Large Eddy Simulation (LES) of Delft Jet-In-Hot-Coflow (DJHC) flame

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Introduction

The diluted combustion, also called flameless combustion or MILD (Moderate or Intense Low Oxygen Dilution) combustion, is a promising combustion technology because it combines low pollutant emissions (e.g. nitrogen oxides NOx) with high combustion efficiency by recovering flue gases energy with a preheating system [1]. It occurs for intense internal flue gas recirculation leading to lower oxygen concentrations and a more uniform temperature. In those conditions of concentrations and temperatures, the reaction rates are lower and the chemical kinetics has a significant impact on the reaction process. Combustion models, such as the Eddy Dissipation Concept (EDC) or its variant, the Partially Stirred Reactor (PaSR) model, were developed to take into account interactions between turbulence and chemistry. The aim of this study is to assess the PaSR model implemented in OpenFOAM® to model diluted combustion.

Flame setup

The Delft Jet-In-Hot-Coflow experiment of Oldenhof et al. [2, 3] was chosen in the present work for two reasons. First, the dimensions of the burner allows to perform LES on fairly small grids. Second, it is an open flame, which enables to avoid radiation modelling.

The system is designed to simulate the diluted combustion conditions. The main burner consists in a central fuel injection with an inner diameter \( D = 4.5 \) mm (see Fig. 1). The fuel jet enters in a hot coflow, distributed in an annulus with a diameter of 18.4\( D \) [2, 3]. The coflow results from the combustion produced by a secondary burner and is composed by a mixture of reactants and flue gases, which leads to low oxygen concentrations (\( Y_{O_2_{av}} = 7.6 \% \)). Moreover, it brings heat to reach the auto-ignition temperature after mixing (Coflow \( T_{\text{max}} = 1540 \) K).

In [2, 3], several parameters were varied such as the Reynolds number and the coflow characteristics. In all the cases, the fuel used in the main burner is Dutch natural gas (81\% \( CH_4 \), 4\% \( C_2H_6 \), 14\% \( N_2 \) and 1\% higher alkanes by volume). The Reynolds number is \( Re_D = \rho U_{\text{bulk}} D / \mu = 8800 \) where density \( \rho \) and viscosity \( \mu \) are taken at \( T = 360 \) K.

Combustion model

The PaSR model assumes that the species react only in a fraction of the computational cell, which is considered as a Perfectly Stirred Reactor (PSR) [5], neglecting turbulent fluctuations. In these reactors, the reaction progress depends on the chemical kinetics. A reaction rate \( \dot{\omega}_k \) is computed for each species \( k \) according to the reaction mechanism. However, this is not equal to the overall reaction rate \( \overline{\dot{\omega}}_k \) of the cell. Indeed, the second cell fraction, in which turbulent fluctuations are not neglected, doesn’t react. To take into account the fraction of the cell that reacts, a coefficient \( \kappa \) such that \( \overline{\dot{\omega}}_k = \kappa \dot{\omega}_k \) is introduced:

\[
\kappa = \frac{\tau_{\text{ch}}}{\tau_{\text{ch}} + \tau_{\text{mix}}},
\]

where the chemical reaction time \( \tau_{\text{ch}} \) is the maximum laminar reaction time among all the species. The mixing time \( \tau_{\text{mix}} \) depends on the flow turbulence.
**Numerical setup**

The computational domain, located at \( z_0 = 0.67D \) downstream of the main burner, consists in a cylinder with a radius of \( 18D \) and is \( 55D \) long in the axial direction. An air inlet is also added around the burner to take into account the air entrainment. The mesh is fully hexahedral and the cells size increases progressively in the radial direction from the axis to the cylinder boundary. It contains about 2.5 million cells.

The profiles of axial velocity, temperature and coflow composition, measured at a distance \( z_0 = 0.67D \) from the fuel injection, are interpolated as inlet conditions. At the fuel inlet, the velocity profile is not imposed. A synthetic turbulence condition adding a time correlated random noise to a constant axial velocity value is applied to better simulate turbulent inflow.

A compressible flow version of the Smagorinsky model is used with the model coefficients values found by Labahn et al. [6] (\( c_k = 0.02 \) and \( c_\epsilon = 0.202 \)). These values provide the best agreement with measurements.

The PaSR combustion model combined with the reduced KEE-58 reaction mechanism (18 species and 58 reactions) [7] is tested in this study.

**Results**

The time-averaged axial velocity, fluctuations and temperature profiles at different axial locations are presented in Fig. 2. The velocity profiles are in good agreement with experimental data, both for the non-reactive flow and the reactive flow, close and far from the fuel injection. The good performances in the non-reactive case could be explained by the same temperature level with and without combustion. The turbulent fluctuations are slightly overestimated at \( z = 6.7D \) but in a right order of magnitude. Far from the burner, the addition of combustion leads to higher temperatures than the experimental ones.

**Conclusion and perspectives**

The results obtained with the PaSR model are promising. This model seems to predict correctly the DJHC flame, which is in diluted combustion conditions. In the continuity of this study, it could be interesting to implement the EDC model in OpenFOAM® and validate it on the same DJHC flame.

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**References**