LES and DNS of autoignition in jet-in-hot coflow CH4/H2 flames

LES and DNS of autoignition in Jet-in-Hot Coflow CH_4/H_2 flames

S.E. Abtahizadeh, J.A. van Oijen, R.J.M. Bastiaans, L.P.H. de Goey
Eindhoven University of Technology
Combustion technology group, Mechanical engineering department
De Rondom 70, 5612 AP, Eindhoven, the Netherlands
E-mail: e.abtahizadeh@tue.nl

Key words: Turbulent combustion, DNS, LES, SGS modeling, Autoignition

ABSTRACT

Autoignition of a fuel mixture by a hot oxidizer plays an important role in Mild combustion; a clean combustion concept. Mild combustion has been introduced as a promising method to increase thermal efficiency and decrease NOx formation. In spite of the enormous potential of the Mild combustion regime, it has been mainly limited to lab-scale burners due to stabilization issues in practical burners. The stabilization mechanism of Mild combustion is often governed by autoignition of a fuel jet in a hot and diluted environment. This mechanism is highly sensitive to variations in the fuel and oxidizer composition and operating conditions. In the laboratory scale Mild burners (JHC burners), stabilization of reaction zone is very often occurred by autoignition. In some burners, methane-based fuel is enriched with H_2. Such conditions require sophisticated models which are able to predict complex autoignition events under significant preferential diffusion effects.

The Delft Jet-in-Hot Coflow (DJHC) burner is chosen as a test case in which methane base fuel has been enriched with 0%, 5%, 10% and 25% of H_2. Studied cases are summarized in Table 1. First, a novel numerical model is developed based on the FGM technique to account for preferential diffusion effects in autoignition. Such development is inevitable since investigations with detailed chemistry indicate that preferential diffusion affects strongly autoignition of the hydrogen enriched mixtures. Igniting Mixing Layer (IML) flamelets are introduced and analyzed to accommodate preferential diffusion effects in a flamelet database. The predictions of this model are then compared with results of the full chemistry mode by performing 3D DNS of igniting mixing layers. Figure 1 shows the comparison of predicted temperature rise ΔT for the Case D25H2 using detailed chemistry and various FGM models. Two FGM models are considered here which employ different types of manifolds: 1) A manifold based on igniting Counter-Flow flamelets (ICF-flamelets) 2) A manifold based on IML-flamelets. From Fig. 1, it is observed that computations based on IML Manifold provide more accurate results compared to those of ICF manifold against the solution of detailed chemistry.

Table 1. Temperature and molar composition of the fuel stream for the different cases. The oxidizer stream has the same composition for all cases: T = 1437 K, X_{O2} = 0.0485, X_{H2O} = 0.1452, X_{CO2} = 0.0727, X_{N2} = 0.7336.

Case	T(K)	X_{H_2}	X_{CH_4}	$X_{C_2H_6}$	X_{N_2}	ζ_{st}
$D00H_2$	448	0.00	0.813	0.037	0.15	0.0178
$D05H_2$	448	0.05	0.763	0.037	0.15	0.0179
$D10H_2$	448	0.10	0.713	0.037	0.15	0.0180
$D25H_2$	448	0.25	0.563	0.037	0.15	0.0183

In the next stage, the IML approach is implemented in LES of the H_2 enriched turbulent lifted jet flames of the DJHC experiments. A presumed β-PDF approximation together with a gradient based model has been used to account for turbulence-chemistry interaction. Figure 2 shows instantaneous Y_{OH} distributions. Predictions indicate formation, growth and convection of ignition kernels in perfect agreement with observations from measurements [1]. Observations from DNS and LES demonstrate that IML approach is a promising method to predict autoignition and preferential diffusion effects for Jet-in-Hot Coflow flames [2].

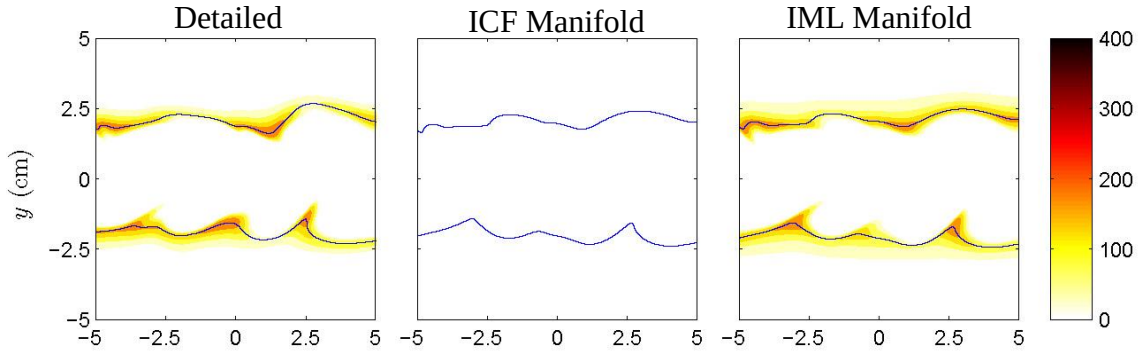

Figure 1 Comparison of the temperature rise ΔT obtained by 3D DNS of mixing layers using detailed chemistry, ICF and IML manifolds for the Case D25H2 at t=0.2 ms. Blue lines correspond to stoichiometric mixture fraction.

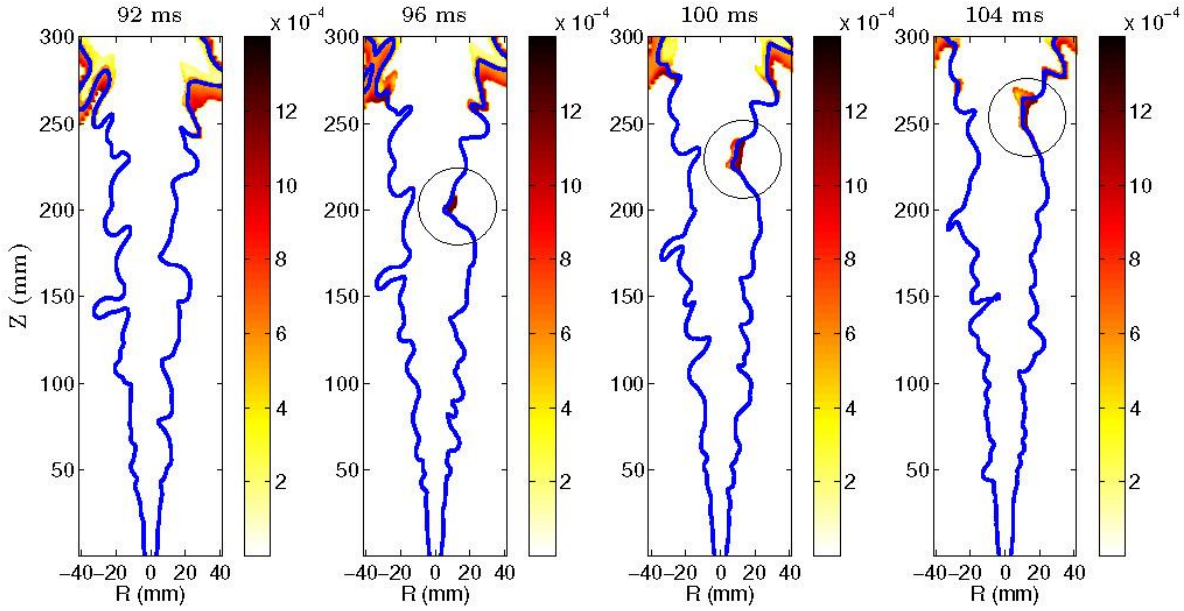

Figure 2 Computed instantaneous snapshots of Y_{OH} using the IML manifold for Case D00H2. Blue lines indicate stoichiometric mixture fraction.

Acknowledgments
The authors gratefully acknowledge the financial support of the Dutch Technology Foundation (STW).

References

[1] L.D.A. Arteaga, M.J. Tummers, E.H. van Veen, D.J.E.M. Roekaerts, *Effect of hydrogen addition on the structure of natural-gas jet-in-hot-coflow flames*, Proc. Combust. Inst. 35, (2014), pp. 3557-356.
[2] S.E. Abtahizadeh, *Numerical study of Mild combustion from laminar flames to Large Eddy Simulation of turbulent flames with Flamelet Generated Manifolds*, PhD Thesis, Eindhoven University of Technology (2014).