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Assessment of the Partially Stirred Reactor model to simulate diluted combustion in a LES approach

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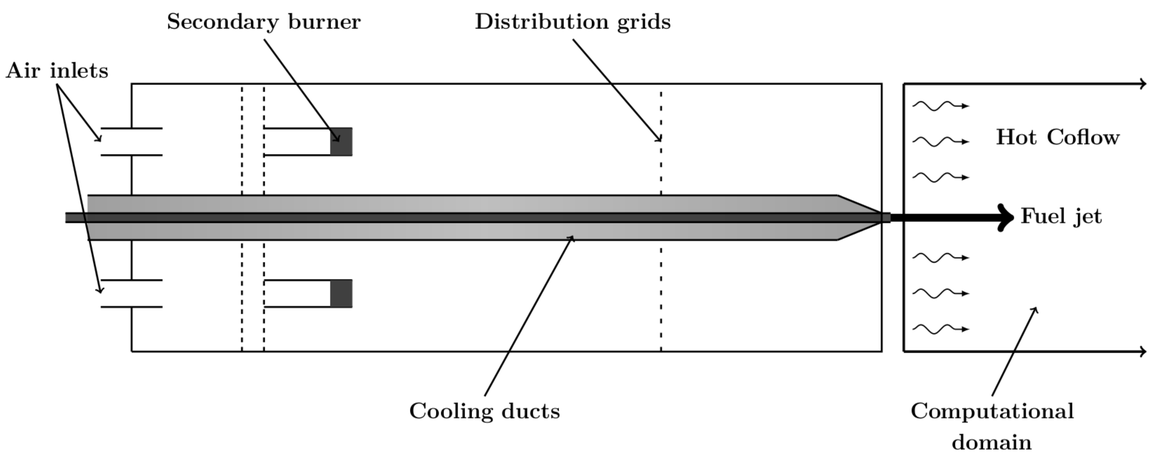
Abstract

Diluted combustion combines high system efficiency (due to the preheating of the reactants) and low NO_x emissions. It is characterized by an intense recirculation of the flue gases, leading to reactants concentrations locally lower than in a standard combustion. Thus, the reaction rates are also lower. Regarding the numerical modelling, it means that the fast chemistry assumption is not valid under these conditions and diluted combustion requires the use of specific combustion models taking into account the turbulence-chemistry interaction. The Partially Stirred Reactor (PaSR) model is assessed in this study on the Delft Jet-in-Hot-Coflow (DJHC), which operates in diluted combustion conditions.

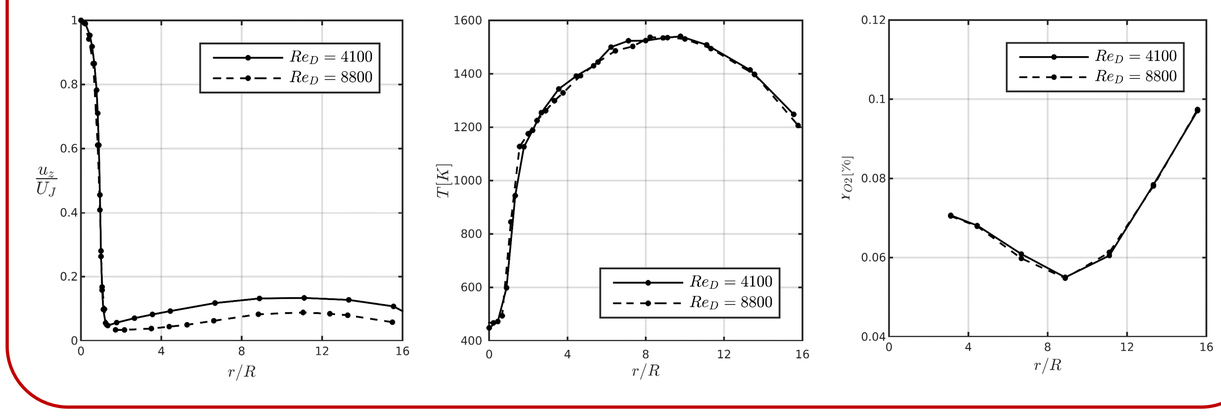
Flame setup

Device designed to produce diluted combustion conditions

- Low oxygen concentration ($Y_{O2,av}$ = 7.6 %)
- Temperature above the auto-ignition temperature ($T_{co,max}$ =1540 K)



Experimental results of Oldenhof [1] (using Dutch Natural Gas)



Numerical simulations using OpenFOAM

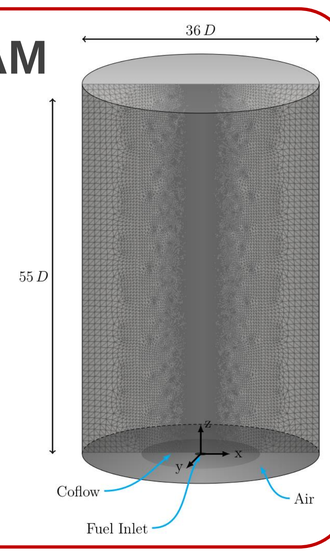
Mesh

- In the fuel region : LES → $Re_h = \frac{vh}{\nu} \approx O(10)$
- 2.5 million hexahedral cells

Static Smagorinsky-like subgrid scale model

Boundary conditions

- Experimental profiles imposed on the inlets
- Synthetic turbulent boundary condition on the fuel inlet
- Pressure outlet on the outlet and the air inlet



Combustion model

Assumption : species react in a fraction κ of the computational cell [2]

- Perfectly Stirred Reactors (PSR)
- Turbulent fluctuations neglected
- Reaction progress depends on chemical kinetics
- One reaction rate $\dot{\omega}_k$ for each species (reaction mechanism)

Second part of the cell

- No reaction
- Turbulent fluctuations not neglected

Overall reaction rate $\bar{\dot{\omega}}_k = \kappa\, \dot{\omega}_k$

Coefficient κ based on time scales : $\kappa = \frac{\tau_{ch}}{\tau_{ch} + \tau_{mix}}$ with $\tau_{mix} = C_{mix}\sqrt{\frac{\mu_{eff}}{\rho\epsilon}}$

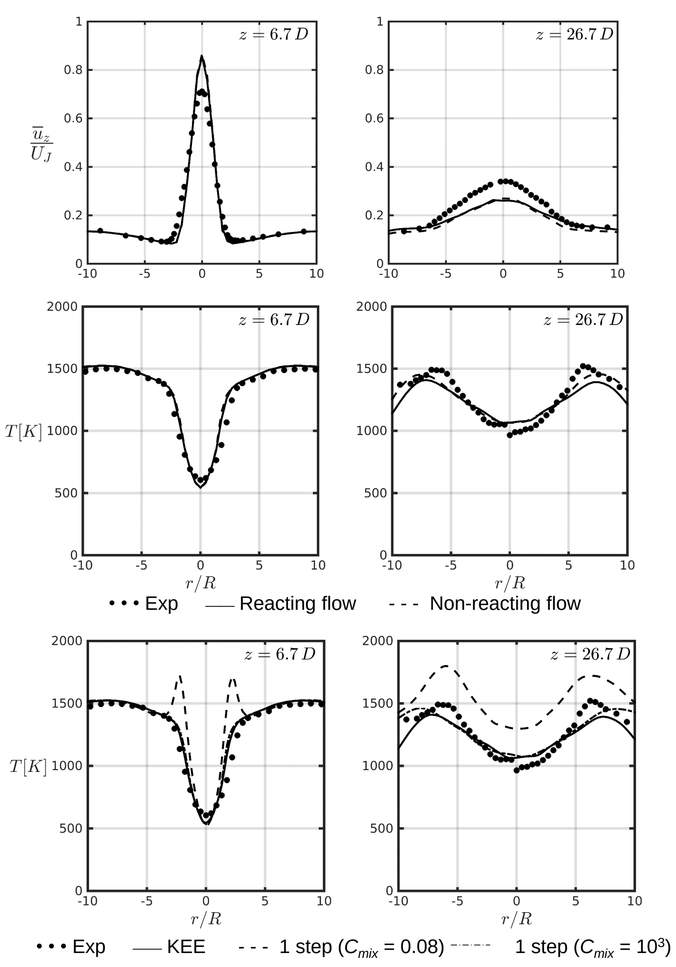
Results

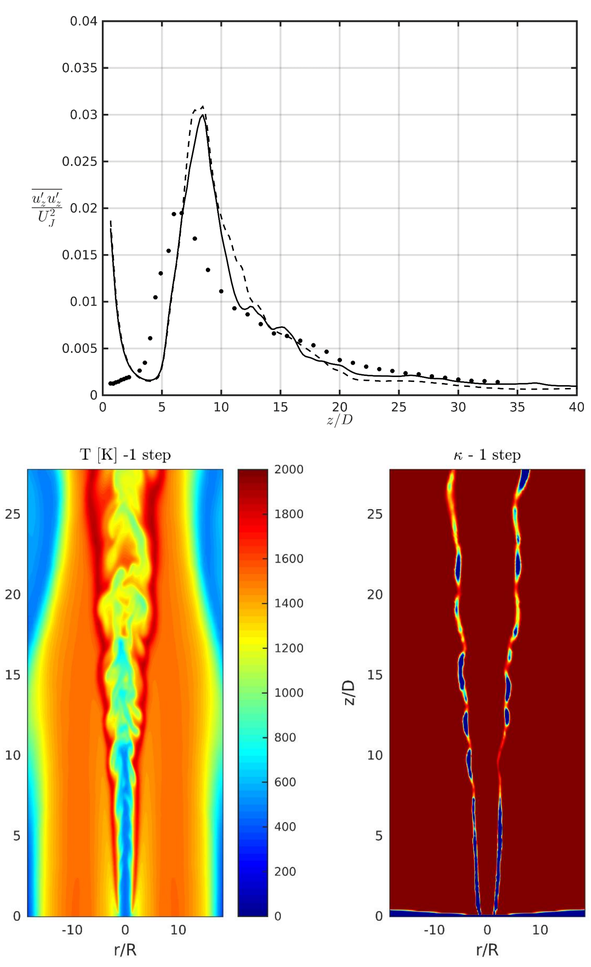
Non-reacting and reacting flows at Re_D = 4100

- Reacting flow : KEE mechanism (18 species, 58 reactions)
- Coincident reacting and non-reacting results (low heat amount released by the reaction)
- Slight overestimations and underestimations of the centerline profiles
- Velocity fluctuations underpredicted close to fuel injection and overpredicted for 6 < *z/D* < 12 (loss of jet momentum) → test of a more realistic turbulent inlet

Influence of the reaction mechanism

- Temperature largely overestimated with the global mechanism (1-step) and the recommended C_{mix} (= 0.08)
- Good order of magnitude with an excessive value C_{mix}
- κ ≠ 1 where the temperature is the highest ($T\nearrow \rightarrow \tau_{ch}\searrow \rightarrow \tau_{ch} \approx \tau_{mix} \rightarrow \kappa \in [0,1]$)





Conclusion and perspectives

A procedure was developed in OpenFOAM to perform LES of non-radiative diluted combustion. The results obtained with PaSR are in a good agreement with experimental data on the DJHC (diluted combustion conditions). Ongoing work concerns the testing of other combustion models as the Eddy Dissipation Concept (EDC). The radiation will be included and applied on a semi-industrial furnace.

Acknowledgment

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References

[1] E. Oldenhof, M.J. Tummers, E.H. van Veen, D.J.E.M Roekaerts, Combust. Flame. 158 (2011) 1553-1563
[2] M. Hallaji, K. Mazaheri, Proceedings of Seventh Mediterranean Combustion Symposium, Italy (2011)