temperature and NO_x emission of a piloted flame burner.

2.0 METHODOLOGY

2.1 Experimental Condition

An experiment of piloted diffusion flame by Brookes and Moss [3] was used for result validation. In Figure 1, the fuel with 99% percent purity flows from the inlet, with the diameter of 4.07 mm. The inlet is enclosed by a pilot nozzle with outer diameter of 4.32 mm.



Figure 1 Piloted methane burner geometry [3] in the present study

The pilot stream is encompassed by moderate air coflow of 1 m/s with coflow diameter of 150 mm. The velocity of fuel stream and pilot are 21 m/s and 2.3 m/s respectively. Table 1 summarises the experimental conditions. The combustion species was measured by method of Raman and laser induced fluorescence techniques while the temperature was measured using Rayleigh measurement.

Table 1Experimental conditions of the piloted diffusionflame [3]

Operating Condition	Fuel	Pilot	Coflow
Temperature (K)	290	290	290

2.2 Numerical Condition

The transport equations of mass, momentum, energy and species are solved by the standard solver in OpenFOAM where the turbulent flow is modelled using the standard k- ϵ model.

The flamelet model that was incorporated in turbulent combustion solver in OpenFOAM offers a wide range of modelling capability of complex fluid flow including combustion, reaction, turbulence, and heat transfer. The combustion model incorporates flamelet library called steady laminar flamelet model (SLFM) that incorporate as steady and laminar counter flow diffusion flame for the flame structure solution in the mixture fraction space [11]. The flame structure is characterized by the scalar dissipation rate that represents the effects of velocity gradient and local strain on turbulent flame. In terms of computational efficiency, the main advantage of flamelet method is the decoupling of flame chemistry from the turbulent stream. This is accomplished by using the passive mixture fraction to model transport of scalars in the mixture. The impact of turbulence on combustion is modelled using presumed probability density function (PDF) [13, 14, 15].

The standard model has various PDF shapes and the possibility to model soot formation as well as heat losses. In that context, the real-gas thermodynamic effects have to be taken into account when calculating the flamelet as shown previously [16]. The new flamelet libraries are incorporated in the existing OpenFOAM framework to guarantee full flexibility. The generation of flamelet library at varying pressure, temperature, and composition is done using published chemical kinetics that is formatted in Cantera.

2.3 Flamelet Library

The flamelet library is developed by solving the temperature and species across different mixture fraction space using the energy and species equation along with the scalar dissipation table. The integration of presumed PDF with the developed library can be used to solve the interaction between turbulence fluctuations and chemistry. The flamelet library will be read during the post processing stage when the mean flow results and presumed PDF are used to calculate the mean species mass fraction and temperature based on the mixture fraction, variance and the scalar dissipation.

Table 2 shows the operating condition of pure methane to generate flamelet library that includes pressure, temperature, mass flow rate of fuel and air, fuel and oxidizer composition, chemical reaction mechanism, and domain length. Using the boundary condition at the fuel and oxidiser inlets in one dimensional reacting flow, the scalar dissipation table is generated. The scalar dissipation tables are used in the flamelet model to calculate the mean species in the turbulent diffusion flame of the present study. Three flamelet libraries are generated under varying fuel composition of 10, 20 and 30 percent of CO₂.

 Table 2
 The parameters for counter-flow diffusion flame for flamelet library generation

Operating Condition	Values	
Pressure	1.013e5 Pa	
Temperature	294	
Mass flow air	0.5 kg/m	
Mass flow fuel	0.1	
Fuel composition (mole	CH4:1	
fraction)		
Oxidizer composition (mole	O2:21 N2:0.79	
fraction)		
Mechanism	GRI 3.0	
Domain Length	0.2	

2.4 Grid Independence Test

Four different mesh have been used for mesh independence study that include 12000, 30000, 51000 and 82000 cells. The mesh independence was achieved at 51000 cells based on the predicted temperature profile in the radial direction at 150 mm downstream of the burner.

3.0 RESULTS AND DISCUSSION

3.1 Validation for Numerical Prediction of Flamelet Model in OpenFOAM

The predicted flame temperatures in the axial and radial direction of methane flame are compared with measurement data in methane flame experiment with coflow burner [3]. The temperature profile was measured using Pt fine wire thermocouple with 50 µm diameter (Type R) [3]. Figure 2 shows the measured and predicted temperature distribution in the axial and radial directions. Referring to Figure 2(a) and 2(b), the flame temperature increases along the flame length in the axial direction and reduces further away from the flame front in the radial direction. The maximum value for the radial temperatures at flame height of 150mm and axis temperature of 1807 K, 1620K was obtained as shown in the Figure 2.

Figure 2 shows that the prediction of temperature is in good agreement with the experimental results with 5 % average error. The trends of temperature in the axial and radial directions are successfully reproduced in the simulation. The validated case is treated as a baseline model before further extension is introduced to simulate the combustion of biogas at different CO2 composition.





Figure 2 Predicted and measured temperature distribution [3] in methane flame jet (a) along the central axis and along the (b) radial direction at 150 mm downstream of the burner

3.2 Effects of CO_2 Dilution on Temperature and NO_x Emission

3.2.1 Temperature Distribution

The flame characteristics at varying CO_2 dilution were investigated at fixed power output. Figure 3 shows the radial profile of temperature at different axial location for flames with different percentage of CO_2 dilution. As expected, the maximum flame temperature reduces at increasing CO_2 dilution. The maximum temperature for biogas with 10%, 20%, and 30% CO_2 are 1835 K, 1756 K, and 1603 K respectively.

The flame height measured as the axial distance from the burner inlets to the highest temperature at downstream region. The decrease of highest temperature at downstream region 400mm indicated the reduction of the flame height. The Figure 3 show the increase of composition of CO₂ reduces the flame height as show by the declining of temperature trend at 400mm away from burner exit. The highest temperature at downstream region as seen in the radial temperature plot occurs at composition 10 percent CO₂ of biogas. Meanwhile, for case composition 30 percent CO₂, the highest temperature region occurs in the near the burner of burner exits and the flame not further extend to downstream.

Explanation of this phenomenon is related understanding of the chemical composition of the fuel. As the CO_2 dilution further increases, the combustion component of the fuel further decrease lead to reduce residence time, mixing time and reaction rate which will produce great reduction in temperature and flame length. As consequence of further increase in CO_2 dilution lead to flame shortening and extinction. In general, the temperature increases in the downstream direction as the flame front is approached. However, the change in the location of flame front at high CO₂ dilution results in the decrease of temperature at downstream region as the flow passes the flame front. The reduction of downstream temperature is due to the dilution effects of methane flame that leads to the reduction of reactant concentrations and reaction rates.

At 400 mm away from the burner, it was observed that the flame with 10% CO₂ dilution has highest maximum temperature followed by the flames with 20% and 30% dilution respectively, as shown in Figure 3. The dilution of the fuel results in more than 200 K reduction in the maximum temperature between the 10% CO₂ flame and 30% CO₂ flame.





Figure 3 Flame temperature for each composition CO_2 dilution as functions of radial position and downstream distance (a) 10% CO_2 (b) 20% CO_2 (c) 30 % CO_2

3.2.1 Mass Fraction of NOx

The level of CO₂ dilution in fuel stream effects the NO emission which is a dominant nitrogen oxide pollution species that is emitted from hydrocarbon combustion. In hydrocarbon flames, NOx is generally made up of approximately 80% NO. Therefore, NO concentration profiles should follow NO_x profiles closely because of the higher contribution of NO in overall NO_x emission. Flamelet model were set up to calculate the mass fraction of NO_x emission. The formation of the NO_x is related by the high temperature during combustion process. It is important to control the emission of the NO_x as to ensure the combustion meet the amount of acceptance of pollution set by government.

The radial profiles of NO_x at different distance from the burner are shown in Figure 4 for different levels of dilution. The trend of NO_x emission follows the trend of temperature where the NO_x increases toward the flame front before reduces in the post flame region. The biogas flame with high composition of CO₂ produces lower NO_x compared to that off the low CO₂ composition due to the same response towards temperature change [18, 19, 20].

Figure 5 shows that the increase level of CO_2 in biogas leads to the reduction of fuel concentration and peak temperature that in turns reduces the formation rate of NO_x. The maximum mass fractions of NO_x at increasing CO₂ concentration are 107 ppm, 102ppm and 90 ppm respectively that imply total reduction of 16 percent, which is quite significant. The highest temperature region are located which directly related with concentration of fuel. Therefore, we can conclude the formation of NO_x happen in highest temperature, the high temperature able to modifying the chemical bond with elements and produce NO_x.

3.2.2 Mass Fraction of CH4

At different composition of CO_2 in methane, there is variation in mass fraction in the axial and radial direction within the flame as shown in Figure 5. The maximum mass fraction of CH₄ located near the burner and subsequently decreases as the fuel is consumed towards the flame front in the axial and radial directions. The dilution effect is seen in terms of the reduction in the mass fraction of CH4 in the near burner region where the maximum mass reaction reduces by more than 60 % as the CO_2 concentration increases from 10 % to 30 %.

Comparing Figures 4 and 5, the NO_x concentration reduces when the local mixture becomes leaner that results in the reduction in the reactant concentration as highlighted in the previous study [5]. Concentration of the fuel leads to lower reaction rate and reduction the mass fraction CH₄.





Figure 4 Mass fraction of NOx for each composition CO2 dilution as functions of radial position and downstream distance (a) 10% CO2 (b) 20% CO2 (c) 30% CO2





Figure 5 Mass fraction of CH_4 for each composition CO_2 dilution as functions of radial position and downstream distance (a) 10% CO_2 (b) 20% CO_2 (c)30 % CO_2

4.0 CONCLUSION

The numerical simulation of the non-premixed turbulent combustion of pure methane was performed and validated with the experimental work of Brookes and Moss [3]. The predicted temperature distribution in axial and radial directions shows good agreement with the experimental results. The combustion of biogas with different composition of CO2 was simulated under fixed power condition and the comparison was made in terms of the predicted temperature, NO_x emission, and fuel mass fraction between different cases. Biogas flame with high percentage of CO2 produces 16 % lower NOx emission compared to that of low percentage of CO₂ due to the dilution effects that reduces the concentration of reactants for NO_x formation. The detailed analysis shows clear relationship between the thermal NOx formation, temperature, and fuel concentration.

Acknowledgement

This work was supported by research student grant University Teknologi Malaysia (R.J130000.7824.4F777). I would like to express my appreciation to my supervisor Dr Mohd Fairus bin Yasin and Assoc. Prof. Dr Mazlan Abdul Wahid for their supervision. Special thanks, Dr Mohd Fairus bin Yasin for his guidance especially in the field of computation of fluid dynamic (CFD) in OpenFOAM.

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