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Advances in modelling in CFD simulations of turbulent gaseous pool fires

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ABSTRACT

Large eddy simulations (LES) using advanced modelling approaches related to thermophysical, turbulence and combustion modelling are presented and their advantages when compared to some of the standard models used in the fire community are analyzed. More specifically, the consideration of a non-unity Lewis number and the Hirschfelder–Curtiss diffusion model, the inclusion of differential diffusion and Soret effects, the application of a dynamic turbulence model with a variable turbulent Prandtl number formulation, along with the EDC combustion model, have been included in a modified version of Fire-FOAM 2.2.x. A comparison between the predictions of the new and the standard models available in the code against experimental data of a medium-scale 24.6 kW methanol pool fire is presented. The predictions with the advanced modelling approaches are qualitatively and quantitatively better when compared to the standard models in the code, while having only a 20% increased computational cost.

1. Introduction

The study of gaseous pool fires remains to date one of the fundamental research topics in fire safety engineering and has received a lot of attention. Large-scale pool fires, often encountered after industrial accidents, can lead not only to severe air pollution due to the release of unburned hydrocarbons and soot into the atmosphere, but can also trigger more severe cascading effects involving explosions, causing huge losses of human lives and material property. The unsteady behavior and flow evolution of pool fires of different scales, even though extensively studied in the past [1–4], still remains even more challenging due to the coupled physical processes involved, e.g., buoyancy-generated turbulence, combustion, thermal radiation and soot generation. Within this framework, accurate modeling of the physics in the gas phase is essential and a prerequisite for performing numerical simulations of fire scenarios involving complex physical processes such as e.g., pyrolysis, flame spread and interaction of fire with sprinklers. A key aspect towards performing reliable numerical simulations of fire scenarios is not only to accurately model turbulence, combustion, radiation and their interaction but to also model all the different local transport phenomena occurring in fires. The use of dynamic turbulence models without any user-input model parameters is preferable and has the advantage that no calibration process is needed before simulating new fire scenarios since they are in principle able to self adjust their parameters depending on the flow conditions of the problem at hand. Improved combustion models are also needed that will not only be robust, accurate and reliable for a wide range of fire applications, but will also still be computationally inexpensive. In addition, the inclusion of fundamental physical processes in fire, often neglected for simplicity or because turbulence is assumed to dominate the flow, such as non-unity Lewis number, differential diffusion effects and the Soret effect (mass diffusion due to temperature gradients) will provide a more accurate description of the transport phenomena naturally occurring in fires.

The use of Computational Fire Dynamics (CFD) has, nowadays, become an integral part of fire protection design of real life applications. Detailed knowledge of the behavior and the dynamics of pool fires is, therefore, essential for fire safety engineers working on everyday life applications involving; fire detection, fire suppression and venting, design of smoke control systems, fire heating of structural elements of buildings or thermal radiation hazards [5]. Thanks to the ever increasing computer hardware capabilities and continuous improvement of software (numerical algorithms and modeling), computer simulations (i.e., well-resolved Large Eddy Simulations (LES) or Direct Numerical Simulations) will play an increasingly important role in engineering applications and research [6]. Therefore, CFD codes will soon be able to shift towards using more state-of-the-art modelling approaches when performing numerical simulations of fire scenarios.

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Nomenclature

c_s	Smagorinsky constant
c_p	heat capacity (J/kg/K)
D	mass diffusion coefficient (m^2/s)
D^T	thermal diffusion coefficient (m^2/s)
g	gravitational acceleration (m/s^2)
h_s	sensible enthalpy (J/kg)
j	mass diffusive flux ($kg/m^2/s$)
k	kinetic energy (m^2/s^2)
N_s	number of species
p	pressure (Pa)
Pr	Prandtl number
$\dot{Q}_c$	heat release rate (W)
$\dot{q}_c'''$	heat release per unit volume (W/m^3)
$\dot{q}_r''$	radiative flux (W/m^2)
S	strain rate (s^{-1})
Sc	Schmidt number
t	time (s)
T	temperature (K)
u	velocity (m/s)
W	molecular weight (kg/mol)
X	mole fraction
Y	mass fraction
Greek	
α	thermal diffusivity (kg/m/s)
Δ	filter width (m)
ΔH_c	heat of combustion (J/kg)
ϵ	dissipation rate (m^2/s^3)
μ	dynamic viscosity (kg/m/s)
ρ	density (kg/m^3)
τ	mixing time scale (s)
$\dot{\omega}'''$	reaction rate ($kg/m^3/s$)
Subscripts	
c	combustion
F	fuel
i, j, k	coordinate index
k	specie
mix	mixture
P	product
r	radiative
sgs	sub-grid scale
t	turbulent
∞	ambient
Superscripts	
0	initial
T	transpose / thermal

Within this framework, the main goal of this paper is to perform Large Eddy Simulations using advanced approaches related to thermophysical, turbulence and combustion modelling, and to report on their advantages when compared to some of the standard modelling choices used in the fire community. Furthermore, it will be examined whether the typical assumption of ignoring molecular diffusion effects in numerical simulations of fire applications is valid or not and report on their significance in the numerical predictions. The present work aims to demonstrate the need of current fire-related CFD codes of shifting towards more advanced modelling choices when performing numerical simulations of fire scenarios. The knowledge gained from the present study can then be applied towards improving the accuracy of numerical simulations of more complex scenarios, e.g., involving compartment fires with the interaction of fire with water sprays. In such scenarios, accurate prediction of the gas phase is crucial since flame suppression will strongly depend on the interaction of the water spray with the fire plume (i.e., there is need for accurate predictions of the flame temperatures and flow field).

The present study aligns with the newly established IAFSS Working Group on Measurement and Computation of Fire Phenomena (i.e., MaCFP Working Group – http://www.iafss.org/macfp/), which emphasizes the need for systematic progress in fire modelling based on fundamental understanding of fire phenomena [7,8]. In well-revolved LES simulations of fire scenarios, it is expected that the contribution of the modelling will be of equal importance as the inclusion of additional physics in the CFD codes, given the use of very fine grid sizes. The use of more advanced turbulence/combustion/radiation models is also more feasible than ever since the increased computational cost associated with them can be compensated by the use of faster computers. Within this framework, the work presented in the paper is expected to be a step forward in fire modelling, leading to improved understanding of fire phenomena and to better predictive capabilities of fire-related CFD codes. The objectives of the paper thus align with the MaCFP initiative. Therefore, the experimental test case considered is a MaCFP target test case. It involves the medium-scale, 30.5 cm in diameter, 24.6 kW methanol pool fire experiments reported by Weckman et al. [9] which include a considerable amount of data suitable for validation of CFD codes.

2. Mathematical approach

2.1. Governing equations

A modified version of FireFOAM 2.2.x, originally developed by FM Global (https://github.com/fireFoam-dev) is employed in this study. It uses a Favre-filtered fully compressible flow formulation and solves for the Navier–Stokes equations, along with transport equations for species mass fractions and sensible enthalpy [10]:

$$\frac{\partial \overline{\rho}}{\partial t} + \nabla \cdot (\overline{\rho}\widetilde{u}) = 0 \tag{1}$$

$$\frac{\partial (\overline{\rho}\widetilde{u})}{\partial t} + \nabla \cdot \left(\overline{\rho}\widetilde{u}\widetilde{u}\right) = -\nabla \overline{p} + \nabla \cdot \left[(\mu + \mu_{sgs})\left(\nabla \widetilde{u} + (\nabla \widetilde{u})^T - \frac{2}{3}(\nabla \cdot \widetilde{u})I\right)\right] + \overline{\rho} g \tag{2}$$

$$\frac{\partial (\overline{\rho}\widetilde{Y}_k)}{\partial t} + \nabla \cdot \left(\overline{\rho}(\widetilde{u} + \widetilde{u}_c)\widetilde{Y}_k\right) = \nabla \cdot \left[\left(\overline{j}_k + \frac{\mu_{sgs}}{Sc_t}\right)\nabla \widetilde{Y}_k\right] + \overline{\dot{\omega}_k'''}, \quad k = 1, \ldots, N_s - 1 \tag{3}$$

$$\frac{\partial (\overline{\rho}\widetilde{h}_s)}{\partial t} + \nabla \cdot \left(\overline{\rho}\widetilde{u}\widetilde{h}_s\right) = \frac{D\overline{p}}{Dt} + \nabla \cdot \left[(\alpha + \alpha_{sgs})\nabla \widetilde{h}_s\right] - \nabla \cdot \overline{\dot{q}_r''} + \overline{\dot{q}_c'''} + \nabla \cdot \left(\alpha \sum_{k=1}^{N_s} (h_{s,k}\nabla \widetilde{Y}_k)\right) + \nabla \cdot \left(\sum_{k=1}^{N_s} (\overline{j}_k h_{s,k})\right) \tag{4}$$

where $\overline{\dot{q}_c'''} = \Delta H_c \cdot \overline{\dot{\omega}_F'''}$ assuming complete combustion, i.e., $\chi = 1$. The last two terms in the formulation of the sensible enthalpy equation account for the differential diffusion and non-unity Lewis number effects.

The mass-diffusive fluxes, accounting for the Soret effect (i.e., the final term in the equation below), are calculated based on the formula of Hirschfelder–Curtiss (here named HC) [11]:

$$\overline{j}_k = -\overline{\rho} D_k \widetilde{Y}_k \frac{\nabla X_k}{X_k} - \overline{\rho} D_k^T \frac{\nabla T}{T} = -\overline{\rho} D_k \nabla \widetilde{Y}_k - \frac{\overline{\rho} D_k \widetilde{Y}_k}{W_{mix}} \nabla W_{mix} - \overline{\rho} D_k^T \frac{\nabla T}{T} \tag{5}$$