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Prediction of Pollutant Emissions from Industrial Furnaces Using Large Eddy Simulation

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Accurate prediction of pollutant emissions from turbulent combustion around complex geometries is of great practical interest. Here, an industrial furnace with rich-burn/quick-quench/lean-burn combustion for NO_x reduction is simulated. Large eddy simulation (LES) is employed as the simulation tool since it outperforms Reynolds-Averaged-Navier-Stokes (RANS) simulations in capturing large-scale unsteady motions and turbulent mixing. A structured LES code with variable staggering in space and time is used for accuracy and efficiency to predict NO_x and CO emissions from the furnace with a cross-flow-jet combustion system. The complex geometry of the furnace is handled by the Immersed boundary (IB) method. A Lagrangian dynamic subfilter model, which is designed for inhomogeneous flow in complex configurations, is employed. Laminar flamelet models are used for subfilter combustion closure. Here, three flamelet models, namely, the standard steady flamelet model, the Flamelet/Progress variable method, and the Lagrangian unsteady flamelet model, are employed. Experimental data obtained from the furnace with propane diffusion burners are used to compare the performance of these three models. Conclusions are drawn regarding the use of these models in combustion LES.

1 Introduction

Industrial furnaces are used in many applications, such as the extraction of metal from ore, or in oil refineries and other chemical plants. In power plants, furnaces play a crucial role in transferring chemical energy stored in fossil fuels into heat. It has been estimated that about 65% of the total electricity generated in the US during 2005 is from power plants using fossil fuels [1]. This percentage is expected to increase in the future as coal becomes a more dominant energy source. The U.S. Department of Energy is developing technologies for ultraclean, 21st century energy plants with efficiency and emission goals well beyond the current state-of-the-art fossil fuel power plants. Control of pollutant emissions such as nitrogen oxides (NO_x), carbon monoxide (CO), and even carbon dioxide is critical for these advanced power plant designs.

Thermal NO_x is an important issue for fuels that have flame temperatures in excess of 1800 K. Staged combustion approaches such as rich-burn/quick-quench/lean-burn (RQL) combustion has been used primarily to minimize NO_x emissions. These approaches usually involve cross-flow air injection into the incomplete combustion products. Figure 1 illustrates the configuration of a low-NO_x RQL furnace that is used in this modeling study. The diffusion burners are operated at fuel rich condition. This is to keep flame temperature low, and hence suppress NO formation. However, the CO concentration is high, since complete oxidation does not occur in the first stage

of rich combustion. Secondary air is injected into the over-fire part of the furnace to complete combustion. The cross-flow air jets introduce rapid mixing, and therefore freeze NO formation reactions. Overall, the combustion process is fuel lean and thermal NO production is reduced.

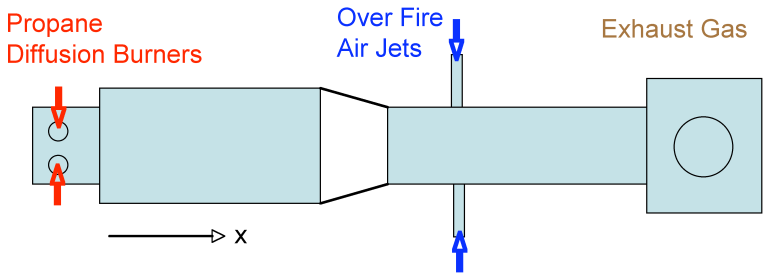

Figure 1: Schematic illustration of a low-NO_x rich-burn/quick-quench/lean-burn furnace

The mixing due to the cross-flow-jets is critical for minimizing NO production. Ideally, mixing between rich combustion products and secondary air should proceed in such a way that the excess CO is fully burned and NO formation is suppressed. If the mixing time scales are too slow, or the cross flow jets cannot penetrate the main flow to distribute the oxidant uniformly across the entire flow area, localized high temperature zones are formed and significant amounts of NO will be produced.

In order to capture the mixing effects of the cross-flow-air-jets, large eddy simulation (LES) is preferred over Reynolds-Averaged Navier-Stokes (RANS) simulation, because of LES's capability in describing unsteady large scale motions and turbulent mixing. LES of furnaces, such as the present cross-flow-jet combustion is rare, as most combustion LES are for laboratory canonical flames or modeled gas turbine combustors [2]. One objective of the present paper is to investigate the mixing process of a cross-flow-jet combustion system in a industrial furnace using LES.

Another objective of the paper is the assessment of laminar flamelet models [3] in LES of cross-flow-jet combustion systems. Due to the separation of chemistry from the flow field solution, laminar flamelet models are computationally very efficient in combustion LES, while still enabling the use of detailed chemistry. This is desirable in industrial applications, where computational turn-around times are usually critical. Flamelet models are also accurate in the sense that chemistry and the molecular mixing process at the small scales are treated simultaneously. Several different flamelet model formulations can be applied to LES with ease. The performance of these models in predicting combustion and pollutant formation is assessed in this study.

2 Physical and Numerical Models

The main features of the LES solver used in the simulation are that it solves the filtered low Mach number formulation of the Navier-Stokes equations on structured grids. The solver employs an energy conserving finite difference scheme, and the numerical discretization in space can be of arbitrary order of accuracy [4]. Variable staggering in both space and time is used [5]. The time advancement is implemented using an Adams-Bashforth predictor-corrector algorithm with second order accuracy [5]. The Lagrangian dynamic subfilter model is implemented for turbulence closure [6].

This structured LES code with staggering in space and time is accurate and computationally efficient, which makes it suitable for engineering applications. However, it is difficult to accommodate complex geometry with structured meshes. The Immersed Boundary (IB) method allows flow simulations around complex objects without restricting grid lines to be aligned with the irregular boundary faces [7]. The no-slip boundary conditions are enforced through body forces added to the right hand side of the momentum equations. The body force terms are applied exactly at the immersed boundary by specifying the velocity values at the nodes closest to the boundary. To allow the structured LES code to handle complex configurations, an IB algorithm developed at the Center for Turbulence Research was implemented. This algorithm is mass conservative, computationally efficient, and sufficiently accurate for large eddy simulations [8].

In most combustion application of LES, the use of laminar flamelet models is straightforward, because of the ease of implementation and the capability of incorporating rather complex chemistry at reasonable computational cost. The basic assumption of flamelet models is that the chemical time-scales are short enough such that reactions occur in a thin layer around stoichiometric mixture on a scale smaller than the small scales of the turbulence. Flamelet models can be divided into steady and unsteady models. The steady models include the classical steady flamelet model and the flamelet/progress variable model. Since the flame structure in steady models is assumed to be in steady state, these models are inaccurate for slow chemical reactions such as NO formation. In order to use steady flamelet models for NO predictions, an appropriate formulation has been proposed for NO [9]. One objective of the present study is to test the accuracy of the proposed formulation. Unsteady flamelet models, such as the Lagrangian flamelet model [10], on the other hand, take the slow chemical/physical process into consideration, and are expected to predict NO formation with better accuracy. In this paper, the performance in predicting NO using the three different flamelet model formulations, namely, the classical steady flamelet model, the flamelet/progress variable model, and the Lagrangian flamelet model will be assessed.

3 Numerical Grid and Procedures

In the simulation, the mixing due to cross-flow air jets is of interets. The experimental data are available only at the over-fire part of the furnace (Fig. 1). It has been verified by experiments that the mixture condition at the location before the air jets is almost uniform across the duct and close to propane equilibrium combustion at 1773K. Therefore, the computational domain in the simulation considers the over-fire part plus a small portion of the main furnace, as shown in Fig. 2. A small portion of the main furnace is included to provide a better flow condition before the cross-flow air jets. The boundary condition for transition from the main furnace to the over-fire part will be treated using the immersed boundary method. The inlet velocity profile is taken from the turbulent solution of a duct flow of the same dimension as the main furnace. The simulation was carried out for about four flow-through times after the flow reached statistically stationary state. The inlet velocity profiles for the cross-flow air jets are plug flow. The mesh size is $256 \times 64 \times 64$ in x, y, and z directions. The simulation time is about 24 hours for one flow-through time on 64 processors.

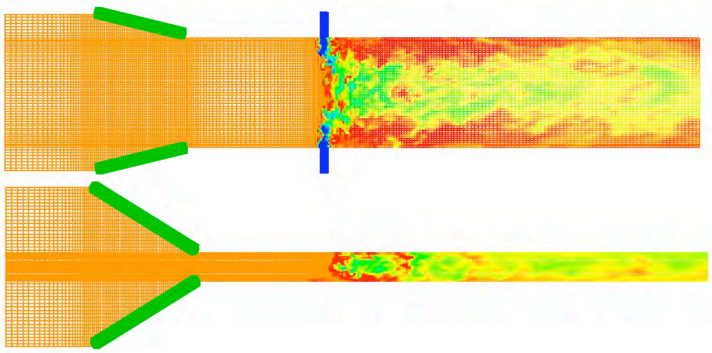

Figure 2: Computational mesh 256 x 64 x64

4 Results and Discussion

In the following, the discussion is based upon the results obtained from the classical steady flamelet model. Figure 3 shows the instantaneous contour plots of velocity and mixture fraction. It can be seen that the high velocity air jets coming from the sides meet in the middle of the furnace. The velocity becomes more uniform further downstream as mixing proceeds. The rich combustion stream from the main furnace is pushed towards the side walls as high momentum fresh air meets in the middle. The mixture fraction contour shows that stoichiometric mixture (at a value of about 0.86, indicated by the black solid contours) is formed near the side walls and the mixture becomes more and more fuel lean downstream as turbulent mixing reveals its effects. Reaction of burning CO will take place mostly along the side walls, where the temperature will be high and the residence time for NO formation will be relatively large due to slow flow motion near the walls.

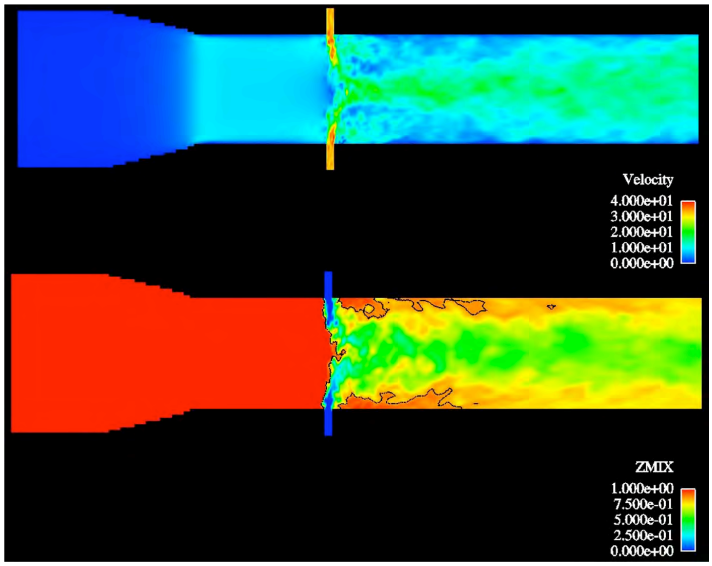

Figure 3: Instantaneous contours of velocity and mixture fraction

Consistent with the contours shown in Fig. 3, the temperature contour shown in Fig. 4 reaches large values in the near wall regions. In these high temperature regions, NO formation is promoted

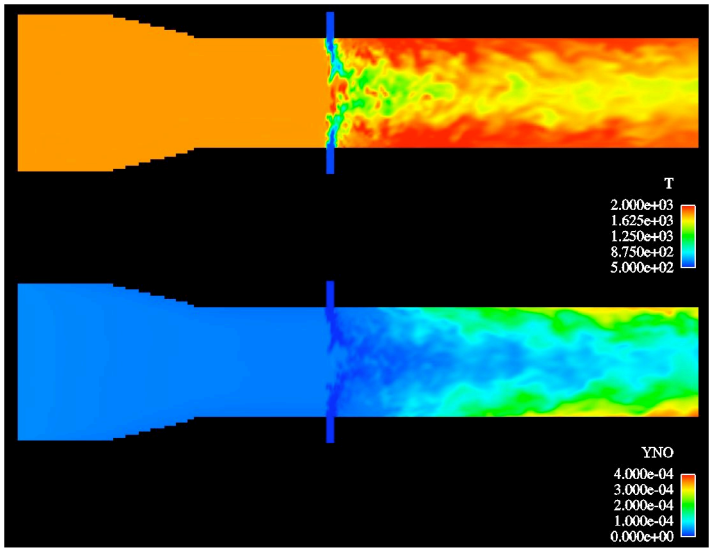

Figure 4: Instantaneous contours of temperature and NO mass fraction.

as shown in the NO mass fraction contours. NO grows and spreads out as it convects downstream. This is consistent with the trend shown in the experiment, where NO peaks in the near wall regions.

Figure 5 shows the calculated mean mixture fractions compared with experiments at three measurement stations: 0.18m, 0.36m, and 0.62m downstream of the air jet inlets. In general, the predicted mixture fraction agrees well with experimental measurements, especially at the second and third measurement stations. At the first station, experimental data show a flatter distribution than that of the simulation, indicating that mixing is under-predicted.

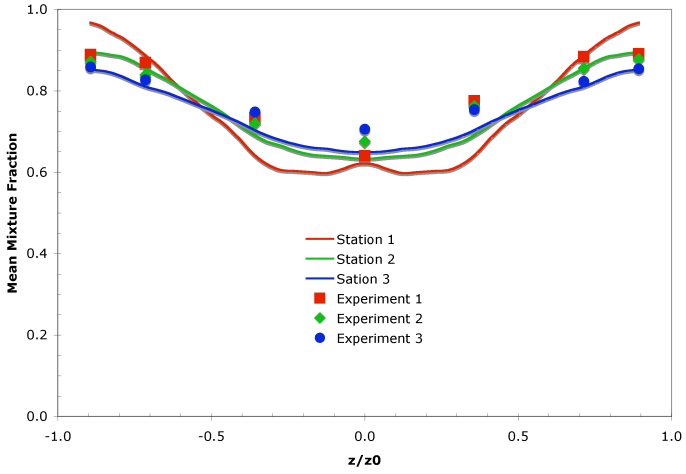

Figure 5: Comparison of mean mixture fractions at 0.18m, 0.36m, and 0.62m downstream of the air jets (station 1, 2, and 3, respectively.)

In contrary to the good agreements in mixture fraction prediction, the calculated mean CO profiles show in Fig. 6 match not well with the experiments: at all three stations, the CO concentrations levels are consistently under-predicted. To understand this discrepancy, CO variations with mixture

fraction are compared with steady flamelet solutions at two values of the scalar dissipation rate in Fig. 7. The experimental values are compared with the flamelet profiles. It can be seen that the experimental data at mixture fractions larger than the stoichiometric value are well above the CO concentrations given by the steady state flamelet solution. This could suggest that either the predictions of the dissipation rate are inaccurate, or that the actual flame structure is not in steady state.

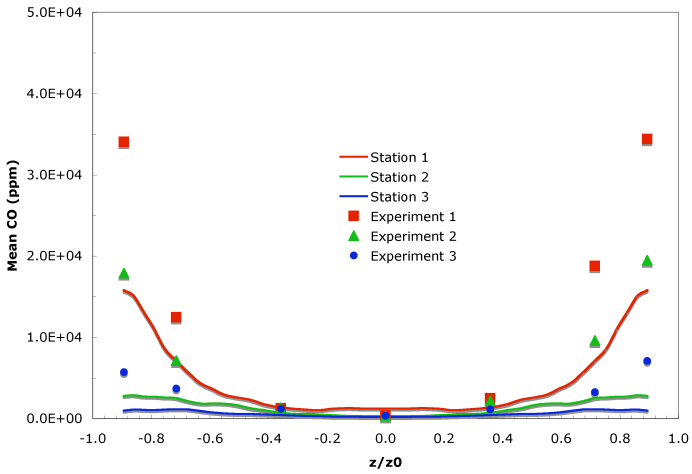

Figure 6: Comparisons of mean CO mole fractions at three measurement stations: 0.18m, 0.36m, and 0.62m downstream of the air jets (station 1, 2, and 3, respectively.)

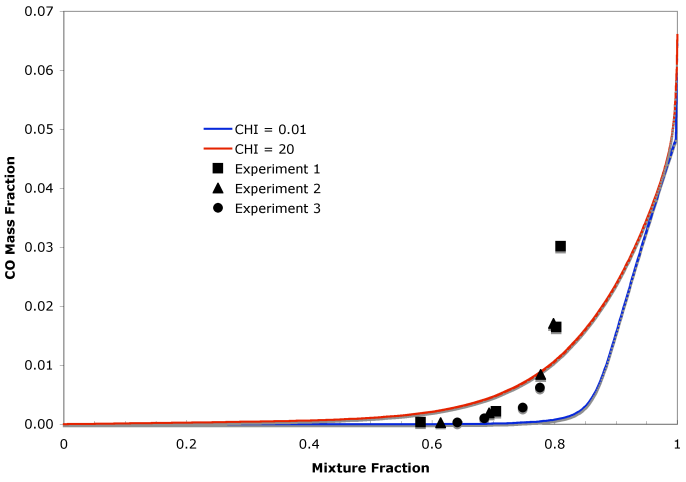

Figure 7: Flamelet profile of CO at two scalar dissipation rate and experimental data at the three measurement stations.

5 Concluding Remarks

A steady flamelet model has been used in the large eddy simulation of pollutant emissions from an industrial furnace with a cross-flow-jet combustion system. The preliminary simulation shows

qualitative agreement with experiments for the flow and combustion behavior. The rapid mixing process in this cross-flow-jet system is well captured by the LES simulation. The under-predicted CO concentration suggests that the flame structures in the actual combustion system are not in steady state. Other flamelet model formulations will be employed and assessed in the simulation, and detailed comparison with experiment will be carried out.

Acknowledgments

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