

FIRE DYNAMICS IN A BUILDING COMPARTMENT – A NUMERICAL STUDY

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Abstract. *Building fires pollute the air heavily and jeopardize human health and life. In this paper, the Large Eddy Simulation method of Fire Dynamics Simulator code has been used to investigate the temperature regime and the pollutant concentrations in a compartment and near a building wall under fire scenario. Numerical results show that the generation of fire products in the compartment is largely dependent on the temperature and the quantity of oxygen available for combustion. The outdoor plume parameters are affected by the temperature difference between the fire flame and plume and the surrounding ambient air.*

Key words: *compartment fire, temperature, pollutant concentrations, air pollution*

1. INTRODUCTION

People can be adversely affected by exposure to pollutants in ambient air. Indoor pollutants jeopardize human health and may even cause serious morbidity and mortality under extreme conditions [2]. Fires and explosions cause a great deal of damage to the property and the environment and their combustion products can very often cause death or injury to people. There are many reasons why accidental fires can be a threat to human life. People exposed to indoor fire and smoke inhalations often die because they are unable to escape from the toxic effects of combustion products.

Combustion products evolve during a fire. The combined effects of carbon monoxide (CO), carbon dioxide (CO₂) as a combustion products, and oxygen (O₂) depletion are the

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main causes of fatalities in smoke. Depending on the degree of ventilation of a compartment, the nature and composition of the smoke can change and produce significantly differing consequences. Fires, in which the amount of O₂ available for complete combustion is low, can be especially hazardous for life of exposed people. Under these conditions, the CO which is the primary toxicant in compartment fires is formed. Namely, the production of CO is promoted by a low O₂ concentration, and as the human body preferentially takes up CO, which is toxic, the threat to life increases as the CO concentration increases [1].

For these reasons, prediction of fire dynamics and generation of fire pollutants in a compartment are very important. In this paper, the fire dynamics and pollutant concentrations under different ventilation conditions has been analyzed. Large Eddy Simulation method of Fire Dynamics Simulator software package has been used to investigate the fire parameters inside a building compartment and into the plume that flows near an outside building wall.

2. NUMERICAL STUDY

2.1. Methodology

With the rapid development of computer technology, Computational Fluid Dynamics (CFD) modelling is widely applied for studies of turbulent flows such as fire. The turbulence methods commonly used in CFD include Reynolds Averaged Navier-Stokes equation, Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS) methods.

Fire Dynamics Simulator (FDS) software package, developed by National Institute of Standards and Technology (USA), is now a popular CFD tool in fire researches. FDS uses LES and DNS methods to calculate the fire parameters. In this study, LES method is used since it can predict the unsteadiness and intermittency of the turbulence structure, which is the most important feature of a strong buoyancy-driven fire-induced flow.

Hydrodynamic model

FDS solves numerically a form of the Navier-Stokes equations approximate for low-speed, thermally-driven fluid. They describe the low speed motion of a gas driven by chemical heat release and buoyancy forces. The governing equations for a thermally expandable, multi-component mixture of ideal gases are, as follows [4]:

Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = \dot{m}_b''' \quad (1)$$

Conservation of individual gaseous species:

$$\frac{\partial}{\partial t} (\rho Y_\alpha) + \nabla \cdot \rho Y_\alpha \mathbf{u} = \nabla \cdot \rho D_\alpha \nabla Y_\alpha + \dot{m}_\alpha''' + \dot{m}_{b,\alpha}''' \quad (2)$$

Conservation of momentum:

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot \rho \mathbf{u} \mathbf{u} + \nabla p = \rho \mathbf{g} + \mathbf{f}_b + \nabla \cdot \boldsymbol{\tau}_{ij} \quad (3)$$

Conservation of energy which is written in terms of the sensible enthalpy:

$$\frac{\partial}{\partial t}(\rho h_s) + \nabla \cdot \rho h_s \mathbf{u} = \frac{Dp}{Dt} + \dot{q}'' - \dot{q}_b'' - \nabla \cdot \dot{q}'' + \varepsilon \quad (4)$$

Equation of state for a perfect gas

$$p = \frac{\rho RT}{M} \quad (5)$$

where ρ – density, \mathbf{u} – velocity vector; T – temperature; D_α – diffusion coefficient; Y_α – mass fraction of α^{th} species; \dot{m}_α''' – mass production rate per unit volume of species α by chemical reactions; $\dot{m}_{b,\alpha}'''$ – production of species α by evaporating particles; p – pressure; \mathbf{g} – gravity vector; \mathbf{f}_b – external force vector; τ_{ij} – viscous stress tensor; h_s – sensible enthalpy; $\dot{\mathbf{q}}''$ – heat flux vector; \dot{q}'' – heat release rate per unit volume from a chemical reaction; \dot{q}_b''' – energy transferred to the evaporating droplets; \dot{q}'' – conductive and radiative heat fluxes; ε – dissipation rate; R – universal gas constant; M – molecular weight of the gas mixture; t – time.

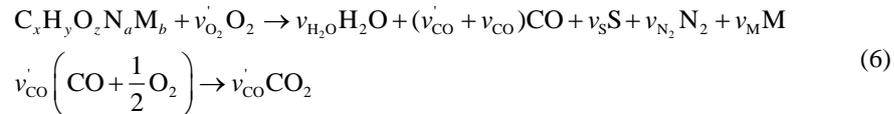
Combustion model

FDS uses the mixture fraction model which includes three different states of fuel to allow for a two-step combustion process. In the first step, fuel is converted to CO while in the second step, CO, as an intermediate combustion product, reacts with O_2 to form CO_2 as follows:

Step 1: Fuel + $O_2 \rightarrow CO$ + Other Products (i.e. H_2O , soot)

Step 2: $CO + \frac{1}{2}O_2 \rightarrow CO_2$

The reaction of fuel and O_2 in terms of all of the species is described as:



The stoichiometric coefficients for other toxic combustion products are:

$$v_{CO_2} = x - v_{CO}' - (1 - X_H)v_S \quad (7)$$

$$v_S = \frac{W_F}{W_S} y_S \quad (8)$$

$$W_S = X_H W_H + (1 - X_H)W_C \quad (9)$$

where v_k - stoichiometric coefficient of species k ; y_k - yield of species k ; W_F - molecular weight of fuel; W_k - molecular weight of species k ; X_H - hydrogen atomic fraction.

The mixture fraction is defined in terms of the mass fractions of fuel ($C_x H_y$) and the carbon-carrying products of combustion:

$$Z = \frac{1}{Y_F^f} \left(Y_F + \frac{W_F}{xW_{CO_2}} Y_{CO_2} + \frac{W_F}{xW_{CO}} Y_{CO} + \frac{W_F}{xW_S} Y_S \right) \quad (10)$$

where Y_F^f – stands for the fuel mass fraction in fuel stream; Y_k – mass fractions of the species in the mixture.

2.2. Model configuration

A computational domain (15 m wide, 30 m long and 30 m high) was designed for CFD LES simulation. The multi-storey residential building was designed at the right side of the domain. The boundaries of the domain were all set to be naturally opened in order for the gases to flow freely in and out of the simulation domain.

The buoyancy source was a compartment fire at the third floor of the building. The compartment had the window (2 m wide and 2 m high), which was closed at the start of the simulation. The other windows at the lower and the upper floors of this building were also closed during the simulation.

Pool fire (i.e. cooking oil) in the kitchen was set as a fire source. Reaction type of "SPRUCE", according to FDS reaction database [4] was specified for generating combustion products from the fire source. The heat release rate (HRR) of the fire is 5 MW.

When applying LES simulation, the grid size is the key parameter that must be considered very carefully, in order to produce reliable simulation results. The grid size is determined by the non-dimensional expression $D^*/\delta x$ where D^* is the characteristic fire diameter and δx is the nominal size of a grid cell. Characteristic fire diameter is defined as [4]

$$D^* = \left(\frac{\dot{Q}}{\rho_\infty c_p T_\infty \sqrt{g}} \right)^{\frac{2}{5}} \quad (11)$$

where \dot{Q} – HRR; c_p – specific heat; T_∞ – ambient air temperature.

Investigations of McGrattan et al. [3] suggest that the grid size must be no larger than $0.1D^*$ to obtain viable simulation results. For the HRR of fire ($\dot{Q} = 5$ MW) used in this numerical study, D^* is computed to be 1.97 m, then $0.1D^*$ is approximately 0.2 m which can be taken as a reasonable grid size. Therefore, the grid was uniform of 0.2 m in the three spatial directions. The number of grid cells was 1,687,500 (75×150×150 in the x , y and z - direction, respectively).

3. RESULTS AND DISCUSSION

3.1. Temperature regime in fire compartment

Smoke temperature was used to represent the fire growth, the HRR and thermal regime in the compartment. Temperature regime of fire which is visualized through time-averaged temperature contour plots of gaseous products is shown in Fig. 1.

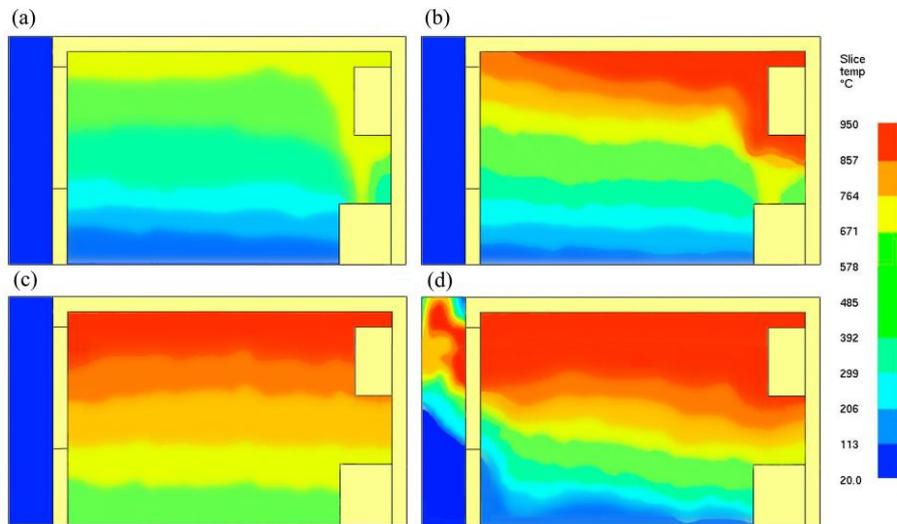


Fig. 1 Temperature regime in fire compartment

The fire originated by ignition of the vapour that was generated over the cooking oil surface in the heating period. Later on, the fire was quickly spread to the whole oil surface. The HRR of the oil was 400 kW and the temperature in the fire source was 450°C (Fig. 1a). The radiative and convective heat fluxes on the kitchen cabinets surfaces were induced by the cellulose pyrolysis and they determined its rate. The volatiles released during the pyrolysis process moved through the pores of the wood particles and mixed with the surrounding air. Piloted ignition occurred when pyrolysis gases were released from the wooden cabinets at a rate which was sufficient to produce a flammable mixture. After ignition, the flame was spread over the cabinets surfaces providing rapid volatilization. Due to combustion of flammable pyrolysed gases, the HRR rapidly grew and consequently, it led to the increase of compartment temperature (Fig. 1b). The HRR further induced the pyrolysis and combustion reactions which influenced the rise of quantity of the hot combustion products in the thermal plume and the increase of the plume layer near the ceiling. Afterwards, the plume moved towards the lower part of the compartment, leading to the increase of the temperature (Fig. 1c). However, the higher portion of the flammable gases burned in the oxygen depleted environment. The limited ventilation reduced the burning rate which caused a decrease in the HRR. But, the accumulated fire plume radiated heat back to the burning cabinets intensifying the wood pyrolysis. As a consequence, the flammable gases of pyrolysis and combustion products were accumulated in the compartment.

Since the double-glazed compartment window was exposed to the fire, its temperature was increased. When the temperature of upper glass surfaces reached 600°C, the window glasses were broken [6]. This can be explained by the following facts: the temperature at the top layers of the glasses was the highest and it decreased gradually towards the lower layers. As a result, due to the temperature difference between the glass layers, uneven thermal expansion was developed. This initiated the crack and the breakage of the glasses.

The outcome of glass breakage was the change of the fire dynamics in the

compartment. The fresh ambient air entered the compartment through the lower part of the window. The quantity of O_2 that is available to the fire increased, which resulted in the combustion of accumulated flammable gases of pyrolysis. Consequently, the HRR and the compartment temperature rapidly increased.

Later on, due to the continuous supply of fresh air, the fire stabilized. A typical stratified fire-induced flow field was developed in the compartment. Namely, the large density variation forced the mixture of the air and the combustion products to rise. These conditions launched consequent entrainment of the fresh ambient air into the compartment through the lower part of the window. The greater air density created a positive pressure in the compartment which was influenced the buoyancy-driven flame and plume to go out through the window and move upwards on the outside building wall (Fig. 1d).

3.2. Gaseous concentrations in fire compartment

As a result of the fire, the combustion products were generated in the compartment. Gaseous products of wood combustion include a large numbers of chemical species. The species of interest in this investigation were CO, CO_2 , and O_2 . Field distribution of CO, CO_2 and O_2 denoted by time-averaged concentrations in the compartment before the glass breakage is shown in Fig. 2.

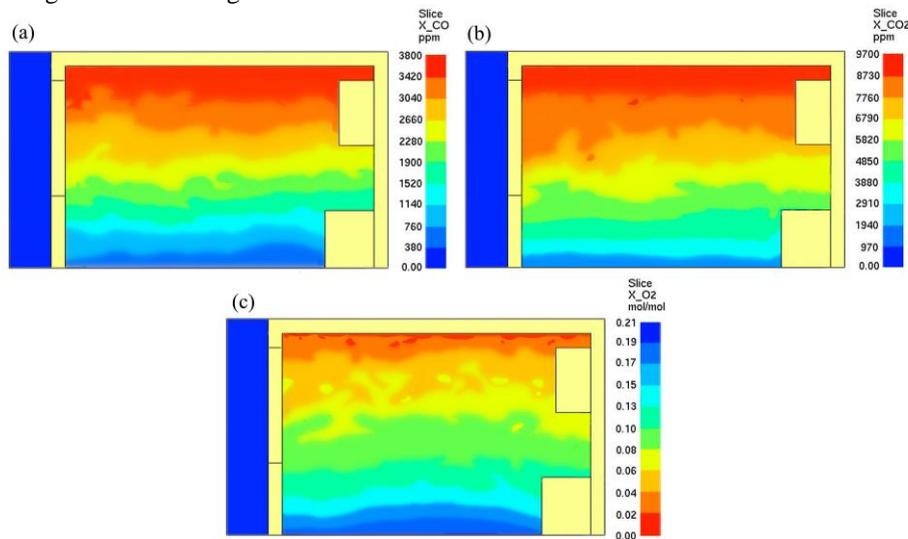


Fig. 2 Gaseous concentrations in fire compartment

The prediction of the CO and CO_2 production, as well as the O_2 consumption was carried out by FDS5 combustion model. Namely, the prediction of CO production, as a first product of hydrocarbon oxidation, has the crucial importance for the two-step reaction scheme. In the first step, hydrocarbon products of wood pyrolysis are converted to water vapour (H_2O) and CO, and depending of the local conditions, in the second step CO is converted to CO_2 .

In general, the generation of fire products depends on the ventilation, i.e. the quantity of available air for combustion and the temperature inside the fire plume.

During the oil combustion, the fire was well ventilated with low CO yield as a result of the combustion. Namely, there was enough quantity of the air and, therefore, CO as an intermediate combustion product reacted with O_2 thus forming CO_2 . Under these conditions, low in the flame, the CO production has been at a maximum, and, high in the flame it decreased to essentially zero because it oxidized to CO_2 (Fig. 2b). After piloted ignition, in the fire growth stage, the larger quantity of pyrolysed hydrocarbons from the wood was burned and consequently the larger CO yield was formed in the fire source. Due to the rise of temperature in the plume layers, there was more intensive oxidation of the post-plume gases. The available quantity of O_2 and the temperature in the fire plume were high enough to accelerate the oxidation of CO to CO_2 .

Later on, in the fire developed stage, there was a jump in the CO yield. This happened because the air quantity was not capable of supporting the rate at which wood was pyrolysed. There was no the sufficient O_2 to allow complete combustion of hydrocarbon products of pyrolysis. For this reason, the incomplete oxidation of unburned hydrocarbons led to the increase of CO generation.

The simulation results show that the large quantities of gaseous fire products were accumulated in the hot smoke layer below the ceiling. The hydrocarbon oxidation is much faster than CO oxidation; however, the unburned hydrocarbon concentrations were increased with O_2 depletion. Consequently, due to the lack of O_2 , the CO quantity also increased. The high temperature dictated post-plume oxidation in the layer; however, the CO oxidation caused by the high temperature influenced a small decrease in CO concentration. Local regions with high equilibrium of CO, which cannot find enough O_2 to burn out, were also present (Fig 2a). The O_2 concentrations were reduced to below 0.01% (Fig 2c). This indicates that the O_2 was utilized entirely for hydrocarbon oxidation and CO oxidation was essentially frozen.

The obtained results indicate that the concentrations of gaseous fire products in the upper hot layer formed below the ceiling depend upon the concentrations of these species in the plume formed above the fire source. The local concentrations are controlled by two mechanisms: their yield through combustion process and transportation of these species in the plume flow.

The factors that affect the CO and CO_2 production in the compartment fire are ventilation and temperature. The temperature effect is dominant only in the case of well ventilated conditions which are typical for the fire growth stage. The change of the fire plume temperature affects the generation of the species. The increased plume temperature correlates with the more complete oxidation of pyrolysed hydrocarbons to CO_2 and H_2O within the plume. The change of compartment temperature affects the oxidation of post-plume fire gases. Under poorly ventilated conditions, the ventilation effect is more dominant than the temperature effect. The ventilation effect is particularly dominant in the fire developed stage when the air quantity inside the compartment is less than its quantity required for complete combustion of the vapourized wood. Since, compared with CO_2 , CO is the first product of hydrocarbon oxidation, quenching of the chemical reactions of oxidation due to O_2 depletion, leads to the higher quantity of CO at the expense of CO_2 production.

3.2. Pollutant temperature and concentrations in outdoor fire plume

In case of the fire within a building compartment, an outdoor spill plume is formed after the window glass breakage [5]. Afterwards, the plume adheres to the external side of the building wall. The entrainment of fresh air into the plume is restricted for fire plume flow along a wall. Consequently, the air enters only the front side and the free ends of the plume. From these reasons, the fire plume behavior along the building wall is dependent on the turbulent and convective flows.

Field distribution of temperature, CO and CO₂ in the outdoor fire plume is shown in Fig. 3.

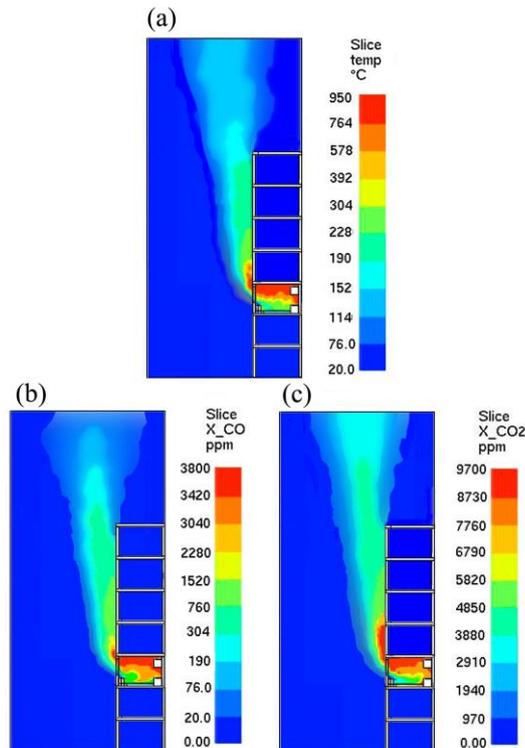


Fig. 3 Parameters of outdoor fire plume

The obtained results indicate that the outdoor plume temperature is affected by the temperature difference between the fire flame and plume regions and the surrounding ambient air. The temperature difference causes the difference of their densities, and consequently, the fresh air enters the plume. Due to the mixing of the cooler air and the hot fire products, the local plume temperatures decrease with the vertical distance away the fire compartment (Fig. 3a).

As the temperature plays an important role on the oxidation of CO, near the window of the fire compartment, the CO oxidizes to CO₂. Consequently, the CO concentrations decrease, while the CO₂ concentrations increase (Fig. 3b and c). Afterwards, when the

temperature of the flame decreases below 520 °C, due to cooling effects of the entrained air into the plume, the concentrations of the fire pollutants also decrease with the height above the fire compartment.

5. CONCLUSIONS

In the paper, FDS LES simulation was performed to study the fire dynamics and the plume parameters inside and outside a building compartment.

The simulation results show that the generation of fire products in the compartment is largely dependent on quantity of O₂ available for combustion. Thermal conditions of the fire plume also play a significant role. The temperature effect is dominant only in the case of well ventilated conditions which are typical for the fire growth stage. Elevated compartment temperature correlates with the increased fire plume temperatures and more complete oxidation of fire load to CO₂ and H₂O within the plume. In the fire growth stage, the combustion is well ventilated with low CO yield and a resulting high CO₂ yield. As the fire reaches its flashover, there is a jump in CO yield. Under poorly ventilated conditions, the ventilation effect is more dominant than the temperature effect. The ventilation effect is particularly dominant in the fire developed stage when the air quantity inside the compartment is less than its quantity required for complete combustion of fire load.

The obtained results also indicate that the outdoor plume parameters are affected by the temperature difference between the fire flame and plume and the surrounding ambient air. Due to the mixing of the cooler air and the hot fire products, both plume temperatures and pollutant concentrations decrease with the vertical distance above the fire compartment.

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DINAMIKA POŽARA U STANU – NUMERIČKA STUDIJA

Požari građevinskih objekata značajno zagađuju vazduh i ugrožavaju ljudsko zdravlje i život. U ovom radu, metod velikih vrtložnih strujanja softvera Simulator dinamike požara je korišćen da se predvide temperaturni režim i koncentracije zagađivača u stanu i pored zida zgrade tokom scenarija sa požarom. Numerički rezultati pokazuju da obrazovanje produkata požara u stanu u velikoj meri zavisi od temperature i količine kiseonika koji je dostupan za sagorevanje. U konvektivnoj struji požara na otvorenom prostoru parametri su pod uticajem temperaturne razlike između plamena i struje produkata i okolnog ambijentalnog vazduha.

Ključne reči: požar stana, temperatura, koncentracije zagađivača, zagađenje vazduha