

Numerical investigation of the Delft Jet in Hot-Coflow burner with EDC model and chemistry reduction in OpenFOAM

Z. Li¹, F. Contino², A. Parente¹

1. Université Libre de Bruxelles, Aero-Thermo-Mechanics Department, Belgium

2. Vrije Universiteit Brussel, Department of Mechanical Engineering, Belgium

Introduction

Moderate or Intense Low oxygen Dilution (MILD) combustion technology has gained increasing attention for the past few decades [1]. It is characterized by very strong mixing between the reactant and product. As a result, the fuel conversion rate is higher and the temperature field is more uniform than that in conventional combustion regime, thereby reducing the CO, soot and NO_x emissions [1, 2]. Due to the intensive mixing and reduced peak temperatures, the reactivity of MILD combustion is reduced. Therefore, chemical kinetics becomes the controlling parameter in the combustion process [3]. This makes it important to include detailed chemistry in the modelling of such flames. In the present work, the Eddy Dissipation Concept (EDC) combustion model is considered, in combination with detailed chemistry. The Tabulation of Dynamic Adaptive Chemistry (TDAC) reduction method is introduced to alleviate the long calculation time associated with high number of species and reactions. Results from a validation test case of Delft Jet in Hot Co-flow (DJHC) burner are shown and discussed.

Numerical models

Eddy Dissipation Concept (EDC) combustion model

The EDC model, proposed by Magnussen [4], has the advantages of including detailed chemistry in the combustion modelling. The EDC model assumes that combustions happens in the fine structures that have the length scales in which dissipation takes place. The fine structures can be described as a Perfectly Stirred Reactor (PSR). The regions without combustion is called as surrounding fluid. The mass fraction of the fine structures (γ_λ) and the mean residence time of the fluid inside the fins structures (τ^*) are described as:

$$\gamma_\lambda = C_\gamma \left(\frac{\nu \epsilon}{k^2} \right)^{\frac{1}{4}}, \quad \text{Eq. 1}$$

and

$$\tau^* = C_\tau \left(\frac{\nu}{\epsilon} \right)^{\frac{1}{2}}, \quad \text{Eq. 2}$$

where ν is the kinematic viscosity and ϵ is the dissipation rate of the kinetic energy, k . The terms C_γ and C_τ are two constants, which equals to 2.1377 and 0.4083, respectively. Finally, the mean reaction rate of specie i is expresses as:

$$\bar{\omega}_i = - \frac{\bar{\rho} \gamma_\lambda^2}{\tau^* (1 - \gamma_\lambda^2)} (\tilde{y}_i - y_i^*), \quad \text{Eq. 3}$$

where $\bar{\rho}$ indicates the mean density of the mixture, \tilde{y}_i is the mean mass fraction of the species i between the fine structures mass fraction y_i^* and the surrounding fluid mass fraction y_i^0 ,

$$\tilde{Y}_i = \gamma_\lambda^2 y_i^* + (1 - \gamma_\lambda^2) y_i^0. \quad \text{Eq. 4}$$

This expression of the EDC model is proposed by Magnussen in 2005, therefore denoted as EDC2005 in the present work.

The EDC2005 model has been reported to over-predict peak temperatures in MILD combustion condition [5, 6]. Adjustments of the C_γ and C_τ constants have been proposed to correct this behavior [5, 7, 8]. Among them, the adjustment proposed by De et al. [8] focused on the DJHC flame, for which C_τ was increased to 3.0 and C_γ decreased to 1.0. The adjusted EDC constants mentioned above [5, 7, 8] are all ad-hoc global approaches, where the choice of the constants is done with a trial and error procedure. In 2016, Parente et al. [5] conducted an analysis on the chemical and fluid dynamics scales in MILD combustion and proposed an approach for the determination of the EDC parameters based on the local Reynolds and Damköhler numbers. They derived the dependence of the constants on the turbulent Reynolds Number, $Re_T = 0.09 * k^2 / \nu \epsilon$ and the Damköhler number (evaluated at the Kolmogorov scale), $Da_\eta = \tau_\eta / \tau_c$, in which τ_η is the Kolmogorov mixing time scale and τ_c is the chemical time scale. The chemical time scale in the present work is estimated using the formation rate of the different chemical species and taking the limiting one [9]. The analytic expressions of C_τ and C_γ are:

$$C_\tau = C_1 \frac{1}{[Da_\eta^2 (Re_T + 1)]}, \quad \text{Eq. 5}$$

and

$$C_\gamma = C_2 Da_\eta^{\frac{1}{2}} (Re_T + 1)^{\frac{1}{2}}. \quad \text{Eq. 6}$$

In Equation 5 and 6, $C_1 = 0.5$ and $C_2 = 1.2247$. The constant C_1 and C_2 can be directly obtained from the energy cascade model, as also indicated by Bao [10]. The version of EDC from Parente et al. [5] is indicated as EDC2016 in the present work.

Tabulation of Dynamic Adaptive Chemistry (TDAC) reduction model

TDAC is a coupling method between a modified In-situ Adaptive Tabulation (ISAT) algorithm and the chemical scheme reduction methods [11], including Dynamic Adaptive Chemistry (DAC) [12], Directed Relation Graph (DRG) [13], DRG with Error Propagation (DRGEP) [14] and similar approaches. The TDAC process can be visualized in Figure 1. When ISAT needs growth or addition instead of retrieve, it provides first the composition ψ^q to the mechanism reduction method, which simplifies the reaction and provides a reduced set of species composition ψ_a^q to the ODE solver. This solver computes the reaction mapping $\mathbf{R}(\psi_a^q)$, and ISAT then builds the full reaction mapping $\mathbf{R}(\psi^q)$ from $\mathbf{R}(\psi_a^q)$ [11].

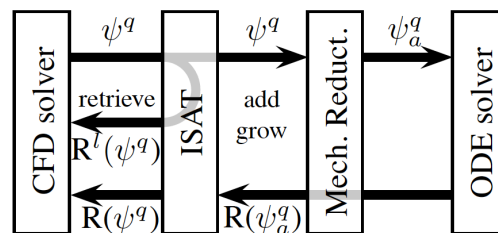


Fig. 1 Tabulation of Dynamic Adaptive Chemistry (TDAC) method flow chart [11].

Validation case set-up

In order to test the EDC2005 and EDC2016 models and the CPU saving potential of the TDAC method, the Delft Jet in Hot Co-flow (DJHC) burner [15] is chosen as validation case. The DJHC burner has a central fuel jet (inner diameter 4.5 mm) with 81% CH₄, 4% C₂H₆ and 15% N₂ by volume. The hot co-flow is provided by a secondary burner mounted in an outer tube with the inner diameter of 82.8 mm. The mass fraction of O₂ in the co-flow is 0.07. The mean and variance of the temperature and velocity experimental values are available for comparison. More details about the DJHC burner can be found in the research done by Oldenhof et al. [15].

Reynolds Averaged Navier-Stokes (RANS) simulation were performed on the DJHC burner using the standard $k - \epsilon$ turbulence model. The simulation domain is extended 160 mm downstream of the burner exit and discretized with a structured 2D axi-symmetric mesh. The OpenFOAM solver reactingFoam combined with Local Time Stepping (LTS) is adopted. The Plug Flow Reactor (PFR) is used to represent the fine structures, although the original model by Magnussen postulates that fine structures shall be modelled as PSR reactors. Previous study has shown that there are no distinguishable differences between using the PSR and PFR canonical reactors [16]. The DRM19 detailed mechanism [17] with 20 species and 84 reactions is used in the simulation. Reduction model of DAC with tabulation is applied, the tolerances of both are set to 1e-04. The seulex ODE solver is used.

Result and discussion

The EDC2005 with standard constants and adjusted constants, as well as the EDC2016 model with TDAC and LTS are compared in Figure 2 and Figure 3. In Figure 2, the mean velocity from the three cases are compared with experimental data. No major differences can be observed between them. The mean axial velocity is relatively well predicted, though with some under-predictions on the axial location of 120mm, 150mm and the centerline.

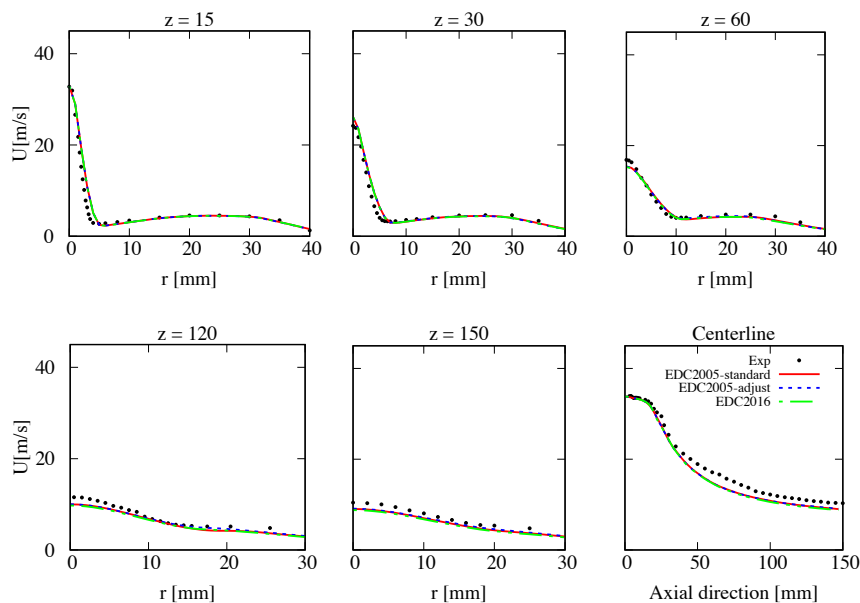


Fig. 2 Mean axial velocity profiles for the cases of EDC2005 standard constants (red), EDC2005 adjusted constants (blue) and EDC2016 (green).

In Figure 3, the mean temperature plots are presented. The EDC2005 model with the standard constants leads to significant over-prediction on the mean temperature profile, especially at the axial location of 60mm, 120mm and 150mm. The temperature peak predicted on 150mm rises up to 1857K, i.e. 27% higher than the experimental peak temperature. This over-prediction can be largely alleviated by using the adjusted EDC constants, in which $C_\tau = 3.0$ and $C_\gamma = 1.0$. From Figure 3, one can also observe that the case with adjusted EDC constants is able to give more accurate mean temperature prediction along the centerline and at the different axial positions. Similar considerations can be made for the EDC2016, albeit some under-predictions at 120mm and 150mm axial locations can be observed. It should be noted, however, that the adjusted constants are optimized for the specific case under investigation while the EDC2016 model self-adapts to the investigated conditions, without need for fine tuning.

As far as the computational time is concerned, the EDC2005 with adjusted constants case is 2.6 times more demanding than the EDC2005 with standard constants case, and 1.6 times than EDC2016 case, because that increasing the C_τ value leads to longer residence time in the fine structures. The adoption of TDAC in the simulation with the current tolerance of $1e-04$ for both the tabulation and chemistry reduction doesn't give visually distinguishable differences on the mean temperature and velocity profiles compared to the case without TDAC. TDAC reduction method is able to provide a calculation speed up, 6-7 times in the simulations ran without LTS and 1.6-1.8 times when using LTS. Moreover, the DRM19 mechanism used in the modelling is already a reduced subset mechanism. The potential of CPU time saving of TDAC method is expected to further increase when larger mechanism is applied.

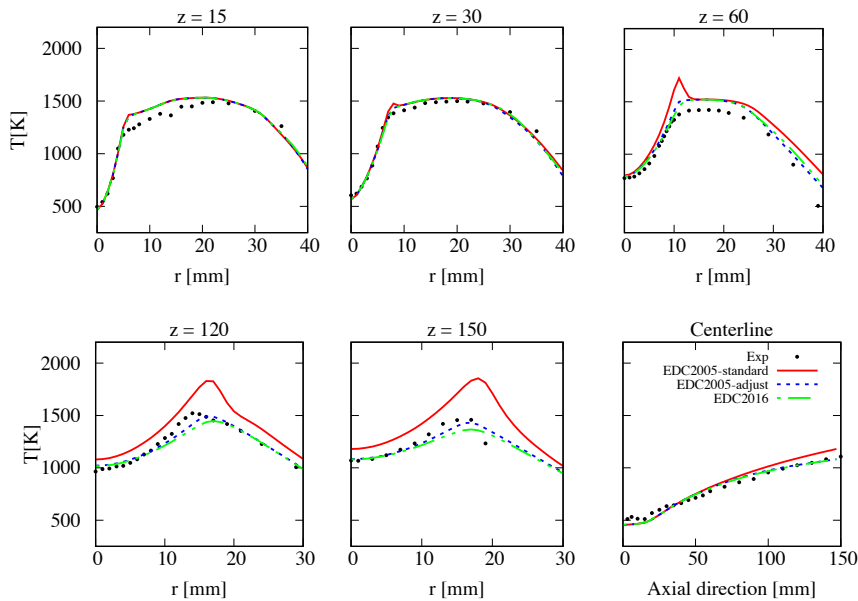


Fig. 3 Mean temperature profiles for the cases of EDC2005 standard constants (red), EDC2005 (blue) adjusted constants and EDC2016 (green).

Conclusion

From the results shown above, the following conclusions can be drawn:

- Adjusted EDC constants in EDC2005 correct the temperature over-prediction using the standard constants.

- The EDC2016 model results in performances comparable to the adjusted EDC2005 model, without need of any fine tuning.
- TDAC provides considerable savings, around 40% of the calculation time, with default tolerance and using LTS.

The current study demonstrates the reliability and affordability of the EDC model in handling the intense turbulence/chemistry interaction condition. Combining EDC and TDAC also provides the possibility of extending the simulation from the DJHC burner that emulates MILD combustion to large scale modelling like industrial burners.

Prospects

In the current abstract, only one chemistry reduction method, DAC, combined with tabulation and the default tolerances are tested. The final work will provide a global view on the results achievable using different chemical reduction methods and solver settings.

Acknowledgement

This project has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 643134. We would also like to show our gratitude to Michał Lewandowski from Polish Academy of Sciences for sharing their DJHC case mesh and boundary conditions with us.

References

- [1] J. A. Wüning, J. G. Wüning, Flameless oxidation to reduce thermal NO-formation, *Progress in Energy and Combustion Science* 23 (1997) 81-94.
- [2] A. Cavaliere, M. de Joannon, MILD combustion, *Progress in Energy and Combustion Science* 30 (2004) 329-366.
- [3] M. Ihme, J. Zhang, G. He, B. B. Dally, Large-Eddy Simulation of a Jet-in-Hot-Coflow Burner Operating in the Oxygen-Diluted Combustion Regime, *Flow, Turbulence and Combustion* 89 (2012) 449-464.
- [4] B. F. Magnussen, The eddy dissipation concept: a bridge between science and technology, *Thematic Conference on Computational Combustion 2005*.
- [5] A. Parente, M. R. Malik, F. Contino, A. Cuoci, B. B. Dally, Extension of the eddy dissipation concept for turbulence/chemistry interactions to mild combustion, *Fuel* 163 (2015) 98-111.
- [6] S. R. Shabaniyan, P. R. Medwell, M. Rahimi, A. Frassoldati, A. Cuoci, Kinetic and fluid dynamic modeling of ethylene jet flames in diluted and heated oxidant stream combustion conditions, *Applied Thermal Engineering* 52 (2012) 538-554.
- [7] A. De, E. Oldenhof, P. Sathiah, D.J.E.M. Roekaerts, Numerical simulation of delft-jet-in-hot-coflow (DJHC) flames using the Eddy dissipation concept model for turbulence/chemistry interaction, *Flow Turbulence Combust.*, <http://dx.doi.org/10.1007/s10494-011-9337-0>.
- [8] M. J. Evans, P. R. Medwell, Z. F. Tian, Modeling Lifted Jet Flames in a Heated Coflow Using an Optimized Eddy Dissipation Concept Model, *Combustion Science and Technology* 187 (2015) 1093-1109.
- [9] J. Chomiak, A. Karlsson, Flame lift-off in diesel sprays, *Twenty-Sixth Symposium (International) on Combustion/The Combustion Institute* (1996) 2557-2564.
- [10] H. Bao, Development and Validation of a New Eddy Dissipation Concept (EDC) Model for MILD Combustion, Master thesis 2017, Delft University of Technology.
- [11] F. Contino, H. Jeanmart, T. Lucchini, and G. D'Errico. Coupling of in situ adaptive tabulation and dynamic adaptive chemistry: An effective method for solving combustion in engine simulations. *Proc. Combust. Inst.*, 33(2):3057-3064, 2011.
- [12] L. Liang, J. G. Stevens, J. T. Farrell, A dynamic adaptive chemistry scheme for reactive flow computations, *Proceedings of the Combustion Institute* 32 (2009) 527-534.
- [13] T. Lu, C. K. Law, A directed relation graph method for mechanism reduction, *Proceedings of the Combustion Institute* 30 (2005) 1333-1341.
- [14] P. Pepiot-Desjardins, H. Pitsch, An efficient error-propagation-based reduction method for large chemical kinetic mechanisms, *Combustion and Flame* 154 (2008) 67-81.
- [15] E. Oldenhof, M. J. Tummers, E. H. van Veen, D. J. E. M. Roekaerts, Role of entrainment in the stabilisation of jet-in-hot-coflow flames, *Combustion and Flame* 158 (2011) 1553-1563.
- [16] Z. Li, A. Cuoci, A. Sadiki, A. Parente, Comprehensive numerical study of the Adelaide Jet in Hot-Coflow burner by means of RANS and detailed chemistry, *Energy* 139 (2017) 555-570.
- [17] M. Frenklach, H. Wang, M. Goldenberg, G. P. Smith, D. M. Golden, C. T. Bowman, R. K. Hanson, W. C. Gardiner, V. Lissianski, GRI-Mech: An Optimized Detailed Chemical Reaction Mechanism for Methane Combustion (Gas Research Institute, Chicago) *Gas Research Institute Tech. Rep. GRI-95/0058*.