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Chemical Engineering Science 60 (2005) 2851–2869

Chemical Engineering Science

www.elsevier.com/locate/ces

Determination of NO_x emissions from strong swirling confined flames with an integrated CFD-based procedure

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Received 29 March 2004; received in revised form 19 November 2004; accepted 23 December 2004

Abstract

The present work is focused on a new procedure for the determination of NO_x emission from combustion processes, which allow using very detailed and comprehensive reaction schemes, on the basis of the results obtained from CFD computations. This procedure is validated in the case of high swirled confined natural gas diffusion flames. The experimental data refer to the work developed within the German TECFLAM cooperation concerning a swirl burner ($0.6 < S < 1.4$) fed with natural gas characterized by 150 kW thermal load and 0.8 equivalence ratio (TECFLAM webpage, www.tu-darmstadt.de/fb/mb/ekt/tecflam; Schmittel et al., Proceedings of the Combustion Institute 28 (2000) 303–309).

The CFD analysis represents a useful technology to provide the flow and temperature fields. The high swirling configuration makes the solution an interesting and difficult task for commercial codes. In particular, previous attempts of predicting the flow and temperature fields with the FLUENT code failed (Meier et al., Applied Physics B 71 (2000a) 725–731). Only a careful attention to the boundary conditions and converging strategy allows to reach a satisfactory modeling of the main characteristics of the flame. The numerical calculation was performed using the commercial code FLUENT6.0. NO_x formation is a chemical process whose time-scale is of the same order of mixing fluid dynamics. For this reason, comprehensive modeling of NO_x reaction processes in combustion systems requires simulation of both the turbulent fluid dynamics and chemical kinetics in the system being modeled. Hundreds of elementary reactions are required to provide a detailed description of the formation and depletion of oxides of nitrogen in combustion systems. However, it is not currently feasible to use such detailed reaction mechanisms to model a turbulent reacting system in which large reaction kinetics schemes are coupled with the turbulent fluid dynamics. Consequently, the difficulties in coupling detailed chemistry and detailed fluid dynamics force to adopt proper simplifications. The prediction of NO_x formation is then obtained by postprocessing the flow and temperature fields, as predicted by CFD, and lumping together computational cells similar in terms of NO_x formation. The resulting macrocells are assumed to be a network of ideal reactors, which are simulated adopting a detailed kinetics. The characteristics and operating conditions of each reactor are defined by a procedure already developed for furnaces and named SFIRN (Faravelli et al., Computers and Chemical Engineering 25 (2001) 613–618). The predictions have been tested on flames at different swirl numbers. Both the CFD and the chemical analysis show a satisfactory agreement with the measured data.

Keywords: Combustion; NO_x prediction; Kinetics; Turbulence; Pollution; Environment

1. Introduction

The optimization of combustion systems in terms of efficiency and reduction of pollutants is considered the main aim of combustor research projects. This result can be achieved through an accurate design of the combustor which also takes heat and mass transfer phenomena into account.

In the last few years, computational fluid dynamic (CFD) has become popular and represents a useful approach for providing preliminary information and facilitating economical combustion systems design. However the phenomena

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doi:10.1016/j.ces.2004.12.038

occurring in burners are highly complex with hot flue gas recirculations, energy exchanges and strong turbulence-chemistry effects which are enhanced still further in the case of swirled combustors. For this reason, CFD analysis of swirling confined reacting flows is one of the most important and challenging areas of modern CFD.

The experimental data developed within the German TECFLAM cooperation project (TECFLAM webpage, www.tu-darmstadt.de/fb/mb/ekt/tecflam; Schmittel et al., 2000) are well documented and they represent useful information for testing CFD. The aim of this article is to investigate NO_x formation from a test burner. The typical time-scale of the chemistry of nitric oxides is of the same order as the fluid dynamic one. Consequently, we were forced to use a detailed kinetic model to quantify these species. At the same time, NO_x is extremely sensitive to both temperature and stoichiometric conditions.

Different mathematical approaches for describing the fluid dynamics and heat transfer can be found in the literature. The main approaches use turbulent combustion models, which make use of the statistical properties of the scalar field. These approaches do yield detailed information on flow and temperature fields in many cases, but their prediction of the concentration of the minor species is less accurate. Unfortunately, even though computer performance and available memory are improving rapidly, it is still difficult to couple detailed kinetics and fluid dynamics especially in the case of combustion of large hydrocarbons. A new way of dealing with this problem has already been proposed for boilers (Faravelli et al., 2001). This approach, referred to as SFIRN, is based on the original concept of the hybrid method. Flow and temperature fields are not influenced by the NO_x chemistry. A few very rapid combustion reactions suffice to describe the heat generation in CFD computations. A network of ideal reactors is defined on the basis of the results obtained by the fluid dynamic simulation. These reactors group together many equivalent cells and are solved by taking a very detailed chemistry into consideration.

The detailed experimental measurements of the TECFLAM project (TECFLAM webpage, www.tu-darmstadt.de/fb/mb/ekt/tecflam, Schmittel et al., 2000) represent a significant test-case in order to validate the capability of the procedure, which can be then more reliably extended to complex furnaces or boilers. In practical combustion devices, common NO_x control technologies include air and fuel-staging, over-fire air, flue gas recirculation, reburning, and thermal $DeNO_x$. These technologies are often used in combination. Most of these NO_x reducing techniques are based on the complex chemistry of interactions between N containing compounds (thermal $DeNO_x$) or between hydrocarbon and NO_x (reburning). Detailed CFD and kinetic modeling is then necessary to give an accurate prediction of NO_x emissions and improve the design and operation of combustion systems.

Our attention turned towards high swirling flames because their application is of interest to furnace combustors and gas turbines. Furthermore, swirled flames represent a promising strategy for minimizing the environmental impact of combustion systems. The application of a tangential velocity component to the flow (W), gives the flow a rotating component, represented by the non-dimensional swirl number (S) defined as the ratio of the axial flow of the tangential component to the axial flow of the axial component (U), which has the form

$$S = \frac{\int_0^{R_{in}} \rho U W r^2 \, \mathrm{d}r}{R_{in} \int_0^{R_{in}} \rho U^2 r \, \mathrm{d}r}. \quad (1)$$

When the swirl number is enhanced (conventional diffusion flames are denoted by $S = 0$) the flow field rapidly changes. The S level in particular affects the turbulent energy, dissipation rate, turbulent stresses and the scale of turbulence. At high swirl numbers ($S > 0.6$) the flow field can be divided into three separate zones as shown in Fig. 1: the mixing zone between the oxidizer and the fuel streams, where exothermic reactions take place (A); the central

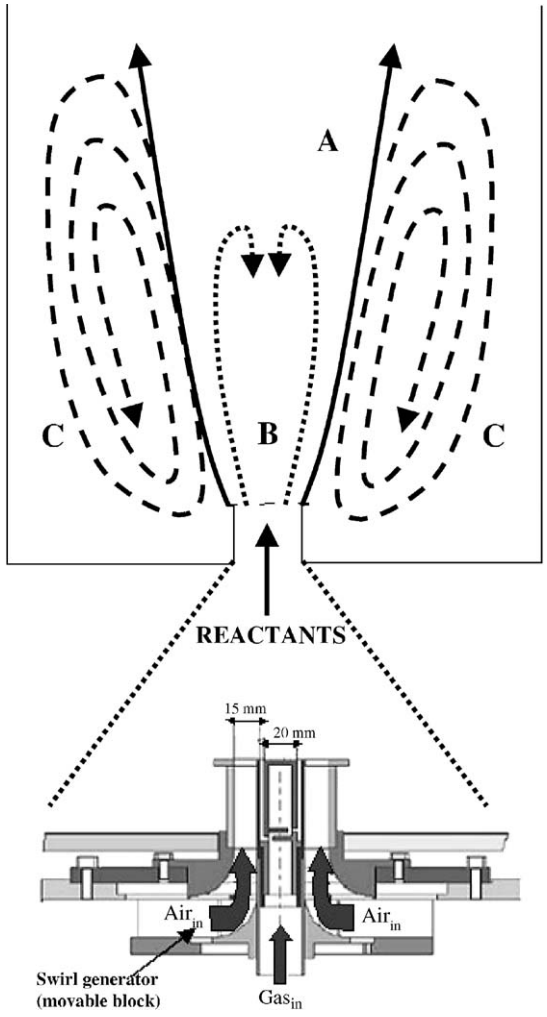

Fig. 1. General pattern of a high swirling confined flame and nozzle geometry (www.tu-darmstadt.de/fb/mb/ekt/tecflam). (A = reaction zone; B = inner recirculating core; C = outer recirculating zone).