Applied Thermal Engineering 76 (2015) 324–334

Contents lists available at ScienceDirect

Applied Thermal Engineering

journal homepage: www.elsevier.com/locate/apthermeng

Research paper

Influence of modelling and scenario uncertainties on the numerical simulation of a semi-industrial flameless furnace

Valentina Fortunato [a], Chiara Galletti [b, **], Leonardo Tognotti [b], Alessandro Parente [a, *]

[a] Service d'Aéro-Thermo-Mécanique, Université Libre de Bruxelles, Bruxelles, Belgium
[b] Dipartimento di Ingegneria Civile e Industriale, Università di Pisa, Pisa, Italy

HIGHLIGHTS

- The significance of turbulence/chemistry interaction closures is demonstrated.
- The impact of simplified and detailed kinetic mechanisms is discussed.
- The impact of uncertainties in boundary conditions and physical model is assessed.
- The N_2O intermediate NO mechanism is found to dominate NO formation.

ARTICLE INFO

Article history:
Received 30 April 2014
Accepted 4 November 2014
Available online 13 November 2014

Keywords:
Flameless combustion
MILD combustion
Turbulence–chemistry interactions
Uncertainty
Validation

ABSTRACT

Flameless combustion is able to provide high combustion efficiency with low NO_x and soot emissions. The present work aims at investigating the role of closure sub-models for the modelling of a flameless furnace, as well as the main NO formation paths. Among the different turbulence models that were tested, modified $k-\varepsilon$ provides the best agreement with the experimental data, especially for temperature measurements. Reynolds stress model leads to smaller deviation for radial velocity predictions. Since in flameless combustion regime the turbulence–chemistry interaction as well as the kinetic mechanism play a fundamental role, the Eddy Dissipation Concept (EDC), coupled with four different kinetic schemes (JL, KEE58, GRI 2.11 and GRI 3.0) was considered. The GRI 2.11 and KEE58 mechanisms perform better, thus confirming the necessity of turbulence/chemistry interaction models accounting for finite-rate chemistry when flameless combustion is studied. As far as NO emissions are concerned, the N_2O intermediate NO mechanism is found to play a major role, while thermal NO formation mechanism is not as relevant as in traditional combustion regime.

An assessment of the uncertainty related to the choice of boundary conditions as well as to the choice of the parameters of the physical models is also performed. Finally the operation characteristics (such as the recirculation rate and the location of the reaction zone) of the furnace are evaluated.

1. Introduction

Flameless combustion [1], also known as Moderate and Intense Low-Oxygen Dilution (MILD) [2] or HiTAC combustion [3] is able to provide high combustion efficiency with low NO_x and soot emissions. The increasing interest in flameless combustion is motivated by the large fuel flexibility, representing a promising technology for low-calorific value fuels [4], high-calorific industrial wastes as well as in presence of hydrogen [5]. Moreover, flameless combustion is very stable and noiseless [6], so it could be potentially suited for gas turbine applications [7] where conventional operations may lead to significant thermo-acoustic instabilities ("humming") and stresses.

Flameless combustion needs the reactants to be preheated above their self-ignition temperature and enough inert combustion products to be entrained in the reaction region, in order to dilute the flame. As a result, the temperature field is more uniform than in traditional non-premixed combustion systems, and it does not

* Corresponding author. Université Libre de Bruxelles, Service d'Aéro-Thermo-Mécanique, Avenue F. D. Roosevelt 50, B-1050 Bruxelles, Belgium. Tel.: +32 2 650 26 80; fax: +32 2 650 27 10.
** Corresponding author. Università di Pisa, Dipartimento di Ingegneria Civile e Industriale, Largo L. Lazzarino 2, I-56122 Pisa, Italy. Tel.: +39 050 22 17 897; fax: +39 050 22 17 866.
E-mail addresses: chiara.galletti@unipi.it (C. Galletti), Alessandro.Parente@ulb.ac.be (A. Parente).

http://dx.doi.org/10.1016/j.applthermaleng.2014.11.005
1359-4311/

show high temperature peaks. Hence, NO_x formation is suppressed as well as soot formation, due to the lean conditions, low temperatures and the large CO_2 concentration in the exhausts.

This combustion regime appears to be still worthy of further investigations and attention. In particular, the fundamental mechanism of the interaction between turbulent mixing and chemical kinetics needs to be elucidated. With respect to conventional flames, turbulence levels are enhanced (due to the high momentum of the gases), thus mixing timescales are reduced; on the contrary chemical timescales are increased due to dilution of the reactants [8]. In flameless combustion, the Damköhler number approaches unity [9], implying that both mixing and chemical kinetics should be taken into account when modelling such a regime, resulting in a very challenging problem. In addition, most of the available models have been derived for conventional flames; hence they need to be validated and eventually revised for non-conventional regimes.

From a computational perspective, the role of the combustion model and the possible degree of simplification of chemical kinetics have not been rigorously and systematically assessed in the context of flameless combustion. Encouraging results in literature on the modelling of such flames have been found using the Eddy Dissipation Concept (EDC) model by Magnussen [10], coupled with detailed chemical mechanism. Such modelling strategy has been successfully applied to the Jet in Hot Coflow burner by Christo and Dally [11] and Aminian et al. [12]. The same approach leads to good results also in presence of hydrogen in the fuel, as reported by Parente et al. [13] and Galletti et al. [14] for a self-recuperative burner and a lab-scale burner, respectively, operating in flameless combustion conditions.

However, recent investigations carried out by De et al. [15] and Aminian et al. [16] have indicated the need for revising the EDC constants in the framework of flameless combustion modelling.

All the works reported above show that the oxidation scheme may strongly impact the results, as indicated by Shabanian et al. [17]. The global schemes are unsuited and generally lead to a strong over prediction of the flame temperatures. Recently Parente et al. [18] applied Principal Component Analysis to a set of measurements taken in flameless combustion conditions, showing that approaches based on single progress variable are not suited for the description of such combustion regime and finite-rate chemistry models are needed.

Finally, the modelling of NO emissions deserves also special attention. The Zeldovich thermal mechanism is the major contributor to NO in most of the conventional combustion system; however, in flameless combustion, the lower temperatures and the absence of large fluctuations inhibit NO formation through such a mechanism. As a result, NO emissions are controlled by other formation routes, such as the Fenimore's prompt NO and/or N_2O intermediate [19]. Therefore, it is necessary to incorporate all potentially relevant formation paths in the numerical model. Moreover, other routes may become relevant with non-conventional fuels, such as the NNH pathway for H_2 containing fuels [14]. The prediction of NO formation in flameless combustion, at low temperatures and with high concentration of H_2 in the fuel stream has been studied by Parente et al. [20]. They found that the inclusion of non-conventional NO formation routes, i.e. N_2O intermediate and NNH, is crucial for characterizing the pollutant emissions.

The elucidation of the above topics needs high fidelity and comprehensive experimental data to validate the numerical models. The Jet in Hot Coflow (JHC) burner [21], the Delft Jet in Hot Coflow (DJHC) [22,23] and the Cabra flame [24] have been conceived to emulate flameless conditions by feeding diluted and hot streams to the burner. They constitute a strong asset for the validation of numerical models as they have been equipped with advanced diagnostics to measure mean and fluctuating variables (e.g. chemical species, temperature, velocities).

However, in the industrial practice, flameless conditions are obtained by means of the massive internal recirculation of flue gases, which allows diluting the fresh gases before they reach the reaction zone. Such recirculation is generally achieved through special designs of the feeding jets as well as of the combustion chamber. A recent review of different designs of flameless combustors is provided by Arghode and Gupta [25,26].

The recirculation affects both mixing and chemical timescales, so that conceptually these burners are different from JHC, DJHC and Cabra flames, which act solely on the chemical timescale. A few experimental investigations of flameless furnaces, based on internal recirculation of exhaust gases can be found in literature. Szegö et al. [19] described the performance and stability characteristics of a parallel jet flameless combustion burner system in a 20 kW laboratory-scale furnace. Mi et al. [27] investigated a 20 kW recuperative MILD furnace, using EDC combustion model with global kinetic schemes for methane and ethane. Plessing et al. [28] and Özdemir and Peters [29] provided a useful set of experimental data (velocity, temperature and NO emissions) on a 5.4 kW furnace fed with methane and operating in flameless regime, subsequently modelled by Coelho and Peters [30] using the Eulerian Particle Flamelet model. Their results showed some discrepancies in the prediction of flow field as well as the overestimation of NO levels at the outlet section. Dally et al. [31] extended the investigation of the same furnace to more fuels and equivalence ratios. Verissimo et al. [32] experimentally investigated a 10 kW reversed-flow cylindrical furnace, for which simulation were performed by Graça et al. [33]. The Authors compared the EDC model coupled with the DRM-19 mechanism and the composition PDF (C-PDF) model, showing a general good agreement between predictions and experiments. Danon et al. [34] performed a parametric study on a 300 kW_{th} furnace equipped with three pairs of regenerative flameless combustion burners with the objective of optimizing the furnace performance. These experimental results were used as validation data for a set of Computational Fluid Dynamics (CFD) simulations of the furnace reported in Ref. [35]. The authors showed that the EDC model in combination with the realizable k–ε model and a skeletal chemistry mechanism allowed reproducing the main furnace performance for all the investigated burner configurations. Rebola et al. [36] performed an experimental investigation on a small-scale flameless combustor, defining the range of operating conditions allowing operating in flameless conditions. Cameretti et al. [37] discussed some aspects related to the employment of liquid and gaseous bio-fuels in a micro-gas turbine operating in flameless regime, showing numerically the energetic and environmental advantages related to the use of those fuels. Recently Huang et al. [38] studied the emissions from a flameless combustion staged combustor. The authors found that the flameless regime yields lower NO emissions compared to the traditional diffusion combustion mode, and the N_2O intermediate mechanism dominates the NO production.

The present work aims at investigating the role of closure submodels for the modelling of the flameless furnace of Plessing et al. [28] and Özdemir and Peters [29], as well as at identifying the main NO formation paths. The selected experiment set-up was chosen as it represents an optimal compromise between lab-scale and industrial systems. It shows, in fact, the typical feature of industrial flames systems, i.e. the internal aerodynamic recirculation, allowing, at the same time, a sufficiently detailed characterization of the system performances.

While existing literature has pointed out the crucial role of finite rate chemistry models and detailed kinetics in flameless regime, little emphasis has been devoted to the quantification of the