17th European Symposium on Computer Aided Process Engineering – ESCAPE17
V. Plesu and P.S. Agachi (Editors)

Axial Dispersion Modeling of Laminar Flames

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Abstract

The reduction of nitrogen oxides (NOx) emissions from an existing burner is a a challenging task requiring the understanding of interactions between burner geometry and flame aerodynamics. Currently, three approaches for NOx control exist: fuel or flue gas treatment and combustion modifications. Low NOx burner design is economically attractive for natural gas and light fuel oil combustion since very low NOx emissions are achievable without the requirement for expensive equipment such as needed for post combustion reduction techniques. This paper deals with the laminar flame modeling through the axial dispersion approach, using the Residence Time Distribution (RTD) analysis. Some small quantity of inert tracer gas is injected upstream the combustor chamber. Downstream, the fluid rich in tracer passes through the detection point, where a mass spectrometer is used to quantitatively measure the tracer's concentration. Then, the analysis of the curves is done and the axial dispersion coefficients are computed. Afterwards, a flow model consisting of a series of a plug flow and an axial dispersion zones is proposed, the model parameters being regressed against the experimental data. This model, combined with a simplified kinetics, is therefore expected to be an interesting tool to reduce NOx in the existing combustors. Model validation against experiments was done.

Keywords: laminar flame, axial dispersion, residence time distribution, helium tracer, flow modeling

1. Introduction

Nitrogen is unique in forming seven molecular oxides, three of which, namely nitric oxide (NO), nitrogen dioxide (NO_2) and nitrous oxide (N_2O), are produced during combustion processes and are quite harmful to environment and human health. They contribute to acid deposition, photochemical smog and ozone layer depletion. There are three approaches for NOx control: fuel treatment, flue gas treatment and combustion modification. Nowadays, the industry tends more and more to process integrated pollution control and low NOx burners can be part of this approach. The different NOx formation mechanisms -the thermal, fuel, prompt and nitrous oxide mechanism- are well known today as well as the measures to avoid its formation in flames (Wendt, 1995). The reduction of NOx emissions from an existing burner, however, requires too the understanding of interactions between burner geometry and flame aerodynamics, which is the subject of this study.

2. RTD Analysis

The RTD influences the formation of emissions and it will be used to describe the quality of the combustor design. The aim of the present paper is to describe the methodology we developed to test and validate the flow model for the sequence combustor-flame, which then will be included into the combustor mathematical model to search for improved operating conditions, permitting the abatement of the pollutant. For this, an experimental set-up was built, to measure and describe the flow patterns in the tandem combustor-flame by generating a stimulus at the entrance, using a tracer, and measuring the response of the system immediately after the flame. From this information, the RTD of the gases, the mean residence time in the combustor and the axial dispersion coefficient can be determined (Levenspiel, 1972). In the past years, two were the tracer type used to carry out the experiments: *inert gases*, mainly Helium, measured by a mass spectrometer, and *radioactive isotopes* ^{41}Argon or ^{81}Crypton M. The inert tracers, especially Helium, have the advantage of being less pollutant and easier to use, without taking anti-radiation special measures (Berkey et al., 2003). The main drawback is the absorption of Helium into the metallic part of the combustor, mainly into the regions with lower temperatures.

2.1. The experimental set-up

Helium injected to the entrance of the burner was set and measured with a graded Hamilton syringe, suitable pre-calibrated, together with an appropriate dispenser (Hamilton's GASTIGHT Repeating Dispenser), since other measur-

ing devices are too expensive, and much too accurate for the scope of this RTD analysis, at least for this stage. Helium concentration at the exit was measured using an appropriate, in terms of precision and accuracy, Helium mass spectrometer (OMNISTAR, Pfeiffer-Vacuum Belgium). The experimental set-up has already being used to characterize thoroughly the laminar flames (Dyakov et al., 2001). Some results of the RTD experiments of the burner-flame tandem have been already presented also (Lavric et al., 2006). Basically, a RTD experiment consists of several (3-4) replicates of a pulse-like injection of 1.5÷2 cc of Helium (this quantity is imposed to maintain the overall flow perturbation under 1%, which is below the acceptable tolerance), followed by a record of the answer of the system, in terms of helium concentration at the exit, in the terminal part of the flame, in one of the five locations we select to test and model the local flow: N, E, S, W and center (care should be taken not to disturb unnecessarily the laminar nature of it). The absence of long tails was considered evidence that Helium was not adsorbed significantly on the internals of the burner. A typical RTD curve (Lavric et al. 2006) shows the presence of a lag-time between the injection of the signal and the moment the first Helium molecules have had been sensed by the mass spectrometer and the presence of the axial dispersion into the chamber and flame. "Cold" (measurements made immediately after the flame was blew out) and "hot" (measurements made in the presence of the flame) experiments showed that the influence of the flame front itself upon the overall dispersion coefficient is rather small. Corroborating these with the time scale difference between the flow through burner chamber and the flame processes (two to three orders of magnitude) we proposed for the system burner-laminar flame a flow model starting with a plug flow zone (this ensures the time delay), followed by a zone with axial dispersion and ending with a perfectly mixed zone, the later corresponding to the flame.

3. The axial dispersion mathematical model

Considering that we can safely assume the gas-mixture has the characteristics of a *microfluid* (Levenspiel, 1972) we will use the flow model following the RTD analysis as the frame for the mass and heat balance equations, the main components of the system's mathematical model.

Burner chamber *– plug flow zone*

The burner chamber has only the role of completely mix the fed-in gases, no chemical process developing inside. More, the laminar condition imposed to the flame is ensured keeping this zone isothermal, so no heat balance will be necessary. Since we deal with a compressible fluid, the mass balance should be written in terms of "*j*" species partial density, in the absence of diffusion/dispersion and chemical process:

$$\frac{\partial \rho_j}{\partial t} + \frac{\partial \left(u_z \cdot \rho_j \right)}{\partial z} = 0 \tag{1}$$

The initial and boundary conditions are ($\rho_{j,inB}$ is the density at the entrance in the burner chamber):

$$t = 0, \forall z, \quad \rho_j = \rho_{j,inB}; \quad t > 0, z = 0, \quad \rho_j = \rho_{j,inB} \tag{2}$$

Burner chamber *–axial dispersion zone*

The axial dispersion process is characterized by the axial dispersion coefficient, D_L; we assume that it has the same value all along the burner chamber and does not depend upon the chemical species. The mass balance reads:

$$\frac{\partial \rho_j}{\partial t} + \frac{\partial\left(\rho_j \cdot u_z\right)}{\partial z} = \frac{\partial}{\partial z}\left[D_L \frac{\partial\left(\rho_j \cdot u_z\right)}{\partial z} \right] \tag{3}$$

The initial and boundary conditions correspond to a closed vessel ($\rho_{j,outD}$ is the concentration at the exit of the plug flow zone):

$$t = 0, \forall z, \quad \rho_j = \rho_{j,inB}$$

$$t > 0, z = 0, \quad \rho_{j,outD} \cdot u_z = \rho_j \cdot u_z - D_L \frac{\partial\left(\rho_j \cdot u_z\right)}{\partial z} \tag{4}$$

$$z = L, \quad D_L \frac{\partial\left(\rho_j \cdot u_z\right)}{\partial z} = 0$$

Since there is no chemical process inside the burner, the order in the sequence is unimportant for the exit concentration of the flowing species (Levenspiel, 1972). The dispersion coefficient comes from RTD measurement analysis, as presented elsewhere (Lavric et al., 2006).

The flame

We can safely assume the validity of two simplifying assumptions, taking into account that the burner chamber has a much larger time scale than the flame. First, the flame can be assumed adiabatic, neglecting the heat transfer through radiation, the only mechanism which could have the same time scale. Second, the flame reaches the equilibrium with respect to any inlet change very fast, so it may be safely seen as in a pseudo-steady state, compared to the burner chamber. Accordingly, its mathematical model reads:

$$\rho_j = \rho_{j,in} - \tau_{flame} \cdot r_j\left(\rho_1, \rho_2, \ldots \rho_S\right)$$

$$T = T_{in} \frac{\overline{\rho}_{in} \cdot \overline{c}_{p,in}}{\overline{\rho} \cdot \overline{c}_p} + \tau_{lame} \cdot \sum_{k=1}^{K}\left(-\Delta H_{r,k}\right) \cdot r_k\left(\rho_1, \rho_2, \ldots \rho_S\right) \tag{5}$$

3.1. Solving the mathematical model

We choose orthogonal collocation as solving algorithm, due to its simplicity robustness, yet preserving the accuracy (Finlayson, 1972). It means replacing the spatial derivatives with their corresponding matrices, thus transforming the PDE into an ODE. Due to the lack of space, the equations are not presented.

4. Results and Discussion

In order to test the model, we solve it in the absence of the chemical process implied by the flame, which means that we considered only the ODEs resulted from orthogonal collocation method. We integrate the system considering a step-like Helium at the entrance (an impulse-like signal is difficult to be modeled numerically and the results are equivalent with what is obtained using the step-like signal) and plotted the results against the experimental ones.

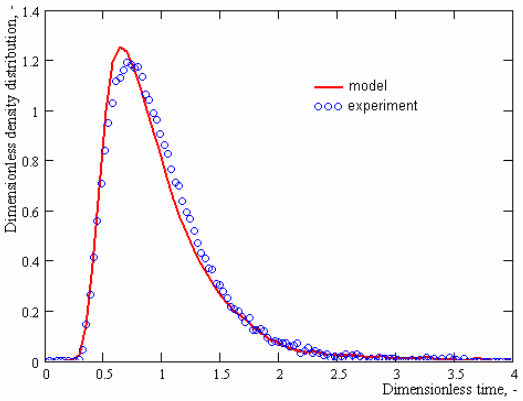

Figure 1. The comparative density distribution profiles for the Helium concentration in the middle of the distributor, in the absence of the flame

We should mention that the axial dispersion coefficient used in computations was the mean value of the experimental dispersion coefficients found along radius. This is mandatory, since our mathematical model is unidirectional, assuming no radial dependency of the state variables. The results are presented in Figure 1, in terms of Helium's density of distribution profiles for the model and the experiment. As it can be seen, the agreement is relatively good, except for the peak zone, but this could be an effect of the simplifications introduced using the mean axial dispersion coefficient value. When we integrated the model for the same situation, but considering the presence of the flame, the results, depicted in Figure 2, were not as good as in the previous case, the disagreement in the peak zone being larger and even displaced. The reason could be not only the actual value of the axially mediated dispersion coefficient, but also the radial distribution of the species concentration, which probably has to be taken into consideration in an improved variant of the model.

5. Conclusions

A stimulus-response technique, based upon Helium as tracer and a mass spectrometer as on-line analyzer, was established then used to characterize the flow distribution, both qualitatively and quantitatively. Then, the flow model of the burner chamber-flame tandem was built, using the RTD analysis and the axial dispersion coefficients were computed, for every operating conditions used into the domain of interest. Based upon the flow model, a mathematical model was developed, using mass and heat balances, where appropriate. The model was validated using "*cold*" experiments, to predict the behavior in the absence of the

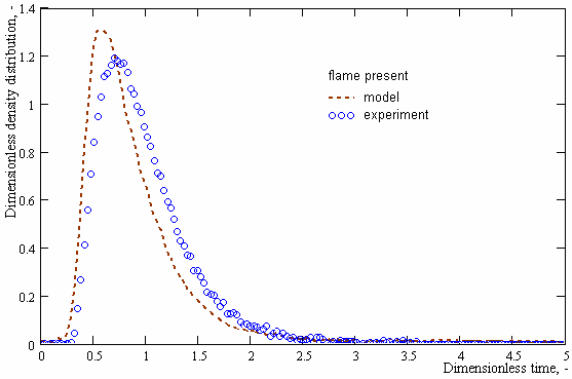

Figure 2. The comparative density distribution profiles for the Helium concentration in the middle of the distributor, in the presence of the flame

burning process, comparing the Helium distributions obtained experimentally and given by the model.

The satisfactory agreement obtained encouraged us to continue with the next step: using the model for "*hot*" experiments. The departure model – experiment was greater due to the simplifications introduced. Yet, the model output is in a good qualitative agreement with the experiment, which is an encouraging conclusion, supporting the decision to implement the kinetic for the flame.

Acknowledgements

The present paper is the result of cooperation between VUB and UPB-CTTIP developed under the auspices of the bilateral agreement between the Flemish and Romanian governments, BWS04/05/MECHWER2- Flame Characterization and NOx Reduction through Residence Time Distribution Analysis. Also, the financial aid of FWO, Belgium is gratefully acknowledged for purchasing the OMNISTAR Pfeiffer-Vacuum, Belgium mass spectrometer.

Bibliography

1. Berkey, J.S., Lachmar, T.E., Doucette, W.J., Dupont, R.R., 2003. Tracer studies for evaluation of in situ air sparging and in-well aeration system performance at a gasoline-contaminated site. Journal of Hazardous Materials. B98, 127–144
2. Dyakov, I.V., Konnov, A. A., De Ruyck, J., Bosschaart, K.J., Brock, E.C.M., de Goey, L.P.H., 2001. Measurement of Adiabatic Burning Velocity in Methane - Oxygen - Nitrogen Mixtures, Combust. Sci. and Tech. 172, 81-96.
3. Finlayson, B. A. The method of weighted residuals and variational principles, Academic Press, New York, 1972
4. Lavric, E.D., Konnov, A., Rybitskaya, I.V., De Ruyck, J., Lavric, V., 2006. Laminar Flames Characterization through RTD Analysis. CHISA'2006, 27-31 Aug., Prague, Czech Republic
5. Levenspiel O., Chemical reaction engineering, Wiley, 1972
6. Wendt, J.O.L., 1995. Mechanism governing the formation and destruction of NOx and other nitrogenous species in low NOx coal combustion systems. Combust. Sci. Technol. 108, 323-344.