Numerical Simulation of Fire Spread in a Compartment Fire: Modelling and Validation

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Abstract

Accurate modelling and simulation of fire and smoke spread in a furnished room is always a challenge due to the various combustion materials in the room and their complex chemical properties. To tackle this issue, fire and smoke spread in a furnished room and its connected corridor was simulated by the Fire Dynamics Simulator (FDS) and calibrated using the test data from an actual room fire test that was reported by the National Research Council Canada. In FDS, a fuel package with combined properties of polystyrene, polyurethane and wood was employed to simulate the combustion of the mixed burning items and furniture in the test room. The fuel packages are prescribed to generate the heat release rates (HRR) measured in the test. The combustion chemistry reaction model was also specified through a number of simulations to properly estimate the indoor conditions. Subsequently, the simulated heat release rate, temperature, visibility, and smoke optimal density as well as CO and O2 concentrations match the corresponding test data.

Introduction

Fire is a serious hazard to the life and safety of the communities. Recently, people have paid attention to the impact of fire and toxic hazards of smoke. Thus, understanding the characteristics of the compartment fires becomes vital in designing building fire protection systems and emergency response and egress plans. Modelling fire starts from quantitatively describing governing chemical and physical reactions of the fire and its spread affected by the room geometry and material nature. Great effort is put into modelling fire in an accurate way to develop those quantitative descriptions for combustion reactions. Several studies conducted zone models in comparison with experimental data to find the extent of their accuracy (Jones, 1983) (Duong, 1990) (Dembsey et al., 1995) (Peacock et al., 1998). Moreover, Yeun (Yuen and Yeoh, 2013) and Beard (Beard, 1997) reviewed field models and their limitations on simulating the fire. The latter includes overall discussion on the CFD code which is limited in modelling detailed combustion reactions during the fire.

A compartment fire is a complex phenomenon consisting of material combustion, turbulent convective heat flow and radiative heat transfer. It gets more complex when one aims to consider close interactions among the three parameters. Therefore, it brings about many shortcomings in the existing models. These shortcomings are related to the fuel pyrolysis and gasification nature which are inherent and extremely difficult to be modelled in complex geometries with multiple burning materials (Xue et al., 2001), while the models predict well buoyancy, convective flows and heat transfer.

These complexities are the reasons that several fire simulators have been released since 2000. For instance, fire dynamics simulator (FDS) was introduced by NIST. Shortly after, PyroSim was brought forward as a user-friendly interface of FDS. PyroSim has been employed for different goals including numerical simulation of a cinema fire (Glasa et al., 2013) to studying the fire risk of different ignition points in a high-speed train (LIANG et al., 2014).

This study simulated a fire test conducted in a room, which was furnished with many typical household items. The items were made of plastics, wood, pressboards, fibreboards and other composite materials including glue and adhesives (Ko, 2021). The material diversity makes it difficult to consider all the combustion, smoke generation and heat transfer in the room fire.

To solve the challenge caused by the diversity of the chemical properties of the many different furniture and burning materials involved in the fire, the diverse materials were modelled as fuel packages with combined properties of polystyrene, polyurethane and wood. Also, the fuel package was prescribed to generate the heat release rate measured in the test. Then, simulation results including temperatures were compared to the real test data for verification of the fuel package model. The gaseous reaction of the fuel package was also investigated for smoke optimal density as well as CO and O2 concentrations in the room.

Methodology

Figure 1 summarizes the key information about the methodology, starting from making the model geometry and defining boundary conditions for the numerical simulations to data extraction and comparisons with the experimental measurements.

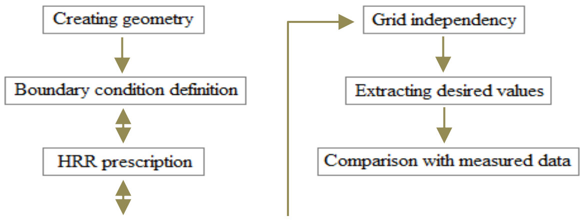

Figure 1. Schematic of methodology

CFD modelling

In this study, Fire Dynamic Simulator (FDS) is employed for the computational fluid dynamics (CFD) modelling. FDS is the product of collaboration led by the National Institute of Standards and Technology (NIST). The CFD tool treats the turbulence by means of Large Eddy Simulation (LES) and is validated for indoor and outdoor flows.

Model geometry

A room and its connected corridor were modelled, as shown in Figure 2, based on the full-scale test descriptions provided by the National Research Council Canada (NRC) (Ko et al., 2019; Ko and Gwynne, 2018).

Table 1 lists general conditions used in the simulation of the room fire. The room and corridor were built in the model using a uniform fine grid size of 0.1 m as shown in *Table 2*.

The connection between the room and corridor is via a door which remains open during the simulation time.

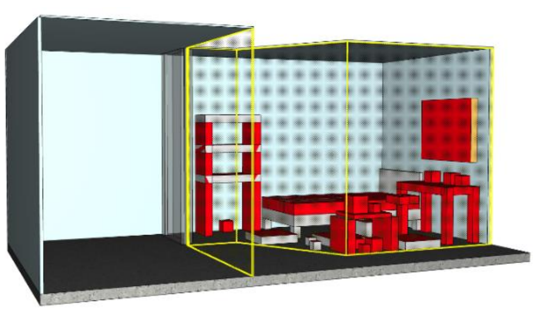

Figure 2. 3D view of the model

Table 1. General conditions used in the simulation

Duration of simulation	Start time: 0 s, End time: 2460 s
Ambient temperature	22.5 ˚C
Ambient pressure	1.01325E5 pa
Ambient oxygen mass fraction	0.232378 kg/kg (Kevin and Glenn, n.d.)
Ambient Carbon dioxide mass fraction	5.95E-4 kg/kg (Kevin and Glenn, n.d.)
Relative humidity	40 %
Ground level	0.0 m

Boundary condition and mesh set up

Following the data reported from the test, the ambient temperature is defined as 22.5 ˚C. While the room and corridor walls were lined with gypsum boards, the walls and concrete floor are simulated as adiabatic surfaces.

The real room was furnished with different pieces of objects/furniture made from plastics, wood, metal, fabric, etc. In the model, these materials were simulated as fuel packages having the fuel properties combined with several types of materials.

The fuel packages were placed in the simulated room, and they were modelled to generate the HRR measured in the test. While the total duration of the real experiment was 60 minutes, the model simulated the first phase of the fire development for 38 minutes, excluding the following phases of the fire going through the flashover (occurred at 40 minutes) and decay. The measured HRR data, which constantly changed over time, was simplified by capturing the critical trends of fire conditions/development measured. The fuel packages were prescribed to generate the simplified HRR curve over time.

The fire spread over the surface of the fuel packages placed in the room was modelled to follow the actual fire propagation observed in the test. Thus, the surface of each material/fuel package was defined in the model to ignite and grow/ramp up to match the fire development observed in the test by prescribing the measured HRR. Using this method and a radiative fraction of 0.35, the simulation resulted in temperature levels in the room and corridor comparable to those measured in the test.

However, accurate modelling of the combustion by-product generation (e.g., carbon monoxide, carbon dioxide) and oxygen depletion, as well as soot generation, requires actual fuel burning properties. Since the fire properties and chemical properties of the furniture and burning items were not available from the test, it was assumed that the fuel package has combined properties of PU, PS and Wood. For a simple reaction chemistry model, the fuel packages were assumed to contain only C, O, H and N, primarily based on Polyurethane and wood combination.

A series of simulations was carried out with varying fire properties for different combinations of various types of PU, PS and wood. Various inputs of soot yield and carbon monoxide yield were simulated. The best combination found with good agreements with the test data for temperature, smoke optical density and carbon monoxide are as follows: Release per unit mass of Oxygen: 1.31E4 kJ/kg. CO yield: 0.06, Soot yield: 0.05, Radiative fraction: 0.35.

Grid independence study

The total grid number in the ultimate case is 39600 which is made of uniform hedral gridding system. The main cell dimension is 10 cm which forms 1.14 cell size ratio. All the simulation cases were run on Mammoth-Mp2b cluster of

Calc Québec located at the Université de Sherbrooke. A per of 24 cores of CPU node is employed to run the simulation in multithreaded environment. Each run took 2 days to finalize, and multiple cases were submitted in parallel.

Table 2. CFD simulation set up

Room	Size	5 m (L) × 3 m (W) × 2.4 m (H)
	Initial indoor temperature	22.5 °C
	Infiltration door	0.8 m × 2.4 m
Corridor	Open vent	4.8 m^2 (between the corridor and outside)
Simulation settings	Domain size	5.5 m (L) × 3 m (W) × 2.4 m (H)
	Total gird number	39600
	Main cell size	0.1m × 0.1m × 0.1m
	Turbulence model	Very Large Eddy Simulation (VLES)
	Division method	Uniform
	Grid type	Hexa (hedral)
	Maximum cell size ratio	1.14
Grid Independence test	Fine grid number	316800
	Fine cell size	0.05 m × 0.05m × 0.05m
	Coarse grid number	11520
	Coarse cell size	0.15m × 0.15m × 0.15m

For the grid independence study, other than the main meshing, two other cell sizes were tested. The fine cell size is 0.05 m × 0.05 m × 0.05 m with a total grid number of 316800, and the coarse size is chosen as 0.15 m × 0.15 m × 0.15 m with a total grid number of 11520. To evaluate the adjacency of the three simulation results, the coefficient of variation - root mean squared error (CV-RMSE) is used (Coakley et al., 2014). The comparison shows the difference in the temperature or mass flow rate values between the three simulation results.

The governing equation of *CV-RMSE* is as follows:

$$CVRMSE = \frac{1}{\theta_{max}-\theta_{min}}\sqrt{\frac{\sum_{j=1}^{n}(\theta_{1,t}-\theta_{2,t})^2}{n}} \quad (1)$$

in which n is the times of observed variables, θ is a series of variables and t stands for time.

Figure 3 demonstrates the temperature values of the grid independence test among the moderate, fine and coarse mesh cases. The comparison shows close results between the fine and moderate grid sizes. At the same time, the coefficient of variation between the coarse and the moderate is more than double, in comparison to the value between the fine and the moderate mesh size. The results between the fine and the moderate cases only have 4.47 percent difference. Therefore, it illustrates that there is no obvious improvement between the moderate and the fine mesh size. In other words, the simulation results are independent of both the moderate and the fine grid resolutions.

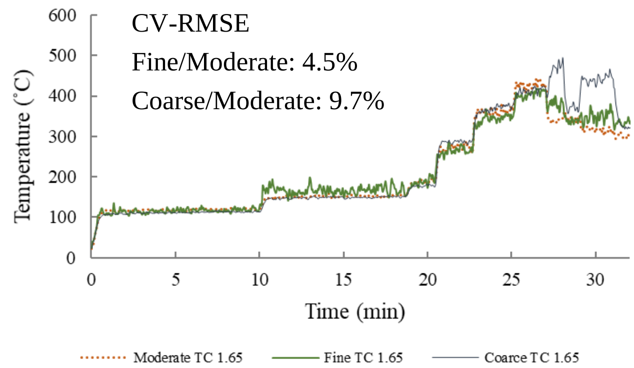

Figure 3. Grid independency test: temperature at a height of 1.65 m in the room for the simulations with the three different grid sizes

Results and Discussion

Comparisons with the actual test data

After creating the geometry and defining the boundary condition, the first step was assigning the same ignition sequence of the real test to the model. Therefore, the agreement in the HRR between the real test and the simulation was first validated by prescribing the actual HRR test data in the simulation.

Considering this agreement, other parameter results from the simulation and the test were compared for temperature, gas concentrations, smoke optical density and visibility. In addition, the simulated oxygen level is acquired.

Figure 4 shows the three curves of the prescribed HRR from the simulation, the actual HRR measured from the test and the HRR of the burner used in the test as an igniter. The prescribed HRR shows a good agreement with the general trend of the test HRR. Specifically, during the most critical period of 20 to 30 minutes, the peak of both curves is hitting the value more than 600 kW.

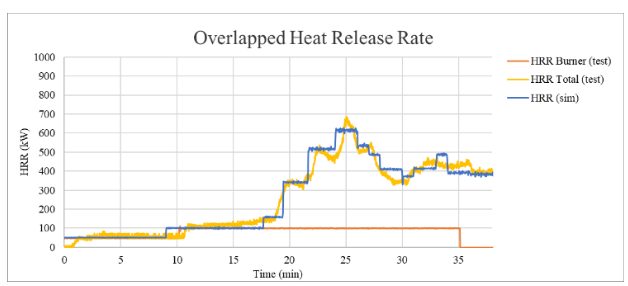

Figure 4. Comparisons of the simulation and test results for Heat Release Rate

In the test, temperatures were measured at different heights using thermocouple trees placed in the room and in the corridor. These measured temperatures are compared in Figure 5 with the simulated temperatures. Among the various heights, the most important one is 1.5 m height from the finished floor surface. This height can be considered as the average height of occupants' eyes and nose while being exposed to the combustion by-products.

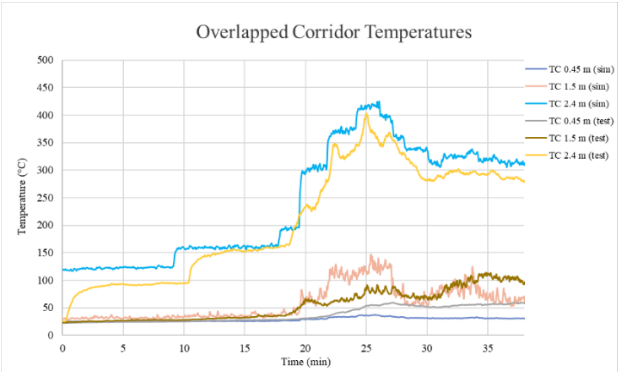

Figure 5. Comparisons of the simulated temperature and the measured temperature in the corridor (TC stands for thermocouple and the adjacent number shows its measurement height)

The NRC test report indicates that at 18.5 minutes from the start, the fire travelled from the bedding and spread to the shelves placed near the door, and the visibility in the room became untenable. Therefore, it can be defined as a critical point of fire growth in the room. Another critical moment was in the corridor at 21 minutes as the visibility became untenable, reaching the limit of 3 m. The following 2D slices in Figure 6 are presented to show the temperature ranges in the above-mentioned critical points.

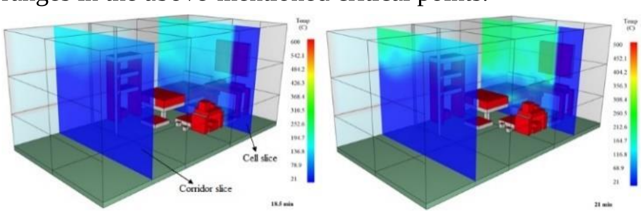

Figure 6. 2D temperature slices in the room and corridor at 18.5 and 21 minutes

The optical density in the model was simulated in the room and corridor at the height of 1.5 m which is the same as in the test. The result is compared with the measured optical density from the test in Figure 7.

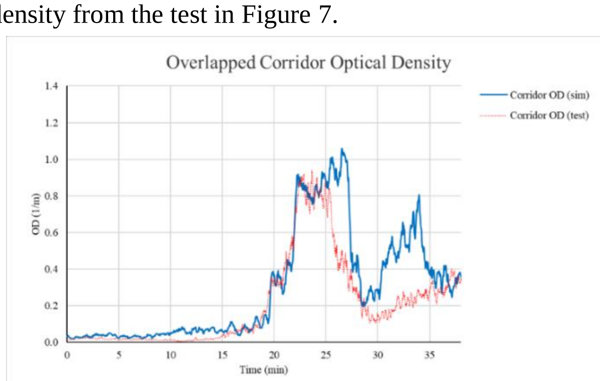

Figure 7. Comparisons of the optical density results from the simulation and the test (at 1.5 m)

The dropped visibility in the room was lower than 3 m around 18 minutes from the beginning of the fire in the test. The visibility in the corridor becomes untenable (3 m) at 21 minutes. The simulated visibility results are also comparable to the test results, as presented in Figure 8.

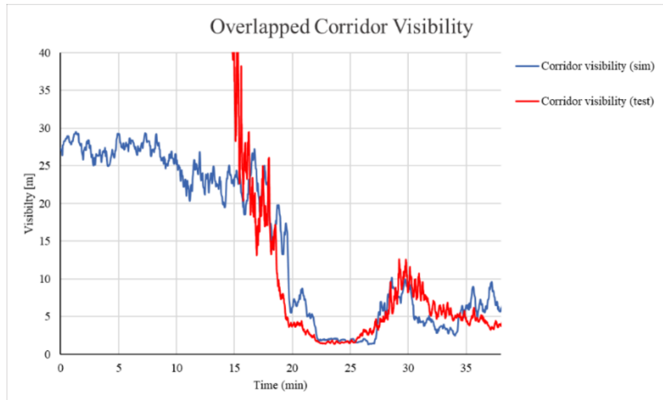

Figure 8. Comparisons of the simulation and test results for visibility in the corridor (at 1.5 m) (Note: FDS uses 30 m as the highest visibility for ambient condition)

Oxygen level estimation

One of the objectives of this simulation study is to estimate the oxygen concentrations in the corridor. While validation is impossible as there is no oxygen data collected from the test, the simulated oxygen levels presented in this section is valid as much as the extent of agreements found for the temperature, smoke optical density and carbon monoxide and carbon dioxide values between the simulated and the test data.

According to Figure 9 and Figure 10, it is observed that the O_2 concentration decreases significantly with the increase of the height, from 0.2 to 0.12 mole fraction. This matter is justified according to the buoyancy-driven nature of the smoke spread and the related density of smoke. Moreover, fire consumes oxygen for its continuity so that the concentration decreases. The lowest oxygen concentration at 26 minutes is related to the maximum HRR measured at the same time.

The results clearly show that the oxygen-level-drop first happens in the room and then in the corridor.

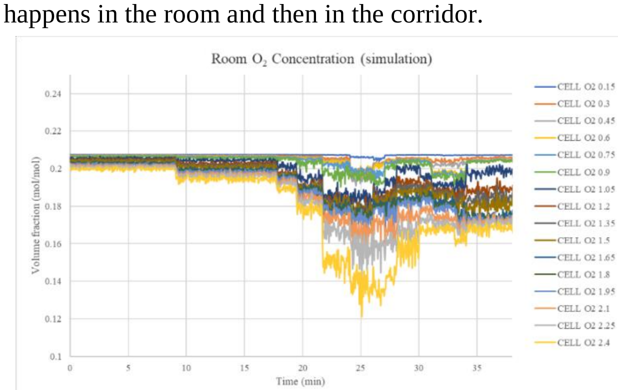

Figure 9. Simulated room O_2 concentration along height

(the numbers in the legend show oxygen sensor height in the room)

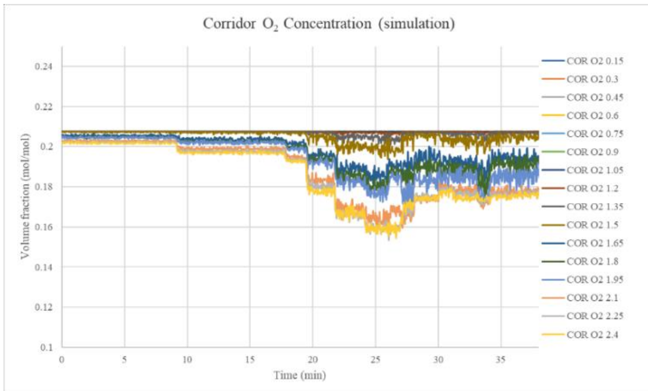

Figure 10. Simulated corridor O_2 concentration along height (the numbers in the legend show oxygen sensor height in the corridor)

Conclusion

A full-scale room fire test is modelled by FDS. The room is furnished with typical household items made of materials including plastics, wood and other composites. The diverse materials were modelled as a fuel package having combined properties, and the fire growth is simulated by prescribing the HRR following the test data. The simplified modelling approach resulted in the simulation results comparable to the test data for temperature, gas concentrations and smoke optical density.

Reaching to acceptable compatibility between the simulation results and the real test measurements mainly for temperature, other required gaseous reactions are also obtained. The obtained information about the fire growth, smoke propagation and the toxic by-products helps to understand the condition inside a room fire.

Acknowledgement

This study was carried out for the Correctional Service Canada and the National Research Council Canada.

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