Stochastic Modeling of a Lifted Methane/Air Jet Flame with Detailed Chemistry

Tommy Starick¹*, David O. Lignell², and Heiko Schmidt¹

¹ Chair of Numerical Fluid and Gas Dynamics, BTU Cottbus-Senftenberg, Siemens-Halske-Ring 15a, 03046 Cottbus, Germany
² Department of Chemical Engineering, Brigham Young University, Provo, UT, 84602, USA

This preliminary numerical study investigates a lifted methane/air jet flame in a vitiated coflow by means of the One-Dimensional Turbulence (ODT) model. In the considered Cabra Burner configuration [Combust. Flame 143 491-506 (2005)], a jet flame issues from a central nozzle into a vitiated coflow of hot combustion products from lean premixed hydrogen/air flames. ODT is a map-based model for turbulent flow simulations which uses a stochastic formulation for the turbulent advection. The diffusion and reaction effects along the one-dimensional domain are considered by temporally advancing deterministic evolution equations. ODT simulations are performed with a representation of the methane/air chemistry by a reduced 19-species mechanism with 15 reactions and a detailed 53-species mechanism with 325 reactions. In this work, we present centerline profiles of temperature and species concentrations obtained from ODT simulations using a cylindrical ODT-formulation. Additionally, two-dimensional renderings of the temperature distribution are shown. Although the simulation of reactive jet configurations by means of ODT is not novel, the complex stabilization region depending on the flow conditions represents a challenge for the model. Considering the reduced order of the model, ODT is able to predict the flow characteristics and reasonably matches the existing experimental data.

1 Introduction and ODT simulation

The recirculation of hot combustion products is a widely used measure to enhance flame stability in practical combustion systems. The accurate prediction of the subtle interactions between the hot combustion products and the cold unburnt jet in complex recirculation flows represents a challenge for most current combustion models. Simplified configurations of a cold unburnt jet issuing into a flow of hot combustion products exhibit similar characteristics for chemical kinetics, heat transfer and molecular transport as recirculation burners, while avoiding their complex recirculating fluid mechanics [1].

At this point, the One-Dimensional Turbulence (ODT) [3] model is an efficient map-based approach for turbulent combustion simulations, resolving all time and length scales along a notional line crossing the turbulent flow field. ODT is characterized by a stochastic formulation of the turbulent advection. Diffusion and reaction effects along the one-dimensional domain are captured by temporally advancing evolution equations.

In the present work, the Cabra burner [1] configuration of a cold unburnt methane/air jet issuing into a coflow of hot combustion products from an array of hydrogen/air flames is investigated. A cylindrical ODT-formulation as detailed in [4] and evaluated in [7] is used for the representation of the round jet flame in a vitiated coflow. The chemistry of the methane/air jet flame is represented by the detailed GRI-Mech 3.0 mechanism [6] with 53 species and 325 reactions and a reduced mechanism with 19 species and 15 reactions [5]. The coflow consists of products from lean premixed hydrogen/air flames and is initialized with an uniform velocity of 5.4 m/s and a temperature of 1350 K. The cold jet is initialized with an instantaneous velocity profile from a pipe flow ODT simulation with a bulk velocity of 100 m/s and a constant temperature of 320 K. The mixture consists of 33% methane and 67% air, by volume. The jet diameter $D$ is 4.57 mm.

The stationary spatially developing round jet flame from Cabra et al. [1] is intended to be compared with ODT results from a temporal ODT-formulation. Since the temporal ODT-formulation is solving for only one spatial direction $r$ and time $t$, a transformation between time and their corresponding downstream position $z$ is required. Following the approach of Echekki et al. [2], for every instant of time a downstream position of the 1D-ODT line can be determined by means of an instantaneous bulk velocity $\bar{u}$.

$$z(t) = \bar{z}(t_0) + \int_{t_0}^{t} \bar{u}(t')dt'$$

$$\bar{u}(t) = u_\infty + \frac{\int_{-\infty}^{\infty} \rho(u - u_\infty)^2 r dr}{\int_{-\infty}^{\infty} \rho(u - u_\infty) r dr}$$

The bulk velocity $\bar{u}$ is calculated by the sum of the free-stream (coflow) velocity $u_\infty$ and the ratio of integrated momentum flux to integrated mass flux. In Equation 1, $z(t_0)$ marks the starting position and $\rho$ the density of the gas mixture.

* Corresponding author: e-mail Tommy.Starick@b-tu.de, phone +49 355 69 4813

1, 2021; 202100237

© 2021 The Authors. Proceedings in Applied Mathematics & Mechanics published by Wiley-VCH GmbH.
2 Results

ODT results are compared to the experimental measurements from Cabra et al. [1]. In the left part of figure 1a), centerline profiles of the Favre-averaged temperature $\overline{T}$ and their corresponding fluctuations $T''$ are shown. In the right part of figure 1a), centerline profiles of Favre-averaged mass fractions of oxygen $\overline{Y_{O_2}}$ and hydroxyl radical $\overline{Y_{OH}}$ are presented. The Favre-averaging of the ODT results is based on an ensemble size of 400 realizations. For all shown results, the ODT model parameters for turbulence intensity $C$ and viscous penalty $Z$ are taken as $C = 18$ and $Z = 400$.

The initial phase up to $z/D \approx 40$ is characterized by non-reactive mixing of the cold jet and the hot coflow from hydrogen/air flames. The initial phase is followed by the flame stabilization phase. That region is characterized by a strong temperature rise, rapid oxygen consumption, hydroxyl radical production and peak in the temperature fluctuations. The ODT results in good agreement with the experimental measurements, which includes the non-reactive mixing process and the reaction process. Additionally, ODT is able to reproduce the trend and magnitude of the Favre fluctuations. The ODT results from the reduced mechanism show a slightly better agreement with the experimental data, since the ODT model parameters were calibrated for the reduced mechanism, which already captures the main combustion dynamics.

Figure 1 b) shows two-dimensional renderings of the Favre-averaged temperature and the temperature distribution of the lifted methane/air jet flame with visualized eddy events from a single ODT realization. Similar to the centerline plots, the initial phase up to $z/D \approx 40$ shows an increase in temperature of the jet only through non-reactive mixing. In the flame stabilization phase, a rapid temperature rise can be seen at the interface between coflow and jet. The error bars in figure 1 b) mark the size and position of the ODT eddy events, which incorporate the effects of three-dimensional turbulence into ODT.

The accurate representation of the subtle interactions of the hot coflow with the cold jet are essential for the reaction and autoignition of the jet. Considering the reduced order of the model, ODT is able to predict the flow characteristics and reasonably matches the existing experimental data.

Acknowledgements Open access funding enabled and organized by Projekt DEAL.

References

[1] R. Cabra, J.-Y. Chen, R. W. Dibble, A. N. Karpetis, and R. S. Barlow, Combust. Flame 143, 491-506 (2005).
[2] T. Echekki, A. Kerstein and T. Dreeben, Combust. Flame 125, 1083–1105 (2001).
[3] A. Kerstein, J. Fluid Mech. 392, 277–334 (1999).
[4] D. O. Lignell, V. Lansinger, J. Medina, M. Klein, A. R. Kerstein, H. Schmidt, M. Fistler and M. Oevermann, Theor. Comp. Fluid. Dyn. 32, 495–520 (2018).
[5] T. Lu and C. K. Law, Combust. Flame 154, 761-774 (2008).

© 2021 The Authors. Proceedings in Applied Mathematics & Mechanics published by Wiley-VCH GmbH. www.gamm-proceedings.com
[6] G. P. Smith, D. M. Golden, M. Frenklach, N. W. Moriarty, B. Eiteneer, M. Goldenberg, C. T. Bowman, R K. Hanson, S. Song, W C. Gardiner, V. V. Lissianski and Z. Qin, GRI-Mech 3.0, http://www.me.berkeley.edu/gri_mech/

[7] T. Starick, H. Schmidt and D. O. Lignell, Proceedings of TSFP-11, Southampton, UK, Session 8C, pp. 1–6.