The effects of density and turbulent Prandtl number variations on the dynamic sub-grid scale modeling of turbulent pool fires

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Abstract
Dynamic sub-grid scale (SGS) modeling offers a modeling methodology to avoid using pre-described constants in Large Eddy Simulation (LES) of turbulent flows. OpenFOAM, as a Computaitonal Fluid Dynamics (CFD) tool box has been used in the numerical simulations of pool fires. The one equation and the dynamic one equation SGS models are available in the latest release of OpenFOAM and have been used in previous studies. In the current work, the uncertainties related to the implementation of the mentioned models and their respective effects are investigated.

Introduction

Large Eddy Simulation (LES) has been used in recent years in most studies on the numerical simulations of the pool fires primarily because of the unsteady and cycling nature of the flow due to buoyant effects. There are major approaches taken in the previous studies toward sub-grid scale (SGS) modeling: non-dynamic and dynamic approaches. In the non-dynamic approach, constants are used to model the effects of sub-grid scales on the resolved scales. Contrary to the non-dynamic methods, the constants involved in the formulations of the SGS model are dynamically determined using resolved information during simulations. Among different dynamic SGS models, dynamic Smagorinski [1–4] and dynamic one-equation [5] models are more prevalent in recent works. OpenFOAM [6] CFD toolbox has been exploited numerously in the past. The dynamic one-equation model (DynOneEq) has already been implemented and used in numerical simulations of turbulent pool fires. In the current paper, the implementation of the DynOneEq in OpenFOAM is under study with respect to the original study of Kim and Menon [7] in which the model is introduced. Thus, the numerical impacts of some discrepancies between the implementation and the theory of the DynOneEq model on results are investigated.

Experimental reference

To achieve the numerical assessment aimed at in the current work, the 30.5 cm-diameter methanol pool fire studied by Weckman and Strong [8] is selected as the experimental reference for data comparison. This flame has been used for validation and evaluation purposes because of the comprehensive available experimental data in terms of time-averaged and Root Mean Square (RMS) of essential variables such as temperature and vertical velocity.

Numerical Methodology

As mentioned, OpenFOAM, an open-source CFD package, is used for the numerical study performed here. The cylindrical (D=1.5m and H=1.8m) computational domain is used in the simulations. The dimensions of doubled mesh cubical enclosure in experiments are $3m \times 3m \times 3m$. The difference between the numerical computational domain and the actual domain did not have any effects on the numerical results. The 1 cm burner lip is considered based on numerical results presented in [3], explaining the effects of the lip on the flame structure. The burner surface is located 30 cm above the floor, and the top and side boundaries are considered to be open boundaries. It is assumed that the fuel is fully evaporated at the fuel inlet surface, and a constant mass flow rate of 1.067 g/s is prescribed for the fuel inlet. [3]. Spatially filtered transport equations are solved using FireFOAM [9]. The PIMPLE scheme is utilized to properly account for the coupling between transport equations and the pressure-correction equation. A single-step combustion reaction is considered in this work. Eddy Dissipation Model (EDM) is applied to close filtered enthalpy and species transport equations. Radiation is modeled using the Discrete Ordinate Method (DOM) with 64 solid angles discretizing the total solid angle. The absorption coefficients of CO_2 and H_2O are computed using RADCAL coefficients. The radiative contributions of other species are ignored. The average grid size in the flaming region (0 cm <Z < 40 cm and 0 cm < r < 30.5 cm) is about 0.25 mm, the mesh is stretched to the side boundaries, and coarser uniform grids are generated beyond the flaming region.

Three SGS models are used here. The first is one the non-dynamic one equation (OneEq) model [9] applied in similar studies like [10]. The second model is the incompressible DynOneEq model [11], where a constant turbulent Prandtl number is applied (Pr_t.=0.5), the same as OneEq model. Mentioned models are available in recent releases of OpenFOAM. The third SGS model is formulated based on the similar assumption of the incompressible DynOneEq model, but several changes are made based on physical attributes of pool fires and discrepancies between the incompressible DynOneEq implemented and the theory of the model. Moreover, the turbulent Prandtl number is also computed dynamically using the method introduced in [12]. The modified model (DynOneEqModified) is implemented in OpenFOAM, and the important changes from the available model can be summarized in the following items;(a) Favre-filtered version of the equations and expressions used to account for the variation of the density due to temperature variation in the SGS modeling, (b) elimination of artificial local averaging in dynamic calculation of constants, (c) dynamic calculation of turbulent Prandtl number, and (d) some minor revisions in implemented formulations.

Results

The methanol flame is simulated, and the mean and RMS of temperature and vertical velocity fields are compared for different SGS models in **Fig. 1**. Based on the mean temperature and vertical velocity distributions obtained by the models, the following results are obtained:

- In general, dynamic SGS modeling makes the predicted flame shorter and wider. The results of both dynamic models are in better agreement with experiments for both radial distributions and centerline profiles.
- The mentioned revisions on the DynOneEq model have slightly widened the flame in lower levels above the burner.
- The difference between RMS fields obtained by DynOneEq and DynOneEqModified models is negligible.
- Utilizing a dynamic approach in SGS modeling is more influential on averaged fields than the RMS fields.
- Apart from the extent of the effects shown in results caused by the modifications, the compatibility of the modified model with the Favre-filtered equations and physical features of turbulent reacting flows avoid introducing any uncertainty.

The other modification that should be introduced in future studies is using a compatible formulation for dynamic determination of the turbulent Prandtl number with the expressions used to compute constants dynamically.

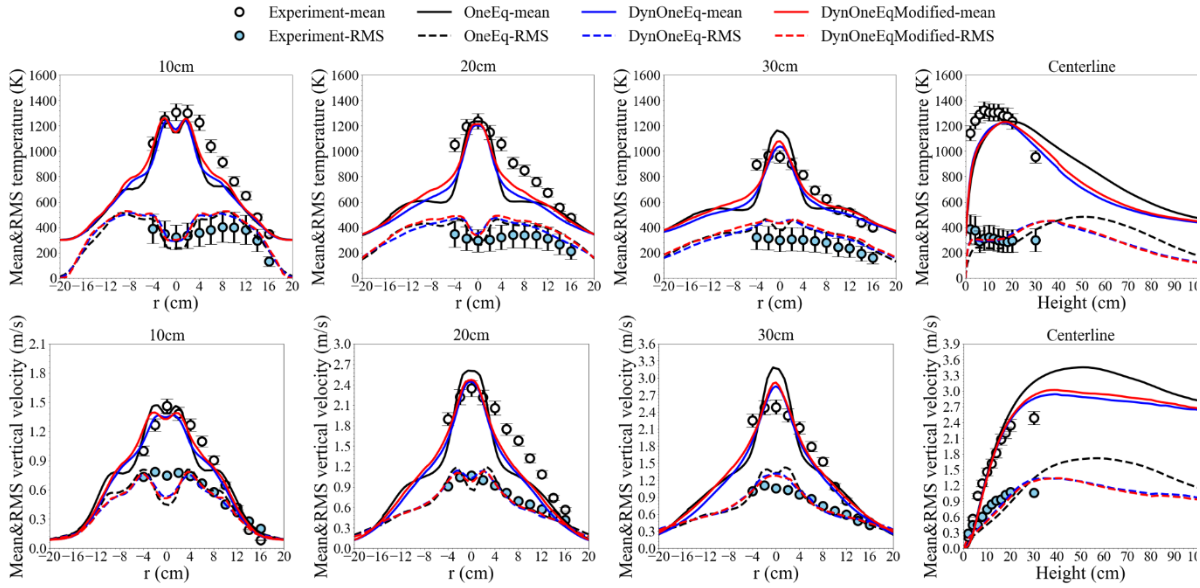

Fig. 1. Mean and RMS distributions of temperature and vertical velocity obtained at various levels above the burner for different SGS models; *OneEq*, *DynOneEq*, and *DynOneEqModified* models.

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