Towards the prediction of the convective and the radiative heat fluxes in turbulent buoyant flames

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ABSTRACT

The present paper aims at describing the flow dynamics of turbulent buoyant flames encountered in gaseous or liquid pool fires or horizontally oriented solid materials. Indeed, the predictive simulations of liquid pools or solid fuel fires requires the prediction of the thermal stress received by the evaporating liquid or the pyrolysing material, and therefore a fine description of the surrounding flame. Yet, reactive Large Eddy Simulation is a powerful tool in fluid mechanics to correctly simulate turbulent flows such as large-scale buoyant flames, so long as the discretization and the numerical schemes allow to resolve the large scale turbulent structures which determine the global flame shape.

Thus, this study is divided into two steps. In the first step, Large Eddy Simulations of the SANDIA FLAME methane pool fire are performed using the CALIF³S-ISIS software, for different grid refinements and convective schemes. The ability of the different numerical choices in correctly describing this flame is compared in terms of velocity variance-to-average ratio, puffing frequency and turbulent structures resolution. In the second step, the flame above a 40×40 cm² PMMA slab is simulated with the best numerical parameters found in the first step. The simulation of the flame is decoupled from pyrolysis aspects assuming by imposing the fuel mass flow rate observed at a particular stage of the experiment. The average temperature axial profile and the transverse profile of convective, radiative and total heat flux at the sample surface are compared to their experimental counterparts.

It is shown that, at least for large scale pool fires such as the SANDIA methane flame, the increasing the mesh refinement permits to reach a good balance between the average velocity and the turbulent kinetic energy and to correctly recover the characteristic flame puffing frequency, whereas using non-dissipative centred schemes allows to catch a wider range of turbulent scales in the flowfield. Unfortunately, for smaller fuel sources such as the 40×40 cm² PMMA slab, the present Large Eddy Simulations do not exhibit fully developed turbulence in most of the combustion zone, in spite of the use of centred schemes and of a fine grid. This uncertainty on the behaviour of the turbulence in such a configuration may be responsible for the observed anomalies, namely the overprediction on the average temperature and the radiative-to-convective heat flux ratio. Further experimental investigations would be useful to better understand the behaviour of turbulence on such mid-scale fires and prescribe relevant numerical model modifications.

KEYWORDS:
Fluid dynamics; Large Eddy Simulation; heat transfer; turbulent buoyant flames; cell size convergence; convective schemes; radiative/convective heat transfer balance
INTRODUCTION

In computational fire dynamics, the fuel load mass loss rate and therefore the total heat release rate are often provided by correlative approaches [1]. However, for more complex fuels, in particular organic materials, predictive approaches are required and two main issues arise: the prediction of the material thermal degradation rate, and the assessment of the thermal stress received by the material surface [2]. The present paper deals with this second issue. More precisely, the assessment of the feedback flux applied by the flame on the fuel load includes radiative and convective effects. The radiative effects mainly depend on the steady flame structure (height, temperature average and variance, optical flame properties). In this respect, the radiative losses can be directly fixed by imposing a flame radiative fraction in the heat transfer equation [3]. But in a predictive approach, special attention must be paid on the combustion model (including soot generation and oxidation) and the resolution of the Radiative Transfer Equation (including the description of the radiative absorption). In the same way, the convective heat exchange between the flame and the fuel interface is often modelled using a heat exchange coefficient depending on the temperature gap between the flame and the surface. But in a predictive approach, the correct evaluation of the convective exchange depends on the relevance of the turbulence modelling and/or simulation. In particular, numerical and experimental studies of the flow dynamics in buoyant turbulent flames [4,5] have highlighted the interaction between several instability mechanisms, which trigger the turbulence in these buoyant flows. Namely, a main puffing phenomenon of well characterized frequency [6] due to the alternate accumulation and ejection of the light injected fluid, and Rayleigh-Taylor and Kelvin-Helmholtz instabilities occurring very close to the light fluid injection which favours the turbulent dissipation and mixing in the flame and the plume. All these phenomena are unlikely to be simulated by RANS approaches even if they have often been used for industrial applications [7]. Conversely, Direct Numerical Simulations of such large-scale configurations is out of reach in terms of CPU capabilities. In this respect, similarly with previous attempts [6,8], Large Eddy Simulations (LES) of these flows can be tentatively performed to accurately evaluate the flame structure related to a restricted period of a fire scenario. Implicitly, one assumes that the high-frequency dynamics of the flame is decoupled to the long-term variations of the flow conditions. Simulations with prescribed, constant injection rate can therefore be performed during a physical duration that is large enough to reach statistic convergence, but that remains smaller than the characteristic time of the fire scenario. Two experimental cases will be simulated with the CALIF3S-ISIS fire simulation software developed by French "Institut de Radioprotection et de Sûreté Nucléaire" (IRSN) [9]: the 1 m diameter methane pool fire performed in the SANDIA FLAME facility [5], which will be used for both physical and numerical model validation; and the pyrolysis experiments performed on 40x40 cm² PMMA slabs in open atmosphere by Kacem et al. [10]. Particular attention will be paid on the flame temperature profiles and the convective and radiative contributions to the flame feedback flux.

CFD MODEL DESCRIPTION

Physical model

The detail of the models used in the present simulations is available in the CALIF3S-ISIS physical documentation [9]. For both simulated experimental cases, the Favre-filtered mass ($\bar{\rho}$), momentum ($\bar{\rho}\bar{u}$), mixture fraction $\bar{Z}$, fuel mass fraction $\bar{Y}_F$ and total enthalpy $\bar{h}$ conservation equations are solved for. The momentum conservation equation is written in Low-Mach number formulation, which allows to uncouple the thermodynamic pressure (which is constant in open flows) and the dynamic pressure, and to only consider density variations related to temperature and mass fractions variations. The subgrid scale momentum stress tensor $\tau_{sgs}$ which appears in the filtered Navier-Stokes equations is modelled using a Boussinesq assumption and depends on the filtered strain rate tensor and the subgrid scale turbulent viscosity $\mu_s$. $\mu_s$ is determined by a Smagorinsky model which general formulation is $\mu_s = \bar{\rho}(C_s \Delta)^2||\mathbf{S}||$, where $\Delta$ is the characteristic cell size and $C_s$ a non-dimensional parameter. Instead of setting a constant value of $C_s$ as in the original Smagorinsky model, the dynamic version based on the Germano identity [11] is used to allow the decay of $C_s$ in laminar and transitional zones, which is particularly important near the injection of fuel. Note that the maximum allowed value of $C_s$ is 0.12. The subgrid scale scalar turbulent fluxes $\tau_{sgs,\phi}$ are also modelled using a Boussinesq assumption and a simple gradient diffusion hypothesis. The ratio between dynamic and scalar mixing is fixed using a turbulent Prandtl or Schmidt number $\sigma_{\phi}$, which is set equal to 0.5. The combustion of a single fuel, namely methane or Methyl Metacrylate (MMA) is modelled using a single step combustion reaction which reads $F + \nu O_2 \rightarrow \alpha CO_2 + \beta H_2O + \sigma S$ in mole formulation. Here $\nu,\alpha,\beta$
and $\sigma$ are the molar stoichiometric coefficients. In particular, the soot production is accounted for here; the mole soot yield $\sigma$ is related to the mass soot yield $y_s = \sigma W_e / W_F$ characterized for a large range of fuels in Ref. [12]. The multicomponent system including the transport of fuel, oxidizer and combustion products mass fractions is reduced to the mixture fraction/fuel mass fraction formulation the under the unit Lewis number assumption. The combustion rate $\hat{\omega}_f$ is described by the EDM approach [13]:

$$\hat{\omega}_f = -\frac{\mu_s}{\sigma C_{LES}} \min\left(\frac{\overline{v_z}}{s}, \frac{\overline{v_d}}{s}\right),$$

where $\sigma_t$ is the turbulent Schmidt number, $C_{LES}$ is a constant which default value is 0.1 and $s = v W_d / W_F$ is the mass stoichiometric ratio (4 for methane and 8.2 for MMA).

The radiative losses are accounted for in the enthalpy conservation equation by solving the Radiative Transfer Equation (RTE). A Weighted Sum of Grey Gases Model (WSGGM) is used for the gas phase radiative absorption $\kappa_G$. Two methods are proposed: for the SANDIA methane flame, the $P1$ approximation of the RTE is chosen because the radiative transfer is not expected to have a major influence on the flame dynamics; the low computational cost of this method therefore allows using relatively large meshes. For the case of PMMA slabs, the Finite Volume Method is used to solve for the RTE, so as to correctly evaluate the radiative transfer, in particular near the sample surface. Considering the large computational cost of this method, it is solved every 20 time steps. Soot formation is accounted for in the flame radiative properties: the molar soot yield is $\sigma = 0.185$, and the additional radiative absorption $\kappa_S$ due to the soot reads $\kappa_S = A T f_v$ where $f_v$ is the soot volume fraction and $A = 1264 \text{ m}^3\text{K}^{-1}$.

**Numerical model**

The integration of the system of equations depicted above is performed using a fractional time step algorithm [14]: the scalar equations are solved for with a backward Euler method as time discretization. Then, the density is updated accounting for its dependence with respect to the updated scalars. Finally, the Navier-Stokes equations are solved for using a pressure correction technique and a second order Crank-Nicolson time discretization. All the above conservation equations are discretized using a Marker-And-Cell staggered discretization. The Navier-Stokes problem and the scalar transport equations. Two couples of space discretisations for scalar/Navier-Stokes equations are considered: (Sch1) MUSCL/centred schemes and (Sch2) MUSCL implicit/QUICK implicit schemes [15]. For (Sch1), the CFL number based on a characteristic velocity $U_{\text{max}} = 5 \text{ m/s}$ and the minimum cell size $\delta_{\text{min}}$ must remain lower than 0.1 because of the instability of the explicit MUSCL scheme and the centered scheme. For (Sch2), the constraint CFL=1 is imposed even if the schemes are implicit and thus stable. The second-order centred scheme used in (Sch1) is assumed to be conservative with respect of the kinetic energy balance for the Navier-Stokes equations, contrary to the upwind third order QUICK implicit scheme used in (Sch2) which is dissipative.

**SIMULATION OF THE SANDIA METHANE POOL FIRE**

The first experimental test case considered here is the 1 m diameter methane pool fire carried out in the SANDIA FLAME facility [5]. The computational domain represents the complete 6.2 m cubic central chamber, including the 2 m diameter flat plate located 2.45 m above the floor, the cylindrical shield surrounding an annular air inlet, the trapezoidal ceiling and the chimney outlet. The cells of the first considered cuboid MAC meshing (M1) are $\delta_{\text{min}} = 2.5 \text{ cm}$ cubic cells near the fuel inlet and are enlarged in the three directions with a maximum cell size of $\delta_{\text{max}} = 20 \text{ cm}$ near the external walls, the air supply inlet, the roof and the chimney outlet. A second refined mesh (M2) with $\delta_{\text{min}} = 1.25 \text{ cm}$ has also been used. In these conditions, the time step is of $8.33 \times 10^{-4} \text{s}$ for (M1/Sch1), $8.33 \times 10^{-3} \text{s}$ for (M1/Sch2), $4.16 \times 10^{-4} \text{s}$ for (M2/Sch1), $4.16 \times 10^{-3} \text{s}$ for (M2/Sch2). For the boundary conditions, a surface inlet fuel mass flux of $0.053 \text{ kg/m}^2\text{s}$ is imposed, which corresponds to a heat release rate of 2.07 MW. The corresponding injection velocity, equal to 0.097 m/s, is not disturbed by synthetic turbulence injection. The inlet temperature is of 286 K. Pure methane is injected with $Y_F = 1$. Note that for this fuel the soot conversion factor can be set equal to 0. Fresh air is injected at the annular inlet with a fixed velocity of 0.327 m/s at the temperature of 290 K. The walls temperature is fixed to an average value of 302 K.

The axial velocity and kinetic energy radial profiles depicted in Fig. 1 show that mesh M2 and convective schemes Sch2 always overestimate the average velocity and the turbulent kinetic energy compared to mesh M1 and schemes Sch1, respectively. For the axial velocity, the gap to experimental data remains in the uncertainty range of 20% [5] for all the simulations. For the turbulent kinetic energy, the use of mesh M2 is required to reach radial profiles which remain within the 30% experimental uncertainty range.
The main “puffing” flame oscillatory behaviour [5] is recovered in these simulations. Quantitatively, considering the High Resolution analysis [16] of the axial velocity recordings at a 0.6 m height on the centreline, the observed puffing frequencies are of 1.25 Hz, 1.3 Hz, 1.45 Hz and 1.5 Hz for M1/Sch1, M1/Sch2, M2/Sch1 and M2/Sch2 respectively, with 20% variations around the average value. These values are underestimated for mesh M1 and are closer from the theoretical frequency of 1.5 Hz for M2; they are slightly underestimated compared to the experimental value of 1.65 Hz. In this respect, the minimal cell size has a larger influence on the puffing frequency than the convective schemes combination. On the contrary, the snapshots of instantaneous temperature depicted in Fig. 2 show that schemes combinations Sch1 and Sch2 exhibit different turbulent structures: Sch2 shows larger, laminar-like fluctuations due to large-scale, toroidal instabilities, whereas Sch1 shows fully turbulent fluctuations which partially hide these characteristic toroidal structures.

Fig. 1. Average axial velocity and resolved turbulent kinetic energy radial profiles at heights 0.3 m (left), 0.5 m (center) and 0.9 m (right) : comparison between simulations (cases M1/Sch1, M1/Sch2, M2/Sch1 and M2/Sch2) and the SANDIA FLAME experimental data.

Fig. 2. Temperature fields in the plane \( y = 0 \) for the simulation cases M1/Sch1 (\( t = 10.62 \) s), M1/Sch2 (\( t = 10.25 \) s), M2/Sch1 (\( t = 10.87 \) s) and M2/Sch2 (\( t = 14 \) s) - from left to right.

SIMULATION OF THE FLAME ABOVE A PMMA SLAB

Here the simulation of the flame above the square 40 × 40 cm\(^2\) PMMA slab studied by Kacem et. al. [8] is presented. Convective schemes (Sch1) are used, the minimal and maximal cell sizes are \( \delta_{\text{min}} = 0.5 \) cm and \( \delta_{\text{max}} = 10 \) cm. A similar mesh as depicted above is used, but this time the external faces are open-air boundaries. The time step is chosen to ensure that the maximum average velocity-based CFL number remains lower than 0.05. A fixed mass flow rate of 0.01 kg/m\(^2\)/s is imposed at the fuel inlet, which corresponds to the
lower limit of the experimentally measured value. This time, 200 random Fourier modes [17] are introduced as inlet velocity disturbances to trigger turbulence near the fuel injection. The simulation is carried out up to 15 s of physical time; statistic averages are performed on the time interval [5, 15] s.

In Fig. 3, the axial average temperature profile is compared to the experimental thermocouple measurements and the spatial evolution of the received convective, radiative and total heat flux over the sample width are depicted. Obviously the simulation overpredicts the temperature in the combustion zone and recovers the correct far field decay after 1 m height. Accordingly, the radiative and total heat flux are underestimated compared to the experimental measurements at the middle of the sample (40 kW/m² and 57 kW/m² numerically against 50±6 kW/m² and 63±4.5 kW/m²). The convective part, defined in the simulations as the sum of the conductive and the turbulent heat flux \(\left(\lambda + \mu_t Pr_T \nabla \bar{T} \cdot \mathbf{n}\right)\), is overestimated (17 kW/m² against 12 kW/m²). Yet, it can be shown that the buoyant flame is characterized by a puffing frequency ranging between 1.5 and 1.9 Hz. Accordingly, the description of the flame puffing over a whole period of Fig. 4 shows that the hot gases accumulation which leads to the flame puffing is triggered by a pure Rayleigh-Taylor-like toroidal structure. This structure, which is more or less strongly dissipated by developed turbulence in the case of the SANDIA methane flame, remains coherent up to \(z = 0.3\) m. This shows that, in spite of the introduction of inlet random Fourier modes on the injected velocity, turbulence is not triggered in this zone. However, further experimental data (high-frequency velocity measurements or flame visualisations) would be necessary to know the actual turbulence behaviour in this zone. This lack of turbulent mixing possibly implies that combustion occurs too far from the sample and that the flame height is too large. Yet, a smaller flame height may induce a larger radiative heat flux received by the sample. It may also induce a lack of mixing with the external fresh air, and therefore explain the overestimation of the convective flux.

CONCLUSION

The Large Eddy Simulations presented in this paper have shown the ability of the CALIF3S-ISIS CFD software to catch most of the phenomena occurring in turbulent buoyant flames, namely the balance between mean and turbulent kinetic energy, the flame puffing and the characteristic instabilities of such flows. In particular, for large pool fires such as the SANDIA methane flame, using upwind high-order schemes allows catching these phenomena, but the non-dissipative centred, second-order centred convective scheme for the Navier-Stokes equations is a better choice to catch more turbulent structures. If the average flame structure is
recovered with 40 points clustered in the pool diameter, twice more points are required to correctly predict the turbulent kinetic energy. For smaller buoyant flames such as the one occurring above a square $40 \times 40$ cm$^2$ PMMA slab, using both 80 points in the slab width and non-dissipative schemes does not allow recovering a fully turbulent flame, which induces an average temperature and a slight radiative heat flux underprediction, and a slight convective flux overprediction. As a consequence, the accurate evaluation of the flame flux received by a pyrolysing sample requires more attention on the behaviour of the turbulence in the near-sample flame zone. From a numerical point of view, imposing inlet temperature fluctuations instead of the velocity fluctuations may be a better mean to trigger turbulence in this zone. Including buoyancy effects in the subgrid scale viscosity model may also help recovering the correct flame shape. But, so as to validate such models, accurate experimental data on smaller flames than those tested in the SANDIA FLAME facility would be useful.

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