A 12-Element Chemical Reactor Network for Carbon Oxide Emission Prediction in Gas Turbine Combustor

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ABSTRACT

This study presents the use of a new chemical reactor network (CRN) model and non-uniform injectors to predict CO emission pollutant in gas turbine combustor. The CRN uses information from Computational Fluid Dynamics (CFD) combustion analysis with two injectors of CH4-air mixture. The injectors of CH4-air mixture have difference lean equivalence ratio, and they control fuel flow to stabilize combustion and adjust combustor’s equivalence ratio. Non-uniform injector is applied to improve the burning process of the turbine combustor. The results of the new CRN for CO prediction in the gas turbine combustor show very good agreement with the experimental data from Korea Electric Power Research Institute.

Key words: Chemical Reactor Networks (CRN), Computational Fluid Dynamics (CFD), Perfectly Stirred Reactor (PSR), Plug Flow Reactor (PFR), Gas Turbine Combustor, Carbon Oxide Emission (CO)

INTRODUCTION

From the nineteen fifties, engineers have used chemical kinetic models to study the combustion process. The concept of modeling the flame by a perfectly stirred reactor (PSR) followed by a plug flow reactor (PFR) was introduced by S.L. Bragg and N.T. Hao (Hao and JungKyu, 2013). Zonal combustion modeling was proposed by Swithinbank as an improvement for combustor design via correlation parameters (Switenbank, J). The flame volume was divided into zones represented by idealized reactor elements, such as PSR, PFR, and MIX (Steel et al, 1997)(Rubin and Pratt).
The concept of modeling the combustor by MIXs and PSRs followed by two PFRs will be applied to predict CO emission in gas turbine combustor. In the PSR the chemical time is assumed to be much slower than the mixing time. Chemical reactor modeling of combustion systems is not necessarily limited to the use of extensive chemical reactor networks. Very simple two/three reactor models have been found useful in modeling research combustion reactors (Nicol et al, 1994) (Hao and JungKyu, 2011). The new chemical reactor network modeling of the gas turbine combustor is constructed based on CFD-predicted flow patterns: flame shape and location, and entrainment of the dome air and gas from main recirculation zone into the flame. The new chemical reactor network modeling is shown the schematic layout of the 12-element CRN developed herein. The chemical reactor network consists of 12 PSR, PFR, and MIX elements. The PSR stands for perfectly stirred reactor (i.e., a continuously stirred tank reactor), in which mixing to the molecular scale is assumed to happen instantaneously compared to chemical reaction. The chemical reaction occurs homogeneously in the reactor. The PFR stands for plug flow reactor, in which the flow is assumed to move as a plug and the chemical reaction proceeds one-dimensionally, longitudinal mixing in the reactor is assumed to be zero. The MIX stands for an element in which the entering streams are uniformly mixed without chemical reaction. This research is somewhat different from the previous ones, being more descriptive and less theoretical. The CFD modeling has ability to provide the valuable insight on the flow and the temperature fields of the combustor, which are difficult to obtain from the experiment. While CFD is a valuable tool to predict the flow and the temperature fields, this method cannot incorporate the complicated chemistry of the detailed chemical kinetic mechanisms.

**CFD Analysis**

The new CRN combustion model is constructed in this study based on the actual experiment and CFD-predicted flow patterns: the flame shape and location, the entrance of the dome air and gas from main recirculation zone into the flame. These flow patterns are treated by adjusting the flow splits between the corresponding elements of the network. The analysis includes a three-step EBU model which was performed using a simple interpretation of the results of the flame. The temperature was used to separate the flame zone which was replaced by simple reactors. The schematic 3D drawing of the combustor with the air flow splits is shown in figure 2. The major design and operating parameters of the modeled combustor are similar to those of typical industrial gas turbine combustor. The modeled combustor consists of the combustor liners, the swirl injector with main circuit, and the swirl pilot circuit. The mean axial velocity profiles of the injector are determined based on the profiles of the swirl ratio and the non-uniform swirl mixture injector. The CRN model is configured from the entrance, consider the mixture of fuel and air to the back-flash phenomenon occur because CH$_4$-air separate analysis is applied to the entrance of the combustor. The k-ε turbulence model is used for wall insulation combustion chamber conditions. In Star-CCM, however, these effects are modeled as in the standard k-ε model. The turbulent kinetic energy and turbulence dissipation rate are determined by solving their modeled transport equations. The simulation performed in the model of CH$_4$-air combustion is repeated using a three-step reaction of the following forms

\[
\begin{align*}
\text{CH}_4 + 0.5\text{O}_2 & \rightarrow \text{CO} + 2\text{H}_2 & \text{(1)} \\
\text{CO} + 0.5\text{O}_2 & \rightarrow \text{CO}_2 & \text{(2)} \\
\text{H}_2 + 0.5\text{O}_2 & \rightarrow \text{H}_2\text{O} & \text{(3)}
\end{align*}
\]

The Reactions (1) $\div$ (3) themselves are defined by specifying the amounts (in kilomoles) of the participating leading reactants, reactants and products. In the properties of Star-CCM window, these amounts are entered into each node for the stoichiometry coefficient. The overall structure of the gas turbine combustor system includes an air compressor, an air heater, a compressed natural gas, a combustor, two gas turbine burners, and an exhaust processing unit. The control instrumentation consists of the ICCD camera and the image processing controller, etc.
Compressed Natural Gas
(a) The Experiment Schematic Measurement

(b) The Control Instrumentation of Gas Turbine Combustor
Figure 1. The Experimental Gas Turbine Combustor Model
The experiment parameters are based on combustion conditions (Figure 1). The external temperature is 298K, after passing through compressor, the temperature is 650K. Pressure and other combustion parameters are based on the maximum load (1.0N load) and minimum load (idle load). In order to understand the effect of the injector CH4-air mixing profile on the flame position and emission levels, this study will calculate profile of non-uniform injector. The mixture between fuel and air in both main injector and pilot injector are not the same. At the idle load, the overall equivalent ratio of the pilot injector is less than 0.7, the lower overall equivalent ratio is 0.166. The overall equivalent ratio of the main injector and pilot injector at the 1.0N load is 0.422, at the 0.8N load is 0.367, and at the 0.6N load is 0.314.

![Figure 2. Computation Grid for CFD Modeling of Gas Turbine Combustor](image)

The combustion chamber boundary is a cylindrical shape using the grid to reduce the computational time is shown in Figure 2. A two-dimensional grid consist of 190,000 cells is used. In order to adequately resolve the gradients that exist in the flame, the grid resolution is refined in the pilot flame region and the boundary layer effect. The results of the mass fraction of the gasturbine combustor at the entrance with overall equivalent ratio of 0.7 are shown in figure 3. The formation of CO emission in the combustor are determined by post-processing CFD solutions of the flow field.

![Flame Temperature Surface](image)

![Ratio of Unburned Fuel in a Premixed Flame](image)
The temperature vectors plot from the 2D CFD simulation of the different load (1.0N, 0.8N, 0.6N, and idle) show the different combustion zones. The highest temperature of the flame in combustion chamber appear on the wall, in this case the temperature is up to 1903.5K. The temperature contours plot from the 2D CFD simulation show the different combustion zones (figure 4): main flame zone, main recirculation zone, pilot inner zone, pilot out post, pilot median zone, pilot recirculation zone. The development chemical reactor network modeling of the gas turbine combustor is constructed based on the CFD-predicted flow patterns such as the flame temperature and the volumetric zones (figure 4), and the entrainment of the dome air and gas from the main recirculation zone into the flame.

(c) Mass Fraction of CO Surface

Figure 3.Temperature, Regress Variable and Mass Fraction of CO Contours Plot from Star-CCM Software Showing the Presence of the Different Combustion Zones

CRN Model Configuration

The CRN model is constructed in this study based on the Figures 3 and 4. First of all, the recirculation zone consists of PSR which was fully mixed assumption. According to the results of Figure 4, the temperature of the flame was broken. At the idle state, the overall equivalent ratio distribution is up to 0.9. More than 0.05 units from overall equivalent ratio of 0.7 are divided into two entrances. The overall equivalent ratio range from 0.6 to 0.7, one of area is subdivided into the entrance, so that the total...
entrances are two. Number of the flame zone is also divided into eight zones. The regions of overall equivalent ratio of 0.7 or more are approximately accounted 20% of the total. At the 0.6N load, 0.8N load, and 1.0N load state, when the overall equivalent ratio distribution is 0.85, the equivalent ratio does not exist and the flame zone is divided into eight zones. The regions of overall equivalent ratio of 0.7 of 0.6N load is accounting approximately 12%, 1.0N load is approximately accounted 9% of the total. The CRN model is separated by a non-equivalent portion of the pilot flame was broken. Area consists of more than overall equivalent ratio of 0.8 is pilot out 2 to simulate the flame was on the wall. Area consists of more than overall equivalent ratio of 0.7 is pilot out 1, flame inside of the wall is modeled. Overall equivalent ratio is less than 0.6 is accounting approximately a medium flame.

(a) The Schematic Layout of the 12-Element CRN Model

(b) The 12-Element CRN Model for Evaluating the CO Emission Based on CHEMKIN Software

Figure 5: 12-Element Chemical Reactor Network of the Gas Turbine Combustor
The schematic layout of 12-element CRN is constructed in this study which based on the CFD-predicted results as shown in Figure 5. The PSR stands for perfectly reactor, in which mixing to the molecular scale is assumed to happen instantaneously compared to chemical reaction. The combustion occurs homogeneously in the reactor. The PFR stands for plug flow reactor, in which the flow is assumed to move as a plug and the chemical reaction proceeds one-dimensionally, longitudinal mixing in the reactor is assumed to be zero. the MIX stands for an element in which the entering streams are uniformly mixed without chemical reaction. The first element in the CRN arrangement is the MIX, which represent the cone shape zone of inlet mixture where the mixture is not ignited yet. The flame zone, the dome and the main recirculation zone, and the immediate post flame zone are modeled by using PSRs, while the post flame zones is modeled by using PFR.

RESULTS AND DISCUSSIONS

Figures 6 ÷ 8 are used to show the mole fraction of CO emission results in three CRN model conditions. The amount of CO at low load appears significantly higher than others. Especially, the mole fraction of CO in cold condition is highest. In this situation, the effect of temperature on the formation of CO into the gas turbine combustor is played the role of great importance. The CO concentrations rapidly fall with temperature, as illustrated by each condition shown in Figures 6 ÷ 8. So that, the CO production mechanisms are also depending on the temperature input such as normal condition, cold condition or hot condition (boundary condition). The CO emission at the exit of the gas turbine combustor is essentially dependent on overall fuel-air equivalent ratio of the idle load, 0.6N load, 0.8N load, and 1.0N load. The formation of CO in the gas turbine combustor non-uniform inlet was applied using the new modified CRN predicts the CO emission is more closely to the experimental data.
Figure 7. Non-Uniformity Mole Fraction of CO in Cold Condition

Figure 8. Non-Uniformity Mole Fraction of CO in Hot Condition

CONCLUSIONS

The 12-element CRN mechanism has been applied CFD modeling of the gas turbine combustor in order to obtain insight on the flow, temperature, and species fields. The flow field information from the gas turbine combustor CFD has been analyzed to determine combustion zones in the combustor. These zones are modeled as chemical reactor elements in the CRN. The methodology of the CRN development is determined based on the agreement between CFD and CRN models.

The new CRN model using 12 idealized reactor scheme modeling has been developed based on CFD results for the gas turbine combustor with overall fuel-air equivalent ratio of the idle load, 0.6N load, 0.8N load, and 1.0N load. The formation of CO emission in turbine combustor non-uniform inlet prediction are more closely to the experimental data, especially at low overall equivalent ratio in normal condition shown in Figure 6.
This research has shown that:

- The combined CFD and CRN approach shows the ability to accurately predict CO emission for lean premixed gas turbine combustor.
- The simple CRN model by applying non-uniform inlet is able to predict CO emission more accurate than uniform inlet.
- The simple CRN model can also be applied to the industrial combustors. The resulting CRN incorporates important flow features and boundary conditions such as: fuel-air distribution, velocity profile, entrainment of the main recirculation zone and the main flame.

REFERENCES


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