Large-eddy simulation of an industrial furnace
with a cross-flow-jet combustion system

By L. Wang and H. Pitsch

1. Motivation and objectives

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 United States during 2005 was from power plants using fossil fuels (Department of Energy Website). 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\textsubscript{x}), carbon monoxide (CO), and even carbon dioxide is critical for these advanced power plant designs.

Thermal NO\textsubscript{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 have been used primarily to minimize NO\textsubscript{x} emissions. These approaches usually involve cross-flow air injection into the incomplete combustion products. Figure 1 illustrates the configuration of a low-NO\textsubscript{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.

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 (Pitsch 2006). One objective of the present paper is to investigate the mixing process of a cross-flow-jet combustion system in an industrial furnace using LES.

Another objective of the paper is the assessment of laminar flamelet models (Peters 1984) 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 easily applied to LES. The performance of these models in predicting combustion and pollutant formation is assessed in this study.

2. Physical and numerical models

The LES code used in the simulation 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 (Morinishi et al. 2004). Variable staggering in both space and time is used (Pierce 2001). The time advancement is implemented using an Adams-Bashforth predictor-corrector algorithm with second-order accuracy (Pierce 2001). The Lagrangian dynamic subfilter model is implemented for turbulence closure (Meneveau et al. 1996).

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 (Fadlun et al. 2000). 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 (Kang et al. 2005).

In most combustion applications 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 (Ihme & Pitsch 2007). One objective of the present study is to test the accuracy of the proposed formulation. Unsteady flamelet models, such as the Lagrangian flamelet model (Pitsch & Steiner 2000), 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, 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 interest. 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 simulation of a turbulent 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, respectively. The simulation time is approximately 24 hours for one flow-through time on 64 processors.

4. Results and discussion

Our preliminary tests (Wang & Pitsch 2007) found that the classical steady flamelet model and the flamelet/progress variable (FPV) model performed similarly well for this over-fire cross-flow combustion system. This can be explained by looking at the solution of the steady flamelet equations, which takes the rich hot combustion product from the main furnace as the fuel stream. Figure 3 shows the maximum temperature of the flamelets as a function of stoichiometric scalar dissipation rate. This figure differs from the S-shaped curves that are generally produced from the steady flamelet equations. This
is because the fuel stream in the flamelet solution is the rich hot combustion product, and therefore, the unstable partially extinguished solution branch does not appear. This is an interesting combustion regime that is similar to the so-called MILD (Moderate or Intense Low-oxygen Dilution) combustion, also called flameless oxidation. In this regime, the fuel is so highly preheated that the non-linear interaction between transport and chemistry, which typically leads to auto-ignition and extinction phenomena, does not reveal these features anymore. Because the fuel is so hot, extinction is no longer possible, no matter how strong mixing is. This implies that using scalar dissipation rate to parameterize the flamelet library provides a unique mapping to the flamelet solutions and makes no difference from using a progress variable as a flamelet parameter. Hence it is expected that the classical steady flamelet model will predict the similar results as the FPV model. In all the latest tests, the PFV model was used exclusively.

It was also observed that the flame appeared at the walls of the over-fire duct and the temperatures in the near wall regions were high. This is unphysical since heat losses to the walls will reduce the temperature such that combustion cannot occur in the near-wall regions. A wall heat transfer model need to be developed and incorporated into the flamelet models.

4.1. A wall heat transfer model

In IC engine simulations using the flamelet approach for combustion modeling, unsteady flamelet formulations are usually employed together with the solution of an enthalpy equation to account for heat losses at the walls. However, usually only one unsteady flamelet is generally considered because of the computational cost and complexity of implementation. In order to keep the computational efficiency of the FPV model, we developed an efficient approach to account for wall heat losses in the framework of steady flamelet formulations. This approach involves the construction of up to third-order derivatives of scalars with respect to enthalpy in the flamelet library.

The basic idea is that we can obtain a series of flamelets that have the same stoichiometric scalar dissipation rate but with different enthalpy values. Since the reference scalar dissipation rate and the reference mixture fraction will be the same for these flamelets,
Figure 4. Instantaneous contours of the difference between enthalpies with and without wall heat losses.

the convoluted scalar dissipation rates, i.e., averaged using the beta subfilter probability density function (FPDF), of different flamelets will be the same for the same filtered mixture fraction and mixture fraction variance. Then, from these flamelets we can obtain the variation of filtered scalar values with respect to the filtered enthalpy. Using Taylor series expansion, the change of the scalars with respect to enthalpy is expressed as

$$
\tilde{\phi}(\tilde{H}_0 + \Delta H) = \tilde{\phi}(\tilde{H}_0) + a_1 \Delta H + a_2 (\Delta H)^2 + a_3 (\Delta H)^3 + \ldots,
$$

where $\tilde{\phi}$ represents filtered chemical composition variables such as species mass fraction, temperature, density, and molecular transport properties, $\tilde{H}_0$ is the filtered enthalpy of the flamelet without heat losses, and $\Delta H$ is the difference between filtered enthalpies with and without heat losses and is called enthalpy defect. The coefficients $a_i$ are related to the derivatives of the scalars. Three additional flamelets with different enthalpy contents may be used to determine the coefficients if third-order derivative is to be retained in the Taylor series expansion, and we have found that third order is required for representing the variations of NO filtered source terms. In our implementation, more than three flamelets are used to construct the coefficients for up to third-order derivatives and a least square minimization algorithm is used to optimize the coefficients. These coefficients are then stored in the flamelet library as a function of filtered mixture fraction, its variance, and filtered progress variable.

During the simulation, a filtered enthalpy transport equation with heat losses is solved. The solution is compared with the enthalpy values from the flamelet library (no heat loss) and the enthalpy defect is computed. Then, according to the filtered mixture fraction, its variance, and the filtered progress variable value, the series expansion coefficients are extracted from the library, and the filtered scalar values including filtered density are obtained using Eq. 4.1.

The flamelets with the same stoichiometric scalar dissipation rate but with different enthalpy values can be obtained by solving the unsteady flamelet equations using the steady no-heat-loss solution as the initial condition, or by solving the steady flamelet equations with different enthalpy contents at the fuel and oxidizer boundaries. For simplicity, the second approach was taken in our implementation.

Figures 4 and 5 show the instantaneous plots of the enthalpy defect and the comparison of temperature contours with and without heat losses from the furnace walls. Since there
L. Wang and H. Pitsch

4.2. Effect of wall heat transfer

Figures 6 to 8 compare the mean profiles at the three measurement stations before and after the wall heat transfer model was implemented. Figure 6 shows the mixture fraction and temperature distributions across the duct. The mixture fractions are in good agreement with experiments indicating that the turbulent mixing process due to the cross-flow jets is captured well by the applied structured LES method. The comparison between temperature profiles shows that the wall heat transfer model is important for predicting the right trend in temperature distribution close to the walls: the bending

**Figure 5. Instantaneous contours of temperature with (bottom) and without (top) wall heat losses.**

**Figure 6. Mean profiles compared with experimental data at the three measurement stations. Symbols are experiments, solid lines are results with wall heat transfer, and dashed lines without. Left: mixture fraction; right: temperature.**

are no experimental data on wall heat transfer, in the simulation a constant heat flux from the walls was assumed for the source term in the enthalpy equation.
of the temperature profile toward walls due to wall heat losses are captured by the wall heat transfer model and the absolute values of temperature are in good agreement with experiments. The agreement worsens at the downstream location. This is probably caused by the artificially specified wall heat flux in the model. More experimental data are required for an improvement in the results.

Figure 7 shows the profiles of the major species, O$_2$ and CO$_2$. The major species are in good agreement with experiments. Figure 8 shows the mean profiles of pollutant species, CO and NO. Compared with experiments, the CO profiles calculated by the wall heat transfer model show qualitative improvement over the profiles without the wall heat transfer model. At the second and the third measurement stations, the simulation without wall heat losses shows a bend of the CO profile close to the walls. This is because without the wall heat transfer model, the simulation predicts high temperatures and reactions occurring near the walls, which cause the CO concentration to decrease. Including the wall heat transfer model eliminates this incorrect behavior at the downstream locations. Figure 8 shows that the CO concentration is over-predicted near the walls by the wall heat transfer model. However, in the middle of the duct, the CO profiles with wall heat
loss have much better agreement with experiments than those without heat losses. The over-prediction near the walls is probably due to the fact that a top-hat inlet profile was used, while in the experiment, the CO concentration near the walls may be lower than that in the middle of the duct.

The NO profiles show that both simulations with and without wall heat transfer over-predict the NO formation, even though including the wall heat transfer model substantially improves the results. The over-prediction may come from two sources of error. The first is the model for NO prediction. This model was developed to address the inherent problem of the steady flamelet model in predicting slow chemical processes such as NO formation. A transport equation is solved for the filtered NO mass fraction and the filtered chemical source terms are obtained from the flamelet library that has a separate treatment for the production and consumption source terms with special considerations for the deficiencies of the steady state assumption. However, this model was validated in simulations of turbulent jet diffusion flames, showing that especially thermal NO, which is the most important formation mechanism for the present case, is quite well predicted.

The second source of error is that thermal radiation was not considered in the formulation. The effect of heat losses via radiation is considered in the following.

4.3. Effect of thermal radiation

In order to evaluate the importance of radiation to the prediction accuracy, an optically thin model was implemented. Because only emission is considered in the optically thin model, the radiation source term for the enthalpy equation can be calculated directly from the solution of the flamelet equations and stored in the flamelet library. Since the optically thin model is known to over-predict radiation heat losses, to minimize the error caused by the simple optically thin model, a factor of 0.2 is multiplied to the radiation source term in the enthalpy equation.

Adding radiation losses to the enthalpy equation increases the enthalpy defect used in the heat transfer model, which caused the temperature to decrease further, as shown in Fig. 9. Heat transfer to the walls is considered in both simulations. There is not much difference in the mixture fraction distribution from the two simulations. The radiation model brings the temperature profiles closer to the experiments. Since absorption was not considered in the optically thin model, the temperatures in the middle are lower than in the experiments.

Figure 10 shows the effect of adding thermal radiation on CO and NO predictions. There is not much difference in CO profiles. For the NO profiles, the change at the first station is small, but the changes at the second and third stations are substantial. This is consistent with the improved temperature distributions. Because of the crudeness of the model, the shape of the temperature profiles was not accurately represented; the predicted temperature was higher closer to walls and lower in the middle. It can be expected that the NO prediction will be improved with a more detailed radiation model.

5. Conclusions and future work

We conclude from the previous discussion that the flamelet model performs well for the prediction of the major species in this cross-flow-jet combustion system. Because of the nature of this combustion system with highly heated fuel stream, there are no major differences between the classical steady flamelet model and the flamelet/progress variable model. In addition, heat losses from the walls and from thermal radiation play
an important role for pollutant species predictions. We have developed a simple wall heat transfer model in the framework of steady flamelet formulation.

The over-prediction of NO species by the current implementation of the NO model needs further investigation. In the implementation, the flamelet library and the Taylor series coefficients for the wall heat transfer model are constructed from steady flamelet solutions, which have been shown to produce large errors in the prediction of slow chemical processes such as NO formation. Unsteady flamelet solutions will be employed in the future for the improvement of NO prediction.

6. Acknowledgments

This project is sponsored by Power & Industrial Systems R&D Laboratory of Hitachi Ltd. The program monitor is Dr. Kenji Yamamoto.
REFERENCES


