Experimental and Modeling Study of NOx Formation in a Turbulent Gasoil Burner

A. Cuoci¹, A. Frassoldati¹, T. Faravelli¹, E. Ranzi¹, C. Accordini², G. Toniato²

¹Dipartimento di Chimica, Materiali e Ingegneria Chimica – Politecnico di Milano, ITALY
²Riello S.p.A – Burners Division, ITALY

Abstract

Aim of this paper is to present and discuss an effective methodology for the prediction of pollutants formation in liquid fuel burners based on computational fluid dynamics (CFD) and detailed chemical kinetics. A commercial turbulent swirl burner (RIELLO RL 85 blu) was simulated using the CFD code FLUENT 6.3.26 and then post-processed by means of a Kinetic Post-Processor (KPP) using a detailed kinetic scheme. The successful prediction of NOx supports the use of this tool to improve the design and scale-up of new burners with a particular attention to pollutants formation.

1. Introduction

The increasingly stringent ambient regulations push research efforts towards the development of new combustion devices with reduced fuel consumption and lower pollutant emissions. The combustion of liquid fuels currently provides the energy used by a variety of power systems such as industrial furnaces and boilers, as well as automotive and aerospace engines. The liquid fuel injection process plays an important role in controlling the performances of numerous combustion processes.

In CFD modeling, accurate sub-models are needed to describe the spray structure since drop sizes are much smaller than practical computer numerical grids. Sub-processes that need to be modeled in sprays include atomization, drop distortion and drag, drop breakup and collision/coalescence, drop turbulence dispersion and turbulence modulation effects, drop vaporization, and possible spray/wall interaction.

An important type of atomizer is the pressure-swirl atomizer, sometimes referred to as a simplex atomizer. The swirling liquid pushes against the walls of the atomizer’s central swirl chamber and develops a hollow air core. A model for pressure-swirl atomizer, available in FLUENT, simply uses observations of external spray characteristics as input variables. The atomization model, in based on the Linearized Instability Sheet Atomization (LISA) model [1], supplies the initial conditions for spray computations, i.e., the drop sizes, velocities, temperatures etc., at the injector nozzle exit.

The fluid-dynamics of the system is solved using the Discrete Phase Model (DPM) [2], i.e. a multiphase model in which the dispersed phase (spray particles) is tracked in a Lagrangian reference frame. The discrete and the continuous phases are properly coupled through sources terms in the governing equations.

Riello Burners owns a new test facility located in Angiari (Italy) with several test rig equipments able to accommodate burners up to 20 kW and comply with the CEN/ISO standards. In this location several experimental tests were made to evaluate the performances of the RL85BLU burner in terms of flame stability and pollutants formation.
2. Burner Geometry - CFD modeling

The liquid-fuelled turbulent swirl burner shown in Fig. 1 is equipped with a central pressure-swirl atomizer which produces a liquid spray of oil droplets. The corresponding whole amount of combustion air is fed to the burner using a fan and is distributed into primary (~25%), secondary (~17%) and tertiary air (~58%) as a consequence of the complex burner geometry. The primary air is forced to flow through a complex swirl generator which induces a recirculation zone close to the burner head and contributes to flame stabilization.

The burner was simulated in the steady-state regime both in cold and flame conditions using initially a complete 3D mesh with more than 2 millions cells. A new mesh of about 800,000 cells describing only one sixth of the physical domain was created by taking advantage of the periodic symmetry of the system. This practice allowed to further increase the detail and to reduce significantly the computational effort. The final mesh is almost entirely structured, with the exception of the inner region of the burner where a high resolution non-structured mesh allowed to improve the description of the elaborate geometry and the very small gaps associated with blades and holes.

Turbulence was modeled by the RANS approach, using the standard $k-\varepsilon$ closure model. A sensitivity analysis on the turbulence model showed a minor impact of this assumption on the predicted air distribution and velocities. For the spatial resolution the First-Order Upwind Scheme was adopted. The algorithms PRESTO! and SIMPLE [2] are respectively used for the pressure interpolation and for the coupling of pressure and velocity, as usually suggested for swirled flows [2]. The radiating heat transfer of the flame is calculated with the DO model [2]. It is worth noting that radiation and spray evaporation are coupled through the radiation absorption by particles.

3. Turbulent Combustion modeling

The description of the turbulence-chemistry interactions represents a critical aspect in modeling turbulent combustion. In this work the Eddy Dissipation (ED) and the Finite-Rate Eddy Dissipation (FR-ED) models were used [3]. The gasoil is described using the surrogate species $C_{16}H_{29}$ already included in the FLUENT code’s database [2]. In fact, this surrogate closely matches the C/H ratio of the actual gasoil used during the experimental campaign. $C_{16}H_{29}$ reacts following a 1-step reaction mechanism, derived form the work of Westbrook and Dryer [5]. To improve model predictions, a 2-step reaction scheme was added to the database always following the previous indications [5]. These kinetics schemes are reported in Tables 1 and 2. The role of the reverse reaction, which becomes significant at high temperatures, is to control the CO/CO$_2$ equilibrium concentration and the heat release intensity.
Table 1: Reaction scheme.

<table>
<thead>
<tr>
<th>REACTION SCHEME</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>1step</strong></td>
</tr>
<tr>
<td><strong>2step</strong></td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

Table 2: Constants used in the 1step and 2step approach. (Units are kmol-m-s-kJ-K)

<table>
<thead>
<tr>
<th>Pre-Exponential Factor</th>
<th>Activation energy</th>
<th>Rate Exponent</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>1-step</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( A_1 = 2.587 \times 10^9 )</td>
<td>( E_{a1} = 1.256 \times 10^5 )</td>
<td>( \alpha_{(C_{16}H_{29})} = 0.25, \alpha_{(O_2)} = 1.5 )</td>
</tr>
<tr>
<td><strong>2-step</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( A_2 = 3.205 \times 10^9 )</td>
<td>( E_{a2} = 1.256 \times 10^5 )</td>
<td>( \alpha_{(C_{16}H_{29})} = 0.25, \alpha_{(O_2)} = 1.5 )</td>
</tr>
<tr>
<td>( A_3f = 2.239 \times 10^{12} )</td>
<td>( E_{a3f} = 1.7 \times 10^5 )</td>
<td>( \alpha_{(O_2)} = 0.25, \alpha_{(H_2O)} = 0.5, \alpha_{(CO)} = 1.0 )</td>
</tr>
<tr>
<td>( A_3r = 5.0 \times 10^8 )</td>
<td>( E_{a3r} = 1.7 \times 10^5 )</td>
<td>( \alpha_{(CO)} = 1.25 )</td>
</tr>
</tbody>
</table>

*In order to better reproduce the CO/CO2 equilibrium [3,6], the concentration exponent was modified.

4. CFD Results and Analysis

The liquid fuel is fed to the pressure-swirl atomizer at 20 atm using different flow rates according to the requested thermal load which can be varied between 0.2 and 1 MW. The air excess is variable between 10 and 30%. The complete set of input data for the atomization model are summarized in Table 3.

Table 3: Input for Atomization model

| Injector Diameter | 1.1 [mm] |
| Spray Angle       | 90 ° ± 60° |
| Upstream Pressure | 20 [atm] |
| Atomizer dispersion angle | 6° |
| Fuel Density      | 840 [kg/m³] |
| Fuel Viscosity (at 20 °C) | 0.0042 [kg/m s] |
| Fuel Mass flow Rate | 18.8 ± 86.2 [kg/h] |

The fuel pressure at the inlet influences the atomization process and the spray mean diameter. At 20 atm \( \bar{D} = 45 \mu m \) and \( D_{Sauter} = 78 \mu m \), while at 30 atm \( \bar{D} = 32 \mu m \) and \( D_{Sauter} = 61 \mu m \). Figure 2 shows the burner and the typical hollow cone of the spray droplets produced by the atomizer in the full load configuration (1 MW).

![Fig. 2 Spray particles: color by particle diameter [m] (left) and temperature [K] (right).](image-url)
5. The Kinetic Post-Processor

The Kinetic Post-Processor (KPP) operates assuming the temperature and flow fields as predicted by the CFD and solves mass balances in the cells with detailed chemistry at fixed temperatures [7]. Two major features make this approach advantageous over the direct coupling of detailed kinetics and CFD. The first is the possibility to lump and group several cells and the latter is to fix the temperature inside the cells. CFD solution provides detailed flow, composition and thermal fields allowing the identification of the zones where the detail of the description can be reduced. The fixed temperature inside the cells reduces the high non linearity of the system, mainly related to the reaction rates and to the coupling between mass and energy balances. Additional details on the KPP are reported elsewhere [7].

The KPP uses a detailed kinetic mechanism (C1C30704NOx) [8] to model combustion and pollutants formation in the gas phase. The fuel evaporation in each cell is calculated by the CFD code and is simply used by the KPP as an external mass flow rate entering the gas phase. The fuel oil is represented by a mixture of n-heptane (59.5%) and benzene (40.5) to match the C/H ratio. The presence of bond nitrogen (0.0176% weight) is taken into account by adding the correspondent amount of HCN to the fuel [9]. It is worth noting that HCN conversion to NO is very sensitive to the local operating conditions. In fuel rich conditions the route leading to N₂ prevails over the oxidation to form NO. Potentially, about 10÷20 ppm of NO could be formed assuming complete oxidation of fuel-N to NO.

6. KPP Results

The results of the KPP simulation are shown in Fig. 3 which displays only a simplified scale based on minimum and maximum values of each contour variable. It is possible to observe the higher reactivity of n-heptane compared to benzene and the relatively high concentration of HCN which is released during the fuel evaporation.

![Fig. 3 Temperature [K], Axial Velocity [m/s] and composition fields [mass fraction] predicted by the KPP (P=0.8 MW, λ=1.37). Major reaction paths under Reburning conditions.](image-url)
The zone close to the burner head is considerably fuel rich due to the spray evaporation. In this region the fuel’s primary decomposition reactions lead to the formation of CH\textsubscript{1} and HCCO radicals which significantly interact with NO according to the reburning mechanism [10] as schematically depicted in Fig. 3.

**Fig. 4**  
HCN mass fraction predicted by the KPP (P=0.8 MW, \(\lambda=1.37\)) using a N-containing fuel (0.0176% weight) and a N-free gasoil.

**Fig. 5**  
NO mass fraction predicted by the KPP (P=0.8 MW, \(\lambda=1.37\)) using only thermal NOx mechanism (left) and the complete NOx mechanism (right).

**Fig. 6**  
Comparison between predicted (line) and measured NOx emissions at different air excess and P=0.2 ±1 MW.

Figure 4 shows that the presence of Fuel-N enhances HCN concentration in the gas phase from 7 to about 21 ppm, especially in the fuel rich region where evaporation largely occurs. The impact on the final NOx emissions is only 2 ppm, confirming that fuel-N is largely reduced to N\textsubscript{2} in this burner. Figure 5 provides a comparison between the major mechanisms involved in NOx formation. A simulation was performed using a kinetic mechanism.
containing only three reactions representing the thermal NOx mechanism (Zeldovich), which is responsible for ~13 ppm of NOx in the flue gases, that is only ~65% of the overall NOx emission. This contribution is expected to increase when reducing the air excess. Figure 6 shows the comparison between measured and predicted NOx emissions using variable air excess and thermal loads. NOx emissions range between 20 and 50 ppm and reveal a significant correlation with the global air excess. This trend is well captured by the model. Moreover, also the agreement with the absolute value of emissions is satisfactory and confirms the overall reliability of both CFD and KPP simulations. A good prediction of the temperature and velocity fields is obviously a necessary condition for the correct application of the KPP: the reliability of the KPP results in terms of pollutant predictions is strongly dependent on the completeness and consistency of the original CFD simulation.

7. Conclusions

A turbulent gasoil burner (RL85BLU) was modeled using a commercial CFD code able to characterize liquid fuel atomization and combustion. The results of the CFD modeling were post-processed using a numerical code called Kinetic Post Processor (KPP) able to handle the complexity involved in the modeling of turbulent reactive flows using detailed kinetic models. The major advantage lies in the reduced computational demands when proper lumping and simplification procedures are applied to the CFD grid to reduce the total number of equivalent reactors. The computed results have been validated in terms of NOx formation and the agreement with experimental measurements is good. The proposed approach seems very encouraging as a solution to manage the complexity involved in the modeling of turbulent reactive flows using detailed kinetic models and can be applied for the design and scale-up of practical combustion systems. Of course, the reliability of model predictions is strongly dependent on the completeness and consistency of the original CFD simulation.

8. References

8. [http://www.chem.polimi.it/creckmodeling/kinetic.html](http://www.chem.polimi.it/creckmodeling/kinetic.html)