

MODELING OF COMPARTMENT FIRE

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Abstract

Fire accident in a containment is a serious threat to nuclear reactors. Fire can cause substantial loss to life and property. The risk posed by fire can also exceed the risk from internal events within a nuclear reactor. Numerous research efforts have been performed to understand and analyze the phenomenon of fire in nuclear reactor and its consequences. Modeling of fire is an important subject in the field of fire safety engineering. Two approaches which are commonly used in fire modeling are zonal modeling and field modeling. The objective of this work is to compare zonal and field modeling approach against a pool fired experiment performed in a well-confined compartment.

Numerical simulations were performed against experiments, which were conducted within PRISME program under the framework of OECD. In these experiments, effects of ventilation flow rate on heat release rate in a confined and mechanically ventilated compartment is investigated. Time dependent changes in gas temperature and oxygen mass fraction were measured. The trends obtained by numerical simulation performed using zonal model and field model compares well with experiments. Further validation is needed before this code can be used for fire safety analyses.

1 Introduction

Fire is one of the complicated subjects in combustion science and is defined as uncontrolled flame spread and growth. Fire within a nuclear reactor is dangerous and must be avoided. The risk posed by fire is larger than the risk posed by internal events within the nuclear reactor. In particular, fire can potentially affect the critical system needed to shut down the nuclear reactor. Several fire accidents are reported in nuclear reactor e.g., fire occurred at the Browns Ferry Nuclear Power Plant (NPP) in 1975, the cause of the fire is attributed to electric cables. Sodium fire accident occurred in sodium fast reactor Monju, Japan in 1985 and it was due to sodium leak in the secondary loop. In order to reduce the risk of fire and frequency of fire occurrence in a nuclear reactor, further research on fire safety analysis is needed. Experimental and numerical investigations are useful approaches for the fire safety analysis. Numerical tools are increasingly being used in risk oriented fire assessments to improve and upgrade fire protection.

There are two approaches of numerical simulations a) zonal model and b) field model, which are based on Computational Fluid Dynamics (CFD). In the past, zonal model was one of the best approach to simulate fire, since it does not require large computational resources. The zonal model divides the geometry into two zones namely a) warm zone and b) cold zone. Equations for conservation of mass, energy and ideal gas law are solved in these zones. The parameters such as temperature and concentration are averaged in each of these zones. This

approach is also used by safety analysis code, however this method is not accurate for highly complicated geometry. An in-depth review of zonal model is presented elsewhere [1].

The alternative method is based on field model which is more accurate than zonal model, however, the simulation of fires using CFD is a challenging task, since a wide range of length scales (diffusion flame of order 1 mm to room dimension of 5 m) must be resolved. In the last decade, several researcher reported such investigation and validation of their code. Fire Dynamics Simulator (FDS) developed by National Institute of Standards and Technology (NIST) is one of the codes, which is widely used. This code is based on Large Eddy Simulation (LES) and mixture fraction based combustion model wherein radiation is accounted by finite volume radiation model. The details of the model are described in FDS manual [2]. Recently, validation of FDS is performed against medium scale pool fire [3], cable fire in Nuclear power plant [4, 5, 6, 7], lifted turbulent jet flame [8], turbulent buoyant flame [9, 10], methane fire [11], enclosure fires [12] and small pool fire [13]. The FDS can also be used for compartment fire [14, 15] and tunnel fire [16, 17, 18] and to simulate extinguishing of fires [19, 20, 21, 22].

Several other codes are also used to perform such analysis e.g., ISIS and FLUENT. ISIS [23, 24] code developed by IRSN (Institut de Radioprotection et de Sûreté Nucléaire) France can also be used to simulate fires in a compartment. The code is based on Favre-averaged Navier-Stokes (FANS) equation and both mixture fraction and eddy-break up combustion models are available [23, 25, 26]. Radiation is accounted by simple and complicated finite volume based model. Commercial CFD code ANSYS FLUENT [27] is also used to simulate fires. Both LES and FANS based turbulence models are available. Three different combustion models based on mixture fraction, eddy break up and laminar finite rate are available [27]. ANSYS FLUENT is validated by Xue et al. [28] for enclosed room fire, shopping mall fires and tunnel fire.

The focus of this paper is to compare zonal model and field model approach against pool experiments relevant to fire in nuclear compartments. In particular, it presents validation of CFD based field model and its comparison with zonal model. The paper is organized as follows. In Section 2, numerical methodology is presented. First in Section 2.1 we present zonal model and describe the governing equations which are solved in zonal model. Second, in Section 2.2 we present governing equations for field model. Furthermore, combustion model, turbulence model and radiation models are discussed in detail. In Section 3, experiments considered for the simulations are described in detail. Section 4 presents the comparison of zonal model and field model simulations against experiments. Finally, conclusion is presented in Section 5.

2 Numerical methodology

2.1 Zone model

Consolidated Model of Fire Growth and Smoke Transport (CFAST) [29] is used here for the validation of compartment fire. The code is developed and maintained by NIST. The code is based on two zones, which means the compartment modeled is divided into zones a) hot layer and) cold layer. This means that the variation of quantities only along the height of the compartment is taken into account. Figure 1 shows control volume of a zonal model. A layer interface divided the lower layer and upper layer This code solves the following equations for pressure, volume and temperature with respect to each layer. These equations are given below. Pressure:

$$\frac{dp}{dt} = \frac{\gamma - 1}{V}(h_L + h_U) \quad (1)$$

Volume:

$$\frac{dV_U}{dt} = \frac{1}{p\gamma} \left[(\gamma - 1)h_i - V_U \frac{dp}{dt} \right] \quad (2)$$

Upper layer temperature and lower layer temperature:

$$\frac{dT_U}{dt} = \frac{1}{c_p \rho_i V_U} \left[(h_U - c_p m_U T_U) + V_U \frac{dp}{dt} \right] \quad (3)$$

and

$$\frac{dT_L}{dt} = \frac{1}{c_p \rho_i V_L} \left[(h_L - c_p m_L T_L) + V_L \frac{dp}{dt} \right]. \quad (4)$$

Here, $i = L$ is the lower layer and $i = U$ is the upper layer, ρ_i is the density, m_i is the mass,

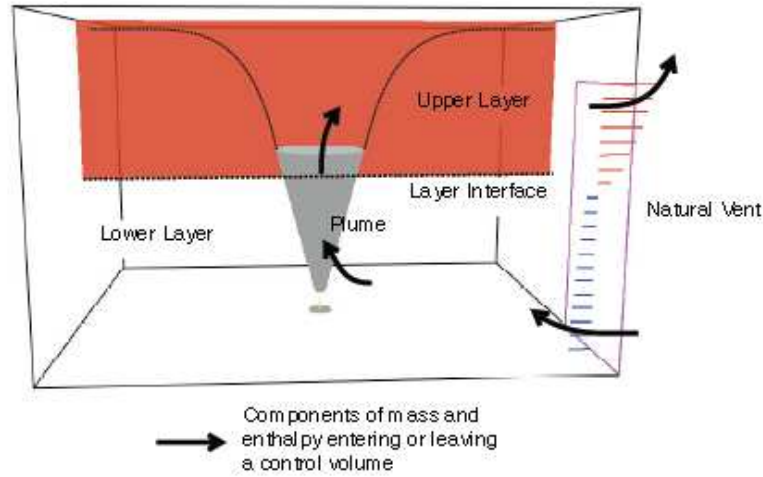


Figure 1: Schematic of control volume in a zonal model.

V_i is volume, T_i is the temperature of the layer i and p is the pressure. V_L and V_U are the lower layer volume and upper layer volume. These sets of equations are derived by conservation of mass, energy and ideal gas law. Fire in CFAST [29] is implemented as a source of mass of fuel released at a prescribed rate. The combustion products are created as it burns. Energy source is equal to product of fuel release rate and heat of combustion released by the fuel. One step reaction is assumed for the reaction of fuel and combustion products. Heat transfer in wall is accounted by solving heat conduction equation normal to the wall.

2.2 Field model

Commercial CFD solver ANSYS FLUENT [27] is used for this purpose. The models and the governing equations are described below in the following subsections.

2.2.1 Governing Equations

Within the ANSYS FLUENT solves the following governing equation for conservation of mass, momentum, energy

Mass:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho} \tilde{u}_i) = S_m. \quad (5)$$

Velocity:

$$\frac{\partial}{\partial t}(\bar{\rho} \tilde{u}_i) + \frac{\partial}{\partial x_j}(\bar{\rho} \tilde{u}_i \tilde{u}_j) = -\frac{\partial \bar{p}}{\partial x_j} + \frac{\partial}{\partial x_j}(\overline{\tau_{ij}} - \bar{\rho} \tilde{u}_i'' \tilde{u}_j'') + g_i \frac{\tilde{u}_i}{\bar{\rho}} S_m. \quad (6)$$

fuel mass fraction:

$$\frac{\partial}{\partial t}(\bar{\rho} \tilde{Y}_k) + \frac{\partial}{\partial x_j}(\bar{\rho} \tilde{u}_i \tilde{Y}_k) = \frac{\partial}{\partial x_j} \left(\frac{\mu_t}{\sigma_t} \frac{\partial \tilde{Y}_k}{\partial x_j} \right) + \tilde{\omega}_k \quad (7)$$

Energy:

$$\frac{\partial}{\partial t}(\bar{\rho} \tilde{E}) + \frac{\partial}{\partial x_j}(\bar{\rho} \tilde{u}_i \tilde{E}) = \frac{\partial}{\partial x_j} \left(\frac{\partial \tilde{T}}{\partial x_j} \frac{k_{eff}}{C_p} \frac{\partial \tilde{T}}{\partial x_j} - \sum_k h_k \tilde{J}_k \right) + S_h \quad (8)$$

Here, $\tilde{u}_i$, $\tilde{Y}_k$ and $\tilde{E}$ are the Favre-averaged velocity, mass fraction of species k and total energy, μ_t is the turbulent viscosity, σ_t is the turbulent Schmidt number and S_m is the mass transfer to the gas phase from liquid droplet or pool due to evaporation, t is the time, ρ is the density, p is the pressure, C_p is the specific heat capacity, g_i is the gravitation acceleration, $\tilde{\omega}_k$ is the reaction rate, S_h is heat of chemical reaction and $\tilde{J}_k$ is the diffusion flux of species k .

2.2.2 Turbulence model

The closure for Reynolds stress terms in Eq. 6 was achieved with the standard $k - \omega$ turbulence model. Following equation for turbulent kinetic energy, k and specific dissipation rate, ω

$$\frac{\partial \bar{\rho} k}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho} \tilde{u}_i k) = \frac{\partial}{\partial x_j} \left(\mu + \frac{\mu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right) + G_k + \underline{G_b} + \bar{\rho} \beta^* f_{\beta^*} \omega k \quad (9)$$

and

$$\frac{\partial \bar{\rho} \omega}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho} \tilde{u}_i \omega) = \frac{\partial}{\partial x_j} \left(\mu + \frac{\mu_t}{\sigma_\omega} \frac{\partial \omega}{\partial x_j} \right) + \alpha \frac{\omega}{k} G_k + \bar{\rho} \beta f_\beta \omega^2 \quad (10)$$

are solved. The turbulent viscosity μ_t is evaluated as follows

$$\mu_t = \alpha^* \frac{\bar{\rho} k}{\omega}. \quad (11)$$

Here, β , β^* , α^* , f_β and f_{β^*} are the constants. The production term in Eq. 9 and 10 is given as follows

$$G_k = \left[\mu_t \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right) - \frac{2}{3} \bar{\rho} k \delta_{ij} \right] \frac{\partial \tilde{u}_i}{\partial x_j}. \quad (12)$$

Buoyancy effects the turbulent kinetic energy given by underlined term in Eq. 9 is taken into account and is implemented in ANSYS FLUENT using User Defined Functions (UDF). The production of turbulence due to buoyancy is given as follows:

$$G_b = \beta g_i \frac{\mu_t}{Pr_t} \nabla \tilde{T}. \quad (13)$$

Here, g_i is the gravitational acceleration, Pr_t is the turbulent Prandtl number and β is the coefficient of thermal expansion and is given by

$$\beta = -\frac{1}{\bar{\rho}} \left(\frac{\partial \bar{\rho}}{\partial T} \right)_p \quad (14)$$

An effect of buoyancy on specific dissipation rate is not taken into account.

2.2.3 Combustion and radiation model

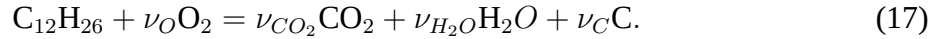
The term $\tilde{\omega}_k$ in Eq. 7 represents the reaction rate which needs to be closed. The eddy-dissipation model proposed by Magnussen and Hjertegar [30, 31] is used to model combustion. The model is based upon the assumption that the overall rate of burning is controlled by turbulent mixing. The net rate of production of species k due to reaction r , $\tilde{\omega}_k$, is given by the smaller (i.e., limiting value) of the two expressions below:

$$\tilde{\omega}_k = \nu'_{k,r} M_{w,k} A \bar{\rho} \frac{\epsilon}{k} \min \left(\frac{Y_R}{\nu'_{R,r} M_{w,R}} \right) \quad (15)$$

and

$$\tilde{\omega}_k = \nu'_{k,r} M_{w,k} A B \bar{\rho} \frac{\epsilon}{k} \frac{\sum_P Y_P}{\sum_j^N \nu''_{j,r} M_{w,j}}. \quad (16)$$

Here, ϵ is the turbulent dissipation rate, A and B are the constants, $M_{w,k}$ is the molecular weight of species k , Y_P and Y_R are the mass fractions of products and reactants, $\nu'_{k,r}$ and $\nu''_{j,r}$ are the stoichiometric coefficients of reactant species k in reaction r and stoichiometric coefficients of product species j in reaction r . Following one step reaction considered for liquid hydrogenated tetra propylene (TPH) which is the fuel burned is considered



Here, ν_O , ν_{CO_2} , ν_{H_2O} and ν_C are the stoichiometric coefficient of O_2 , CO_2 , H_2O and soot. To account for radiation loss, Discrete Ordinate (DO) radiation model is used here. The absorption coefficient of the soot, CO_2 and H_2O must be taken into account. To calculate the absorption coefficient of soot and gas, respectively following equation is used

$$\alpha_{soot} = 1262 f_v T \quad (18)$$

and

$$\alpha_{gas} = P(k_{CO_2} x_{CO_2} + k_{H_2O} x_{H_2O}). \quad (19)$$

Here, f_v is the soot volume fraction, P is the absolute pressure, k_{CO_2} , k_{H_2O} are the temperature dependent absorption coefficients of CO_2 and H_2O are taken from [32], x_{CO_2} and x_{H_2O} are the mass fractions of CO_2 and H_2O . The absorption coefficients are implemented in the solver using UDF.

To summarize, at each time step Eq. 5, 6, 7, 8, 9, 10 and 11 are solved to obtain density, velocity, mass fraction of species, k , temperature, turbulent kinetic energy and turbulent dissipation rate.

2.2.4 Numerical scheme

3D simulations were performed using ANSYS FLUENT, which employs a finite volume method. The spatial and time discretization of the conservation equations were performed with second order upwind scheme and second-order implicit method, respectively. The pressure-velocity coupling was performed with SIMPLE and discretized equations were solved using a segregated solver in an iterative manner.

3 Results and discussion

The aim of this work is to compare zonal model approach against field model. For this purpose, the experiments performed in confined and mechanically ventilated fire compartment are selected. This is described below.

3.1 Experiment

Within the framework of PRISME (French acronym for “Fire Propagation in Elementary Multi-room scenarios”), several experiments were performed starting from single room to fires in three rooms with ventilation. These experiments were performed in DIVA facility in IRSN, France. The Diva facility shown in 3.1 essentially contains a room (floor area 5×6 and height 4 m) which is mechanically ventilated. The floor of the room containing pool of liquid hydrogenated tetra propylene (TPH) is burning at specified mass loss rate (see Fig. 3). The pool surface is 0.4 m^2 before ignition and the fuel depth is 0.05 m. The pool is ignited by propane gas burner. The room has inlet and outlet branches of the ventilation system. The inlet branch supplies fresh air at a ventilation rate of $560 \text{ m}^3\text{h}^{-1}$. The properties of the room and the liquid fuel are mentioned in Table 1 and 2 and 3. More details of the experiments are provided in paper by Pretrel et al. [33].

Table 1: Experimental condition

Atmospheric temperature	287 K
Absolute Pressure	99kPa
Fuel temperature	306.5 C
Temperature in fire compartment	307
Temperature in JUPITER compartment	304
Wall temperature	305

Table 2: Diva compartment

Material	Thermal Conductivity $\lambda [\text{Wm}^{-1}\text{K}^{-1}]$	Heat Capacity $C_p [\text{Jkg}^{-1}\text{K}^{-1}]$	Emissivity $\epsilon [-]$	Density $\rho [\text{kgm}^{-3}]$
Concrete	1.5	736	0.7	2430
Rockwool	0.102	840	0.95	140

Table 3: Hydrogenated tetra-propylene properties

Formula	Density ρ [kgm^{-3}]	Heat of vaporisation h_{fg} [kJkg^{-1}]	Heat of combustion ΔH_c [Jkg^{-1}]	Ignition temperature T_{ign} [K]	Radiative fraction β [-]
$\text{C}_{12}\text{H}_{26}$	749	362	42.106	473	0.7

The point measurements of temperature performed at different locations $x=2.375$, $y=0.0$ $z=[0.05, 0.3, 0.55, 0.80, 1.05, 1.30, 1.55, 1.80, 2.05, 2.30, 2.55, 2.8, 3.05, 3.3, 3.55, 3.80, 3.85, 3.90]$. Additionally, oxygen concentrations are measured for entire fire duration of 3500 s. The uncertainty in measurement for gas temperature and oxygen concentration are 10 % and 2 %.

3.2 Simulations

The experiments are simulated using CFAST and ANSYS FLUENT. The computational domain and boundary conditions used in ANSYS FLUENT are described here. Commercial

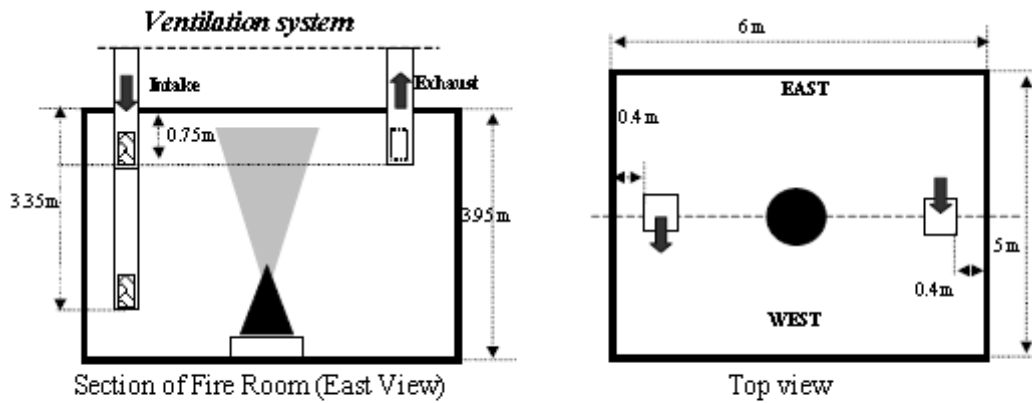


Figure 2: Schematic of DIVA facility

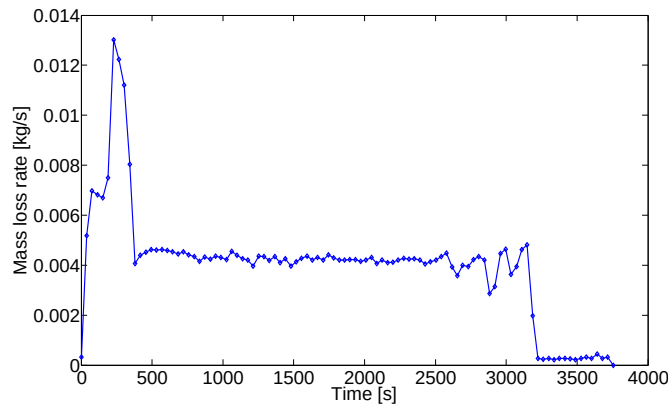


Figure 3: Measured mass loss rate

Meshing software ANSYS GAMBIT is used to mesh the geometry. Two different meshes (cell size of 10 cm and 20 cm results) were compared to obtain grid independent results. Time dependent mass flow inlet boundary condition is specified in the fire inlet (see Fig. 3), while constant mass flow rate is specified for the air inlet. The thickness of the wall on the roof and adjacent walls were resolved and heat conduction equation was solved for this purpose.

Figure 4a and b) shows the comparison of gas temperature at two location $z = 0.155$ m and $z = 0.205$ m. Curves 1 and 2 were obtained using CFAST and ANSYS FLUENT simulations, respectively. Filled symbols in Fig. 4 represent experimental data. The results are plotted only from time $t = 0:500$ s since the peak in mass flow rate occurs in this time range (see Fig 3) . The results obtained from CFAST over-predict the gas temperature, while ANSYS FLUENT results are in good agreement with experiment. It is worth mentioning here that the uncertainty in measurement in gas temperature is 10 %. Both CFAST and ANSYS FLUENT results show peak in temperature at the same time as in the experiments.

Figure 5a) and b) shows the comparison of gas temperature at location $z = 0.28$ m and $z = 0.33$ m. Curves 1 and 2 were obtained using CFAST and ANSYS FLUENT simulations, respectively. Filled symbols represent experimental data. The results obtained from both these simulations tend to over-predict the gas temperature, however, the trends are predicted very

well. Further investigations are needed to ascertain the cause of over-prediction in gas temperature.

The oxygen concentration plays a major role in fire propagation. As the oxygen concentration decreases, burning rate also decreases and hence the gas temperature. Figure 6a) and b) shows the comparison of oxygen concentration at location $z = 0.08$ m and $z = 0.33$ m. Curves 1 and 2 were obtained using CFAST and ANSYS FLUENT simulations, respectively. Filled symbols represent experimental data. Results from ANSYS FLUENT match very well with the experiments. It is worth mentioning here that the uncertainty in measurement in oxygen mass fraction is 2%.

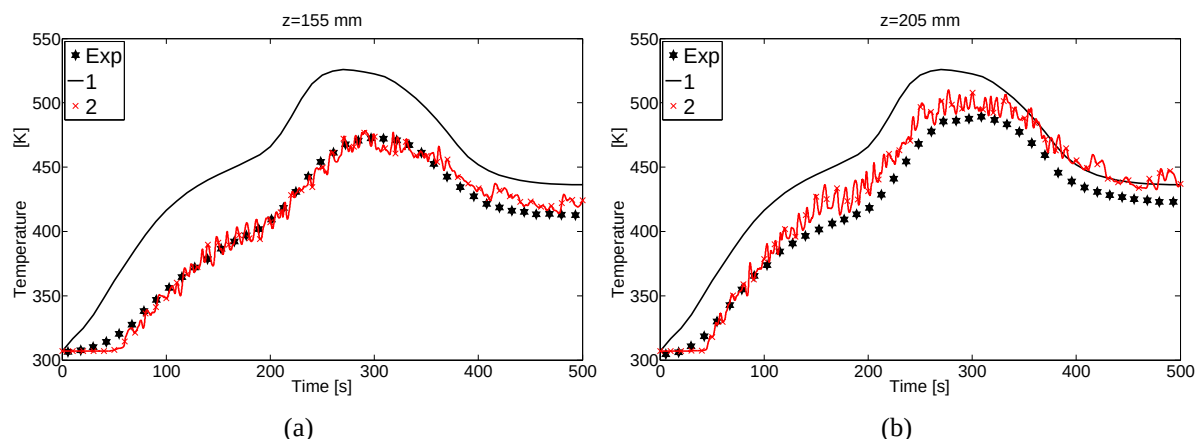


Figure 4: Gas temperature $T(k)$ versus time, t a) $z = 0.155$ m b) $z = 0.205$ m. Curves 1 and 2 were obtained from CFAST and ANSYS FLUENT simulations, respectively. Symbols represent experiments.

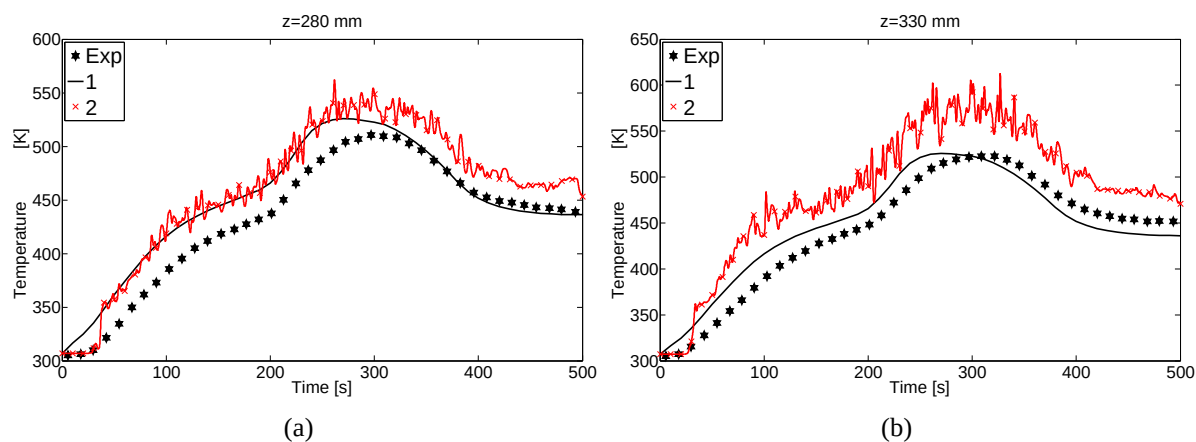


Figure 5: Gas temperature $T(k)$ versus time, t a) $z = 0.28$ m b) $z = 0.33$ m Curves 1 and 2 were obtained from CFAST and ANSYS FLUENT simulations, respectively. Filled symbols represent experimental data.

4 Conclusion

Fire accidents in nuclear reactors must be prevented to avoid the risk of release of harmful radioactive materials in the environment. Numerical tools based upon zonal and field model

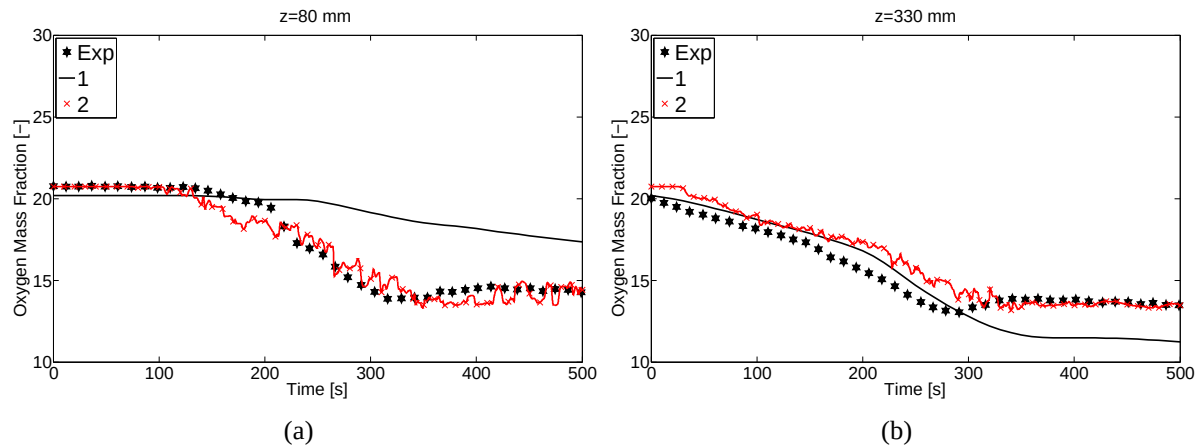


Figure 6: Oxygen concentration versus time, t a) $z = 0.28 \text{ m}$ b) $z = 0.33 \text{ m}$. Curves 1 and 2 were obtained from CFAST and ANSYS FLUENT simulations, respectively. Filled symbols represent experimental data.

approaches are commonly used for the safety analyses of nuclear reactors. The aim of this work is to compare both these simulation approaches against experiment. For this purpose, simulations were performed and compared against liquid pool fire experiments conducted in confined and mechanically ventilated compartment. Zonal model simulations performed using CFAST and field model simulations performed using ANSYS FLUENT are compared. The gas temperature and oxygen concentration at different locations obtained using simulations show similar trends as in experiments. However, CFAST over-predicts the gas temperature and oxygen concentration in comparison to ANSYS FLUENT.

Further validation must be performed before this code can be used for the fire safety analyses of nuclear reactors.

5 Acknowledgment

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Nomenclature

Roman Symbols

C_p	:Gas mixture heat capacity at constant pressure [J/kg.K]
g	:Gravitational acceleration [m^2/s]
H_c	:Heat of combustion [kJ]
h_j	:Enthalpy of species, j [J/mole]
h_L	:Enthalpy of lower layer [J/moles]
h_U	:Enthalpy of upper layer [J/moles]
k	:Turbulent kinetic energy [m^2 / s^2]
k_{eff}	:Gas mixture thermal conductivity [W / m.K]
m_i	:mass of layer i [kg]
Nu	:Nusselt number [-]
P	:Absolute pressure [Pa]

p	:Pressure [Pa]
R	:Universal gas constant [J/K.mol]
r	:Radius [m]
Re	:Reynolds number [-]
S_h	:Energy source [-]
S_m	:Mass source [-]
Sc	:Schmidt number [-]
T	:Temperature [K]
t	:Time [s]
T_L	:Temperature of lower layer [K]
T_U	:Temperature of upper layer [K]
u	:Velocity [m/s]
V	:Control Volume [moles]
V_i	:Volume of layer i [m ³]
V_L	:Volume of lower layer [m ³]
V_U	:Volume of upper layer [m ³]
x_j	:Coordinates in j [m]
Y_k	:Mass fractions of species, k [-]
z	:Height [m]

Greek Symbols

ϵ	:Emissivity [-]
μ	:Laminar viscosity [Pa.s]
μ_t	:Turbulent viscosity [Pa.s]
ω	:Specific dissipation rate [1 / s]
ρ	:Density [kg/m ³]
ρ_g	:Density of gas [kg/m ³]
σ	:Stefan-Boltzmann constant [.]
σ_t	:Turbulent Schmidt number [-]

Acronyms

CFAST	:Consolidated Model of Fire Growth and Smoke Transport
FDS	:Fire Dynamics simulator
IRSN	:Institut de Radioprotection et de Sûreté Nucléaire
NPP	:Nuclear Power Plant
RHS	:Right Hand Side

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