CFD Investigation of Pollutant Emission in Can-Type Combustor Firing Natural Gas, LNG and Syngas

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Abstract. CFD investigation of flow, combustion process and pollutant emission using natural gas, liquefied natural gas and syngas of different composition is carried out. The combustor is a can-type combustor commonly used in thermal power plant gas turbine. The investigation emphasis on the comparison of pollutant emission such in particular CO₂, and NOₓ between different fuels. The numerical calculation for basic flow and combustion process is done using the framework of ANSYS Fluent with appropriate model assumptions. Prediction of pollutant species concentration at combustor exit shows significant reduction of CO₂ and NOₓ for syngas combustion compared to conventional natural gas and LNG combustion.

1. Introduction
Global warming has become an important issue around the world with recent unpredictable weather condition that has affected human lives. This issue is always associated with uncontrolled CO₂ emissions from various hydrocarbon combustion sources. Among the largest contributor for CO₂ and NOₓ emission power generation industries. It is known that most of the power generators around the world still depends on hydrocarbon as the main source of combustion. With increasing stringent environment policy to limit pollutant emissions, an alternative cleaner source of fuel is widely researched and studied. Among others, synthetic gas or syngas has becoming a fuel of choice and has the potential to become a major fuel towards zero pollutant emission [1]. Syngas has the potential to replace conventional fuel used in power station gas turbine and attempt has been made to study the combustion behaviour when this fuel is used [2]. In the open literature, many works have been made to investigate the combustion behaviour when hydrogen or syngas is used [3-6]. However, majority of these works were carried out on small or lab-scale at which the combustion characteristics might vary differently with the actual process inside large scale combustor. Thus, this paper attempts to numerically investigate the combustion, flow and emission in full scale gas turbine combustor firing syngas. Emphasis is made to the prediction of pollutant emission, in particular CO₂ and NOₓ with comparison made to pollutants from natural gas and LNG.

2. Model Descriptions
The can-type combustor model geometry is obtained by 3D scanning of the actual combustor used in thermal power plant. The cloud data for the combustor is then transferred to a more readable format of
surface data, which is later transformed into CFD model. Detail modelling of the actual combustor model has been thoroughly explain and describes in [7].

3. Model Assumption and Boundary Condition
The calculation of flow and combustion uses pure methane, ethane, propane, liquefied natural gas (LNG) of different composition and syngas the fuel. In reality however, the fuel is made up from several other species and this will be considered into the simulation in an increasing complexity manner. The combustion model was based on eddy dissipation model which compute the rate of reaction under the assumption that the chemical kinetics are fast compared to the rate at which the reactant are mixed by turbulent fluctuations. The mixture fraction model involves the solution for one or two conserved scalars (the mixture fractions). In this approach, the transport equations for individual species are not solved. Instead, the individual component concentrations for the species of interest are derived from the predicted mixture fraction distribution. Physical properties of chemical species and equilibrium data are obtained from the chemical database. The connection of turbulence and chemistry is derived with the probability density function (PDF), which describes the fraction of time that the fluctuating variable, $f$, takes in a value between $f$ and $f + \Delta f$. The mixture fraction/PDF model is computationally efficient because it does not require the solution of a larger number of species transport equations. This approach has an additional benefit of allowing a more accurate estimation of the flow field mean density than is possible using the finite rate formulation. The flow is also assumed to follow the ideal gas behaviour and the specific heat values are assumed to obey the mixing law. These assumptions are general for most gaseous combustion found in the open literature.

4. Results and Discussion
Two pollutant species are calculated at combustor exit which are CO$_2$ and NO$_x$. Detail comparison is made on the emission of these pollutants when fuel compositions are altered. In this case, the CH$_4$ combustion is treated as a reference case.

4.1. CO$_2$ and NO$_x$ Emission for Natural Gas
The distribution of CO$_2$ inside the combustor for different natural gases is shown in figure 1. General trend illustrates that the maximum CO$_2$ concentration is approximately 17% (by mass fraction) and is given by propane, followed by ethane and methane. Theoretically, this agrees well with the theoretical value which indicates that the CO$_2$ emission is highly dependent on fuel carbon number. In this case, propane is expected to produce the highest CO$_2$ due to its highest carbon number compared to methane and ethane. At the combustor exit however, the trend does not agree with the maximum CO$_2$ concentration and this is given in figure 2. The emission for all cases shows almost identical trend with only a slight difference of less than 4%. The average emission of CO$_2$ is approximate 1080 ppm. In terms of NO$_x$ emission methane shows the highest emission at combustor exit with an approximate value of 670 ppm. This is followed by ethane and propane with 545 ppm and 262 ppm respectively.

4.2. CO$_2$ and NO$_x$ Emission for LNG
In this simulation, the species were varied by retaining CH$_4$ as the major source of fuel. The other species such as C$_2$H$_6$, C$_3$H$_8$ and C$_4$H$_{10}$ are treated as minor and their composition were varied such that the volume fraction does not exceed 5%. Therefore the resulting CO$_2$ distribution does not differ much as compared to the one produced by pure methane combustion. Detail CO$_2$ distribution at combustor exit is shown in figure 3. The fraction of CO$_2$ ranges from 950 ppm to 1117 ppm. No clear trend could be deduced from the comparison of different LNG compositions due to the fact that the majority of component species that make up the fuel consist of CH$_4$. Thus it is anticipated that all cases will follow the CH$_4$ combustion emission. The NO$_x$ emission for different LNG composition at combustor exit is shown in figure 4. Due to the uncertain variation of temperature magnitude at combustor exit, similar
trend for NOx is also anticipated. Comparison with methane shows slightly lower NOx emission for different LNG composition at combustor exit.

4.3. CO2 and NOx Emission for Syngas

Figure 5 shows the CO2 emission of syngas combustion at combustor exit for different syngas composition. It is well acknowledged that coal, natural gas and most hydrocarbon combustion is the biggest CO2 producer in the world. Thus it is anticipated that CH4 combustion results in the maximum CO2. For syngas combustion however, the CO2 production does not depend on the H2 composition. The trend shows that it is highly dependant on the composition of CO, i.e. higher CO in syngas results in higher CO2. Nevertheless, the difference in CO2 production is very little between different syngas composition thus could be neglected. The distribution of thermal NOx at combustor exit for different syngas composition is illustrated in figure 6. Compared to CH4, syngas combustion produces much less NOx. For syngas, the fuel element consists primarily on fixed CH4 and varied composition of H2/CO ratio. In this case, the amount of CH4 is very minimal (fixed to 10% mole fraction). The volume fraction occupied by the syngas within the primary combustion region is higher thus limiting the occupation of N2 element in air which is known to contribute to the production of NOx.

Figure 1. CO2 distribution at combustor mid plane for different Natural Gas

Figure 2. CO2 emission at combustor exit for different natural gas

Figure 3. CO2 emission at combustor exit for different LNG compositions

Figure 4. NOx emission at combustor exit for different LNG compositions
5. Conclusions
The prediction of combustion gas temperature for natural gas agrees reasonably well with theoretical stoichiometric value for flame temperature. The emission of CO$_2$ at combustor exit is highly dependent on the fuel composition. Highest emission of CO$_2$ at combustor exit is given by natural gas combustion, followed by LNG and syngas. Different compositions in LNG do not significantly influence the CO$_2$ emission as the major species mole fraction was occupied by CH$_4$. Similarly for syngas, different syngas composition does not significantly influence the CO$_2$ emission since the controlling parameter was conventional hydrocarbon, $C_nH_m$. Despite having higher flame temperature, the thermal NO$_x$ generated at combustor exit for syngas is relatively low compared to CH$_4$. It is approximately 70% lower than the NO$_x$ produced by conventional CH$_4$ combustion.

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6. References
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