Large Eddy Simulation of a Mechanically Ventilated Compartment Fire for Nuclear Applications

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ABSTRACT

This paper deals with the modelling of a mechanically ventilated compartment fire which is a commonplace in nuclear fire scenarios. An advanced Computational Fluid Dynamics (CFD) field model with a wall conjugate heat transfer treatment is proposed. It simultaneously solves the compartment fire flow and the wall heat conduction. The flow solver is based on the Large Eddy Simulation (LES) based fire simulation solver FireFOAM within the frame of open source CFD code OpenFOAM®. An extended eddy dissipation model is used to calculate the chemical reaction rate. A soot model based on the concept of smoke point height is employed to model the soot formation and oxidation. A finite volume method is adopted to model the radiative heat transfer. The ventilation flow is modelled by a simplified Bernoulli equation neglecting the detailed information on the ventilation system. The proposed model is validated against a single room fire test with forced mechanical ventilations. The predictions are in reasonably good agreement with experimental data.

KEYWORDS: Compartment fire, large eddy simulation, conjugate heat transfer, forced ventilation.

INTRODUCTION

A confined and mechanically ventilated compartment fire is a commonplace in nuclear fire scenarios, where fire compartments are connected to ventilation networks to prevent radio-active releases. The mechanically ventilated compartment fires differ from the naturally ventilated ones in that fires are confined in enclosures with forced ventilations, leading to significant thermodynamic pressure variations [1]. Although naturally ventilated compartment fires have been extensively studied in the literature [2-5], mechanically ventilated compartment fires are less documented due to the lack of large-scale fire tests. A fire test program PRISME [6] was designed to investigate the fire growth in full-scale confined and mechanically ventilated compartments. The test results have been widely used as benchmark data for the validation of fire models [1, 7-10].

The underlying physics of the mechanically ventilated compartment fires are complex. Combustible solid/liquid material is firstly pyrolysed into gaseous phase and then ignited by heat sources, resulting in a buoyant fire accompanied by the formation and oxidation of soot particles. Soot particles enhance the radiative heat transfer, and the radiative heat feedback to the surfaces of combustible material can modify the fire burning rate. The time-varying burning rate induces pressure variations which alter the ventilation flow rates. Combustion heat is extracted from the confined compartment in two ways: one is through ventilation exhaust flows; the other is via heat transfer to the walls.

The modelling of the above mentioned fire scenario is challenging. Some simplifications have to be made. There are generally two fire modelling approaches: integral zone models [11, 12] and CFD field models. In the zone models the fire compartment is normally divided into an upper hot zone and a lower cold zone, where a homogeneous mixture is assumed in each zone. The zone properties...
such as pressure, temperature, species concentrations, etc. are solved by the integrations of the mass and energy balances in each zone. The field models solve differential transport equations of mass, momentum and energy, closed by more elaborate physics-oriented models such as turbulence model, pyrolysis model, combustion model, soot model, radiation model, ventilation model and conjugate heat transfer (CHT) model etc. In this study, an advanced CFD field model with a wall CHT model is proposed and validated against PRISME Source test data [6].

**NUMERICAL DESCRIPTION**

Fire spreading in a compartment is a low Mach number flow of variable density. A fully compressible flow solver becomes inefficient due to the need to capture acoustic waves; hence a low Mach approximation is widely adopted to speed up simulations in the fire modelling, by dividing the pressure into a time dependent thermodynamic pressure for the energy equation and a spatial and time dependent hydrodynamic pressure for the momentum equation. The flow solver in this study is based on our previous studies on fire modelling [13, 14], in which the eddy dissipation concept (EDC) was extended to the framework of large eddy simulation (LES) by taking into account the distinctive roles of the sub-grid scales (SGS) and using the partially stirred reactor (PaSR) concept to relate the filtered soot formation rate to the soot chemical time scale which is assumed to be proportional to the laminar smoke point height (SPH). The turbulent mixing time scale for soot is computed as a geometric mean of the Kolmogorov and integral time scale. A finite volume based radiation model is adopted for radiative heat transfer. More details about the LES solver for fire modelling can be found in the reference [13, 14].

A major feature of mechanically ventilated compartment fires is in that fire rooms exchange mass, momentum and energy with the ambient environment through ventilation networks. The ventilation networks are usually rather complex, composed of different types of components such as ducts, bends, valves and fans etc. Computing the ventilation flow of the whole networks requires detailed information of all the components. To simplify the ventilation calculation, the flow resistance coefficient between network nodes can be calculated using test pressure data if the detail of the ventilation structure is known [9]. The ventilation flow is usually solved separately from the flow solver, and the ventilation flow is coupled to the compartment flow via boundary conditions. In this study a simplified ventilation model [1, 8] based on a general Bernoulli equation is adopted, which neglects the detailed information on the ventilation system. Because of the pressure variation, reverse flows are observed at both admission and exhaust ventilation branches. Therefore, the ventilation model can be written in a general form as follow:

\[ P_{\text{vent}} - P_{\text{room}} = R_{\text{vent}} \rho |Q|, \]  

where \( P_{\text{vent}} \) is the pressure of a node inside the ventilation system, which keep nearly constant during operation; \( P_{\text{room}} \) is the pressure at the ventilation openings connected to the compartment; \( R_{\text{vent}} \) is the resistance coefficient; \( Q \) is the ventilation volumetric flow rate and keeps positive if ventilation flow is directed into the compartment and otherwise keeps negative; \( \rho \) is the upstream density, i.e. taken as the density at the ventilation openings if the ventilation flow is directed out of the compartment. The resistance coefficient \( R_{\text{vent}} \) is priori calculated using test data and keeps constant during the simulation.

The hot fire smoke exchanges heat transfer with wall surfaces in the forms of radiative and convective heat transfer. The most accurate method to calculate the heat transfer is the CHT approach which solves the gas phase flow in the compartment and the wall heat conduction simultaneously and the wall surface heat flux is used as a coupled boundary condition between the two phases. The modelling of the convective heat transfer in the confined compartment is not a straightforward task. The convective heat transfer can be calculated from the empirical heat transfer coefficient which is related to the properties of gas phase, the type of convection, the orientation of solid wall. However, there lacks of well-defined large-scale fire tests for determining the coefficients in the literature. Therefore,
a fixed coefficient or one-dimensional heat conduction calculations [9] were normally adopted in previous studies. In this study, a three dimensional CHT model, which solves a 3D heat conduction Eq. (2) for the solid wall, is proposed to calculate the wall heat transfer. At the wall surface a balance Eq. (3) of heat flux is used as a coupled thermal boundary condition between the solid and gas phases.

\[
\rho_s c_s \frac{\partial T}{\partial t} = k_s \left[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right], \tag{2}
\]

\[
k_s \left( \frac{\partial T_s}{\partial n} \right)_{\text{wall}} = k_g \left( \frac{\partial T_g}{\partial n} \right)_{\text{wall}} + Q_r, \tag{3}
\]

where \(\rho_s, c_s\) and \(k_s\) are respectively density, specific heat and heat conductivity of solid phase and assumed to constant; \(k_g\) is effective heat conductivity of gas phase corrected by SGS turbulence, counteracting the under-prediction of the temperature gradient at the under-resolved wall boundary, \(Q_r\) is radiative heat flux.

VALIDATION CASE AND PROBLEM DESCRIPTIONS

The numerical models in the second section are validated against PRISME Source test PSR-SI-D3, which is a single room test. The test room has an internal dimension of \(5 \times 6 \times 4\) m ventilated by an admission branch and an exhaust branch. The ventilation branches enter the room through two \(0.4 \times 0.4\) m rectangular ducts. The test room consists of 30 cm thick concrete walls and the ceiling is covered by an insulation layer of 5 cm thick rock wool. A fuel pan of a surface area \(0.4 \, m^2\) is situated in the room centre and hydrogenated tetra-propylene \((C_{12}H_{26})\) is used as fuel. The detailed information on the test facility and test conditions can be found in [1, 2].

The computational domain shown in Fig. 1 is divided into two regions, a fluid region enclosed by a solid region (black). The fluid region is meshed using non-uniform grids with a maximum grid size of 5 cm, clustering at the wall surfaces. Uniform mesh is created for the solid region, 10 grids are placed in the thickness direction. The simulation starts from zero velocity, an initial pressure of 98384 Pa and an initial temperature of 307 K for the two regions. No pyrolysis model is attempted for modelling the fuel burning rate in this study, in order to avoid its uncertainties affecting the predictions. The burning rate is defined by the experimental data as shown in Fig. 2, and applied as an inflow boundary condition at the fuel inlet. Reverse flows were observed at both the admission and exhaust branches in the fire test, an inlet-outlet boundary is applied at the ventilation openings where inflow/outflow velocities are calculated using the ventilation model in Section 2 according to the room pressure. On the all the wall boundaries of the fluid region, a no-slip velocity boundary condition and a coupled thermal boundary condition (Eq. (3)) are applied.

![Figure 1. Computational domain.](image)

![Figure 2. Fire burning rate of the test.](image)

A one-equation SGS turbulence model [15] is employed to represent the SGS stress and turbulent Viscosity, and two model coefficients are set to be \(C_k=0.05\) and \(C_v=0.4\). An extended Eddy dissipation combustion model [14] and a soot model based on smoke point concept [15] are used to model the
chemical reaction rate and the formation and oxidation of soot particles, and the smoke point height of \( \text{C}_{12}\text{H}_{26} \) is set to 0.029 in the simulation.

A finite volume method (FVM) [14] is used for radiative heat losses, in which the radiative transfer equations within multiple solid angles are solved to evaluate radiative absorption and emission. With the Gray assumption, the total absorption coefficient is decomposed into the gas absorption coefficient and the soot absorption coefficient. A total of 16 solid angles covering a hemisphere is used for the radiative transfer equations (RTE) as a compromise between computational time and accuracy.

For the heat conduction of the solid region, Eq. (2) is spatially discretized using a second order Gauss linear scheme and the solution is marched in time using a first order explicit scheme. The thermal properties of solid region are assumed to be constant in the simulation, and can be found in the Ref. [1]. The outer boundaries are assumed to thermally adiabatic.

RESULTS AND DISCUSSION

Fig. 3 shows the comparison of the room pressure variations. The predictions follow closely with the changing trend of the experimental data. Three factors contribute to the pressure variations: combustion heat release, ventilation flows and wall heat transfer.

![Figure 3. Comparison of the pressure variations.](image)

After the ignition, the combustion heat release induces a rapid pressure rise due to the increasing burning rate. The predicted variation is initially higher than the experimental data, which increases the exhaust flow rate and reduces the admission flow rate resulting in an early reverse flow at the admission branch (see Fig. 4). The first pressure peak, which occurs at \( t = 65 \) s corresponding to the first peak of the burning rate, is under-predicted by 700 Pa due to the over-prediction of the pressure variation which increases the energy and mass losses through the ventilation system. After the first peak, owing to the increasing heat losses via the wall heat transfer and the ventilation system, the room pressure then drops to a valley value which is well predicted by the current simulation. As the burning rate increases again after \( t = 160 \) s, the pressure variation increases and reaches to another peak because the combustion heat release outnumbers the heat losses. The extinction at \( t = 370 \) s induces the lowest valley value which is also moderately under-predicted by about 700 Pa due to the under-prediction of the wall heat transfer resulting from the inadequate grid resolution at the wall boundary layers.

Comparisons of the volumetric flow rates at the admission and exhaust branches are shown in Fig. 4. The ventilation flow is closely coupled with the pressure variations and its changing pattern resembles
that of the pressure variations. The predictions are generally in reasonable agreement with the experimental data. Over-predictions of the ventilation flow rates are observed prior to \( t = 250 \) s for the admission flow rate and \( t = 300 \) s for the exhaust flow rate. After the ignition, a reverse flow quickly establishes at the admission branch due to the initial pressure increase, and the reverse flow last for approximately 250 s. A reverse flow is also observed for the exhaust branch after the extinction, but it only lasts for 80 s. The predictions agree rather well with the experiment data after \( t = 300 \) s.

**Figure 4.** Comparisons of the admission flow rate (left) and exhaust flow rate (right).

Fig. 5 shows the comparisons of oxygen molar fraction at three locations. Overall, the predictions agree well with the experimental data at all the locations. The fire smoke tends to spread towards the ceiling due to the buoyancy effect and then forced to move downward. Therefore, the oxygen concentration starts to drop sooner close to the ceiling, and then almost drops linearly with time to a minimum value before the extinction. After the extinction, the concentration starts to gradually recover due to the intake of fresh air from the admission branch. The moments when the oxygen molar fraction starts to drop and the final oxygen concentration are well predicted in current simulation.

**Figure 5.** Comparisons of oxygen molar fraction at three locations: (a) \( X = -0.8 \) m, \( Y = 0 \) m, \( Z = 0.35 \) m; (b) \( X = 1.5 \) m, \( Y = -1.25 \) m, \( Z = 0.8 \) m; (c) \( X = 1.5 \) m, \( Y = -1.25 \) m, \( Z = 3.3 \) m.

Fig. 6 shows the comparisons of temperature at three locations. One peak value is observed almost at the same moment \( t = 300 \) s for each location, which is higher close to the ceiling. The peak value and its location are well predicted for all the locations. After the ignition the temperature is over-predicted, and after the peak moment the temperature is moderately under-predicted, except at the location of NE380 which is significantly over-predicted after \( t = 400 \) s due to the over-heating from the heated ceiling. The discrepancies of the temperature can be mainly attributed to the imperfectness of the ventilation model, wall CHT model and the combustion model. Among these causes, the error
resulting from the CHT model due to the less resolved boundary layer is the most possible reason responsible for the discrepancies.

**Figure 6.** Comparisons of temperature at three locations: (a) $X = 1.5$ m, $Y = -1.25$ m, $Z = 1.8$ m; (b) $X = 1.5$ m, $Y = -1.25$ m, $Z = 2.8$ m; (c) $X = 1.5$ m, $Y = -1.25$ m, $Z = 3.8$ m.

Fig. 7 displays the contours of temperature in the middle plane at four different moments. After the ignition, a fire plume establishes and spreads towards the ceiling. The maximum flame temperature is observed around 1300 K. The temperature is higher inside the plume, and a hot upper layer is developed and extended towards the floor. After the extinction a temperature gradient still prevails inside the room.

**Figure 7.** Contours of temperature in the middle plane at $t = 100$ s, 200 s, 300 s, and 400 s.

Fig. 8 displays the contours of oxygen mass fraction in the middle plane at four different moments. The fire plume consumes oxygen inside the room. As the fire plume induces pressure rise causing a reverse flow at the admission branch, which prevents the intake of fresh air, the depletion of oxygen results in the fire extinction.
Fig. 8. Contours of oxygen mass fraction in the middle plane at \( t = 100 \) s, 200 s, 300 s, and 400 s.

Fig. 9 displays the contours of carbon dioxide mass fraction in the middle plane at four different moments. The maximum of carbon dioxide mass fraction is found to be 0.18 inside the fire plume. After the extinction, a nearly uniform distribution of carbon dioxide mass fraction around 10% is observed.

Fig. 10 displays the contours of soot mass fraction in the middle plane at four different moments. The maximum of soot mass fraction is found to be 2.4% inside the fire plume. After the extinction, a nearly uniform distribution of soot mass fraction around 0.5% is observed.
CONCLUSIONS

An advanced CFD field model has been proposed for modelling of mechanically ventilated compartment fires. The field model is based on a LES flow solver coupled with a wall CHT model. The LES flow solver adopts a one equation SGS turbulence model, an extended eddy dissipation combustion model, a soot model based on the concept of smoke point height, a FVM radiation model, a ventilation model based on a general Bernoulli equation.

The proposed model is validated against a single room fire test, ventilated by an admission branch and an exhaust branch. The predictions of the pressure variation, the volumetric flow rates at the admission and exhaust branches, oxygen concentration and temperature are compared with experimental data. Overall, these predictions are in reasonably good agreement with the experimental data, closely following the experimental changing patterns. The ventilation flows and the wall heat transfer are two important features of the mechanically ventilated compartment fires, their model accuracies greatly affect the predictions and responsible for the discrepancies in the current simulation. To improve the accuracies of the proposed field model, a detailed ventilation model by solving the ventilation flow in the whole ventilation system and a CHT model based on empirical correlations on the convective coefficient needs to be implemented, if the detailed information of ventilation networks and large-scale fire tests on the empirical correlations is available.

REFERENCES


