Soot formation in turbulent, non-premixed flames using OpenFOAM

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Abstract

The problem of soot formation in combustion devices is attracting the attention of many researchers because of its negative effects on human health and for the increasingly stringent limitations concerning the emissions of pollutants in the atmosphere. Moreover, soot formation has a strong influence on the radiative heat transfer in furnaces and various practical applications. Detailed kinetic models can be successfully used to help identify the conditions that reduce soot formation. However, the direct coupling of detailed chemistry and CFD is a very difficult task, especially when considering the typical dimensions of the computational grids used for complex geometries and industrial applications. Unfortunately, kinetic post processing procedures, largely adopted for describing the formation of slow pollutant species (nitrogen oxides, for example) and based on the decoupling between chemistry and fluid dynamics, cannot be used for soot, because its important effects on flame structure and radiation. As a consequence, the numerical modeling of soot formation in turbulent flames requires simplified, semi-empirical models for describing its chemistry (inception, growth, coagulation and oxidation).

This paper mainly describes the implementation in OpenFOAM of a Method of Moments (MOM) for predicting the formation of soot in turbulent non premixed flames in the context of steady state RANS simulations. Two additional transport equations are solved in OpenFOAM for the soot particle number density and its volume fraction. The source terms in transport equations are calculated using semi-empirical models taking into account nucleation, surface growth, coagulation and oxidation phenomena. The effect of soot radiation on the flame structure is also considered.

The attention was focused on the effects of turbulent fluctuation on the formation of soot. For this purpose, besides the *mean approach* (neglecting the influence of turbulent fluctuations), two additional strategies for the closure of source terms in the transport equations were implemented and compared [1]. In both cases, the mixture fraction, its variance and the enthalpy defect are required, but this does not mean that the CFD simulation must be necessarily performed using the Steady Laminar Flamelet Model (SLFM). In particular, the so-called *uncorrelated approach* assumes that mixture fraction and enthalpy defect are completely uncorrelated with soot properties [2]. On the contrary, the *correlated approach* imposes a perfect correlation between soot properties and mixture fraction. The application of these closure strategies require the construction of a look-up table, based on four independent variables: mixture fraction, its variance, scalar dissipation rate and enthalpy defect. This look-up table contains only the source terms for the soot transport equations, calculated in steady state, laminar counter flow diffusion flames.

In order to verify the implementation in OpenFOAM and to validate the proposed approach, two turbulent jet flames fed with ethylene and natural gas were numerically simulated. The results evidenced that turbulent fluctuations must be carefully taken into account to obtain a reliable prediction of soot volume fraction. Moreover, it was confirmed that the coupling between the soot production and the radiative heat loss cannot be neglected. Several sensitivity tests to the semi-empirical models of soot chemistry were performed. The predicted soot amount was relatively insensitive to the nucleation model. On the contrary, growth and oxidation models significantly influenced soot formation.

Key words: Combustion, soot, pollutants, turbulence-chemistry interactions

References

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