Fuel 163 (2016) 98–111

Contents lists available at ScienceDirect

Fuel

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

Extension of the Eddy Dissipation Concept for turbulence/chemistry interactions to MILD combustion

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ARTICLE INFO

Article history:
Received 10 April 2015
Received in revised form 8 September 2015
Accepted 9 September 2015
Available online 25 September 2015

Keywords:
Eddy Dissipation Concept
Energy cascade model
Flameless combustion
MILD combustion
Turbulence/chemistry interactions

ABSTRACT

Over the past 30 years, the Eddy Dissipation Concept (EDC) has been widely applied in the industry for the numerical simulations of turbulent combustion problems. The success of the EDC is mainly due to its ability to incorporate detailed chemical mechanisms at an affordable computational cost compared to some other models. Detailed kinetic schemes are necessary in order to capture turbulent flames where there is strong coupling between the turbulence and chemical kinetics. Such flames are found in Moderate and Intense Low-oxygen Dilution (MILD) combustion, where chemical time scales are increased compared with conventional combustion, mainly because of slower reactions (due to the dilution of reactants). Recent modelling studies have highlighted limitations of the standard EDC model when applied to the simulation of MILD systems, noticeably a significant overestimation of temperature levels. Modifications of the model coefficients were proposed to account for the specific features of MILD combustion, i.e. an extension of the reaction region and the reduction of maximum temperatures. The purpose of the present paper is to provide functional expressions showing the dependency of the EDC coefficients on dimensionless flow parameters such as the Reynolds and Damköhler numbers, taking into account the specific features of the MILD combustion regime, where the presence of hot diluent and its influence on the flow and mixing fields impacts on the reaction rate and thermal field. The approach is validated using detailed experimental data from flames stabilized on the Adelaide Jet in Hot Co-flow (JHC) burner at different co-flow compositions (3%, 6% and 9% O_2 mass fraction) and fuel-jet Reynolds numbers (5000, 10,000 and 20,000). Results show promising improvement with respect to the standard EDC formulation, especially at diluted conditions and medium to low Reynolds numbers.

1. Introduction

New breakthroughs in clean energy are needed to provide our society with the necessary resources in a way that also protects the environment and addresses the climate change issue. The need for innovation is particularly important in combustion, considering that the energy derived from burning fossil fuels (coal, petroleum or natural gas) supplies over two thirds of the total world energy needs. A certain number of new combustion technologies have been proposed in recent years. Among them, Moderate or Intense Low-oxygen Dilution (MILD) [1–3] combustion is certainly one of the most promising, as it is able to provide high combustion efficiency with low pollutant emissions. This mode of combustion is achieved through the strong exhaust gas and heat recirculation, achieved by means of the internal aerodynamics of the combustion chamber in conjunction with high-velocity burners [1]. Heat recovery by preheating the oxidant stream can also help in improving thermal efficiency and maintaining the MILD regime. The resulting combustion regime features reduced local oxygen levels, distribution of reaction over the whole combustion chamber, no visible or audible flame and thus the name flameless. The temperature field is more uniform due to absence of temperature peaks, which drastically reduces NOx formation [1,2,4–6], while ensuring complete combustion and low CO emissions [7–10]. MILD combustion can accommodate large fuel flexibility, representing an ideal technology for low-calorific value fuels [11–14], high-calorific industrial wastes [15] as well as for hydrogen-based fuels [16,17].

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http://dx.doi.org/10.1016/j.fuel.2015.09.020
0016-2361/

In recent years, attention has been paid to MILD combustion modelling, due to the very strong turbulence/chemistry interactions of such a combustion regime. The Damköhler number in MILD conditions usually approaches unity [17] and both mixing and chemistry need to be taken into account with appropriate turbulent combustion models. This has also been proven by Parente et al. [18], who analysed the correlation structure of MILD combustion data [19] using Principal Component Analysis (PCA) and showed that the standard flamelet approach is not suited for such combustion regime. Recently, successful predictions of different MILD combustion cases have been reported [17,20–22] using Reynolds-Averaged Navier–Stokes (RANS) modelling and the Eddy Dissipation Concept (EDC) [23]. However, several studies of the Jet in Hot Co-flow (JHC) configuration [19] also reported that the standard EDC tends to over-predict maximum temperatures when applied to the MILD combustion regime [24,25]. Recently, De et al. [26] carried out a detailed study on the performance of the EDC model on the Delft Jet in Hot Co-flow burner (DJHC) emulating MILD conditions. The authors showed that the model described correctly the mean velocity profiles and the Reynolds shear stress distributions, but showed significant discrepancies between measured and predicted temperatures. The mean temperature field showed systematic deviations from experimental data, due to the under-prediction of the lift-off height and the over-estimation of the maximum temperature level. This is mainly due to the over-estimations of the mean reaction rate in the EDC model. The authors showed that the prediction could be improved by adapting the standard coefficients of the classic EDC model, in particular increasing the time scale value, C_τ, from 0.4083 to 3. The results were further confirmed for the analysis of the Adelaide JHC flames with methane/hydrogen mixtures [27] and with several ethylene-based blends [28]. Recently, Evans et al. [29] showed that adjusting the EDC coefficients C_τ and C_γ from their default value, 0.4083 and 2.1377, to 3.0 and 1.0, respectively, results in significantly improved performance of the EDC model under MILD conditions. Although the modification of the coefficients was shown to provide improved agreement between experiments and numerical simulations, it is still necessary to identify clear guidelines for the modification of the model coefficients in the context of MILD combustion, based on the specific turbulence and chemical features of such a regime. Shiehnejadhesar et al. [30] showed, for instance, that the standard EDC is not applicable for turbulent Reynolds values below 64 and proposed a hybrid Eddy Dissipation Concept/Finite-rate model calculating an effective reaction rate weighting a laminar finite-rate and a turbulent reaction rate, depending on the local turbulent Reynolds number of the flow.

The purpose of the present paper is to provide functional expressions showing the dependency of the EDC coefficients on dimensionless flow parameters such as the Reynolds and the Damköhler numbers. After a brief description of EDC and of the energy cascade model it relies on, the novel approach for the determination of the EDC coefficients will be presented. Results for the Adelaide JHC at different co-flow composition (3%, 6% et 9% O_2 mass fraction) and fuel-jet Reynolds numbers (5000, 10,000 and 20,000) will be presented, to assess the soundness of the current approach.

2. Eddy Dissipation Concept

The Eddy Dissipation Concept (EDC) by Magnussen [23] for turbulent combustion has found wide application for the simulation of turbulent reacting flows, especially for cases where combustion kinetics plays a major role, as it happens for MILD conditions. EDC has the advantage of incorporating detailed kinetics at a computational cost which is affordable when compared to more sophisticated models such as the transported PDF methods. This advantage is maximised when EDC is used in conjunction with *in-situ* adaptive tabulation (ISAT) [31].

According to the EDC model, combustion occurs in the regions of the flow where the dissipation of turbulence kinetic energy takes place. Such regions are denoted as fine structures and they can be described as perfectly stirred reactors (PSR). The mass fraction of the fine structures, γ_λ, and the mean residence time of the fluid within them, τ^*, are provided by an energy cascade model [32], which describes the energy dissipation process as a function of the characteristic scales:

$$\gamma_\lambda = \left(\frac{3C_{D2}}{4C_{D1}^2}\right)^{\frac{1}{4}}\left(\frac{\nu\epsilon}{k^2}\right)^{\frac{1}{4}} = C_\gamma\left(\frac{\nu\epsilon}{k^2}\right)^{\frac{1}{4}} \tag{1}$$

and

$$\tau^* = \left(\frac{C_{D2}}{3}\right)^{\frac{1}{2}}\left(\frac{\nu}{\epsilon}\right)^{\frac{1}{2}} = C_\tau\left(\frac{\nu}{\epsilon}\right)^{\frac{1}{2}} \tag{2}$$

where ν is the kinematic viscosity and ϵ is the dissipation rate of turbulent kinetic energy, k. C_{D1} and C_{D2} are model constants set equal to 0.135 and 0.5, respectively, leading to fine structure volume and residence time constants equal to $C_\gamma = 2.1377$ and $C_\tau = 0.4083$. Fine structures are assumed to be isobaric, adiabatic perfectly stirred reactors. The mean (mass-based) source term in the conservation equation for the ith species is modelled as suggested by Gran and Magnussen [33]:

$$\overline{\dot{\omega}}_i = -\frac{\overline{\rho}\gamma_\lambda^2}{\tau^*(1-\gamma_\lambda^3)}(\widetilde{y}_i - y_i^*), \tag{3}$$

where $\overline{\rho}$ denotes the mean density of the mixture, y_i^* is the mass fraction of the ith species in the fine structures and $\widetilde{y}_i$ represents the mean mass fraction of the ith species between the fine structures and the surrounding state (indicated as y_i^0):

$$\widetilde{y}_i = \gamma_\lambda^3 y_i^* + (1-\gamma_\lambda^3)y_i^0. \tag{4}$$

As indicated above, the expressions for γ_λ and τ^* used in the mean reaction rate for the ith species are obtained from an energy cascade model, based on Kolmogorov's theory. In the following the model is briefly summarised, to highlight the main hypothesis behind it. Then, the proposed modification of the EDC standard coefficients will be presented and discussed.

2.1. Energy cascade model

The energy cascade model for EDC [32] starts with the transfer rate of mechanical energy, w', from the mean flow to the large turbulent eddies. The sum of the heat generated at each level, $\sum_i q_i$, is assumed to be equal to the turbulent dissipation rate ϵ. The first cascade level is characterised by a velocity scale $u' = \sqrt{2/3k}$ and a length scale L', giving a strain rate $\omega' = u'/L'$, and it represents the whole turbulence spectrum because it contains the effect of smaller scales. In the energy cascade model, it is assumed that the strain doubles at each level, so that $\omega'' = u''/L'' = 2\omega'$. The strain rate at level n is $\omega_n = 2\omega_{(n-1)}$. In the original model formulation, the last level is described by scales $\omega^*,\ u^*,\ L^*$, which are considered to be of the same order of Kolmogorov scales, $\omega_k,\ u_k,\ L_k$.

The rate of production of mechanical energy, w_i, and the rate of viscous dissipation, q_i, at each level of the cascade are expressed [32] in analogy to the production and dissipation terms appearing in the equation of turbulent kinetic energy, k. This implies, for level n:

$$w_n = \frac{3}{2}C_{D1}\omega_n u_n^2 = \frac{3}{2}C_{D1}\frac{u_n^3}{L_n}, \tag{5}$$