CFD simulations of compartment fires

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This study provides an overview of the CFD modelling of compartment fires in chemical-engineering practice. We focus on comparing simulation results from specialized solvers SmartFire and FDS with experimental data obtained during large-scale fire experiments. The distribution of temperature and concentration of monitored gases are compared in the case of a non-spreading compartment fire for two model situations: burning of a gas (propane-butane) and combustible liquid (heptane). We study the influence of a combustion model on simulation results and estimate the differences between the used solvers in terms of obtained results.

1. Introduction

Computational fluid dynamics (CFD) modelling of compartment fires is a fast developing part of the fire safety engineering. The present usage and future ambitions of the fire modelling can be divided into two groups. The first area is the design of commercial buildings, where fire simulations can be helpful tools to design ventilation systems for smoke exhausts and to assess data for evacuation analysis (Shi et al., 2009). The second part is fire investigation, namely testing various hypotheses on a location and cause of a fire.

Venart (Venart, 2007) used mathematical modelling for an investigation in the case of the accident at Flixborough in 1974. Markatos et al. (2009) address the potential impacts of fires in large reservoirs in the petrochemical industry. Many authors are focused on large-scale compartments, including atria under fire scenario and/or smoke spread (Qin et al., 2009), and other structures, which can be found in commercial buildings (Sun et al., 2009).

It is possible to perform a fire simulation either by general CFD solver or by codes specialized to compartment fires. General CFD codes are, for example, PHOENICS and ANSYS Fluent. The most common CFD software tools specialized to fire simulations are FDS, SmartFire, SOFIE and JASMINE. Validation of CFD codes with respect to experimental data provides information on their capabilities for reasonably accurate predictions. A lot of authors have been studying the influence of a grid resolution and

sub-models i.e., the turbulence, radiation and combustion models, which may have significant impact on obtained results (Lin et al., 2009; Van Maele and Merci, 2008).

FDS and SmartFire are the most commonly used solvers in the case of fire modeling. In this contribution, we focus on comparing the temperature and concentration fields obtained by these two CFD codes with experimental values in the case of the non-spreading gas and liquid fire.

2. Experiments

A set of large-scale fire experiments were conducted by The Fire Technical Institute, Prague, in a single compartment of size 3.3 x 3.0 m in plan and 2.6 m in height, including a single door opening of size 0.8 x 2.0 m. The compartment was provided with K-type thermocouples to measure temperatures in several positions, 0.32 m from the wall with the door opening. The thermocouples were placed 0.58, 0.94, 1.24, 1.4, 1.54, 1.69 and 2.07 m high. The concentrations of selected gases were measured by the portable analyzer TESTO 350XL. A sampling probe for chemical analysis was placed in the door of 1.92 m high.

Two different fire scenarios representing a non-spreading fire were carried out:

- A gas fire was simulated by two propane-butane burners located in the corner of the room. The total time of propane-butane burning was 1020 s. 2.205 kg of propane-butane were burned by burner No. 1 and 0.945 kg by burner No. 2. The heat of combustion of propane was determined to be 46.03 MJ/kg and butane 45.64 MJ/kg.

- A fire of a spilled liquid was carried out by the combustion of heptane in a tank of circular cross section with 0.34 m in diameter located in the corner of the room. The total time of heptane burning was 1367 s. 4.595 kg of heptane were burned during this experiment. The heat of combustion of heptane was determined to be 44.6 MJ/kg, (Steinleitner, 1988).

3. Simulations

The simulations of propane-butane and heptane combustion were performed using FDS with a graphical interface PyroSim and SmartFire.

First, the geometry of the compartment was defined as it is described in the experimental section. The walls and ceiling were considered as inert objects. The circular cross sections of the propane-butane burners and of the tank with heptane were approximated by square cross sections, because both SmartFire and FDS use structured mesh.

SmartFire generated a computational mesh automatically after defining a geometry. In FDS, a mesh with cell size of 0.1 m was used with a finer mesh in the combustion area with cell size of 0.02 m (propane-butane) and 0.05 m (heptane).

Combustion was represented as an exothermic reaction between fuel and oxygen. Therefore, it is necessary to define a fuel and its mass loss rate (m_f, in kg/s). The average mass loss rate m_f was estimated from the weight of the burnt fuel (m, in kg) and total time of the experiment (t, in s)

$$m_f = \frac{m}{t}.$$

(1)

We considered constant mass loss rates during the simulations. The thermal properties of the fuels were defined by the heat of combustion.

In SmartFire, it is also necessary to define a combustion efficiency which is the ratio between the effective heat of combustion and the complete heat of combustion. In the cases studied here, we assume that combustion efficiency is equal to 1 to provide better comparison between the CFD codes.

In SmartFire, we used default setting of the parameters for prediction of carbon monoxide concentration. In FDS, we used values of CO yields from FDS database for heptane and from literature (Karlsson and Quintiere, 2000) for propane.

4. Results

We compared the experimentally obtained temperatures and temperatures simulated by FDS and SmartFire for both fire scenarios described in experimental section. Figs. 1 and 2 show the dependence of the temperature on the vertical coordinate z of the thermocouples for the selected simulation time. We chose $t=400$ s because measured temperatures reached maximum or almost constant values at this time.
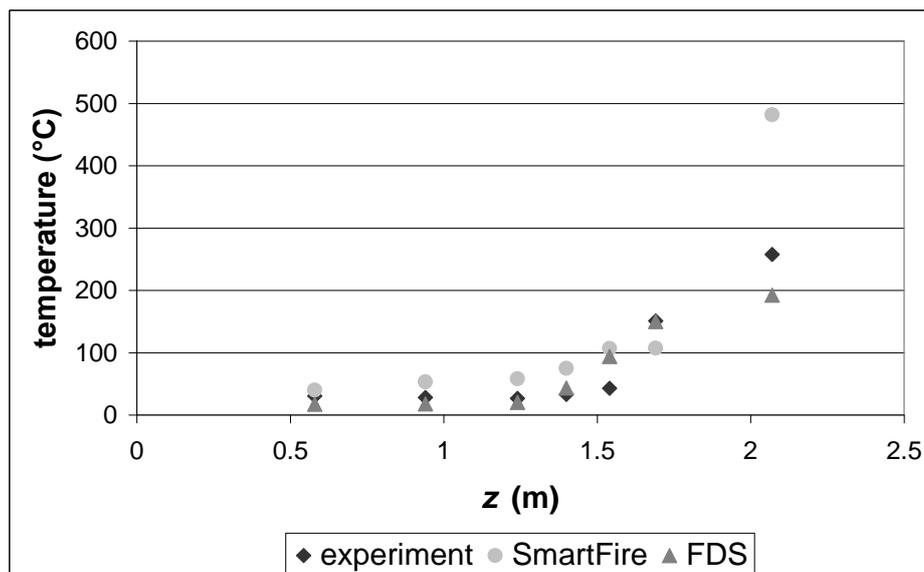
Fig. 1: Propane-butane, thermocouple tree at time t=400 s (temperature dependence on the vertical coordinate)

Both FDS and SmartFire reached reasonable qualitative agreement with experimental data in the vertical temperature distribution. Assessing the computed temperatures, it is necessary to bear in mind that we assume constant mass loss rates during the simulation, but the situation was different during the fire experiment. This difference is significant

especially in the case of propane-butane, when the bottles were freezing in the second part of the experiment. On the other hand, we decided to set up constant mass loss rates because this choice enables us to compare the results from two different CFD codes. Differences between measured and computed temperatures appear in the upper layer from a height of approximately 1.5 m, where SmartFire predicted higher temperatures. The main reason for this overprediction is probably the value of combustion efficiency, which was set to 1 in SmartFire.
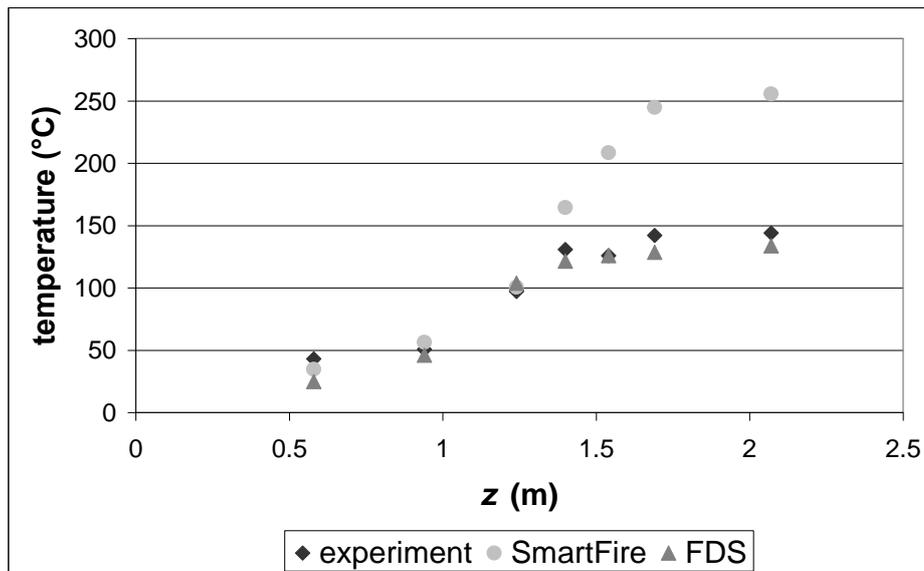
Fig. 2: Heptane, thermocouple tree at time t=400 s (temperature dependence on the vertical coordinate)

Figs. 3 and 4 show the comparison of experimental and computed concentrations of carbon monoxide, which are generally in good agreement. Concentration values obtained from SmartFire are in better agreement with measured data in a sense that they provide more realistic approximation of maximum measured concentration values. However, results from FDS depend on the CO yield, which has to be found in literature if the fuel cannot be found in the FDS database.
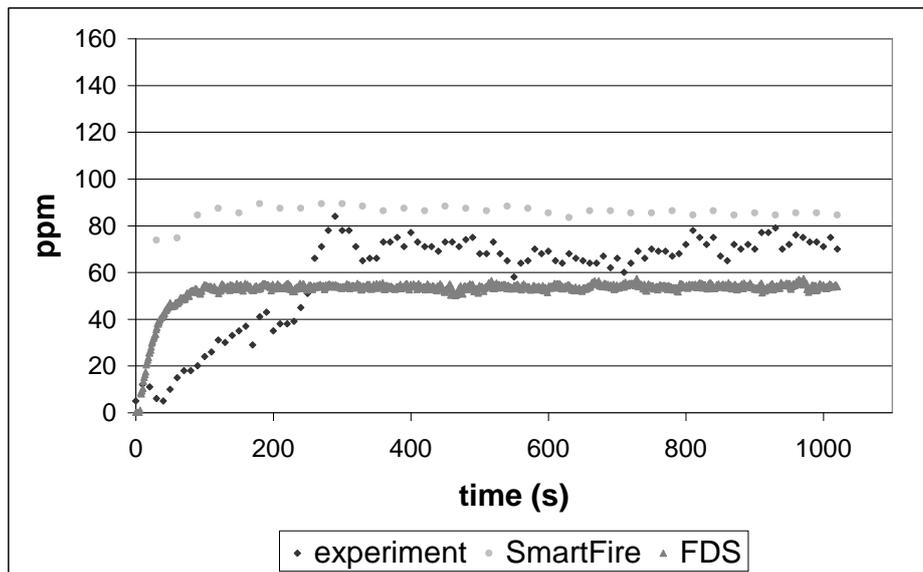
Fig. 3: Propane-butane, the content of CO
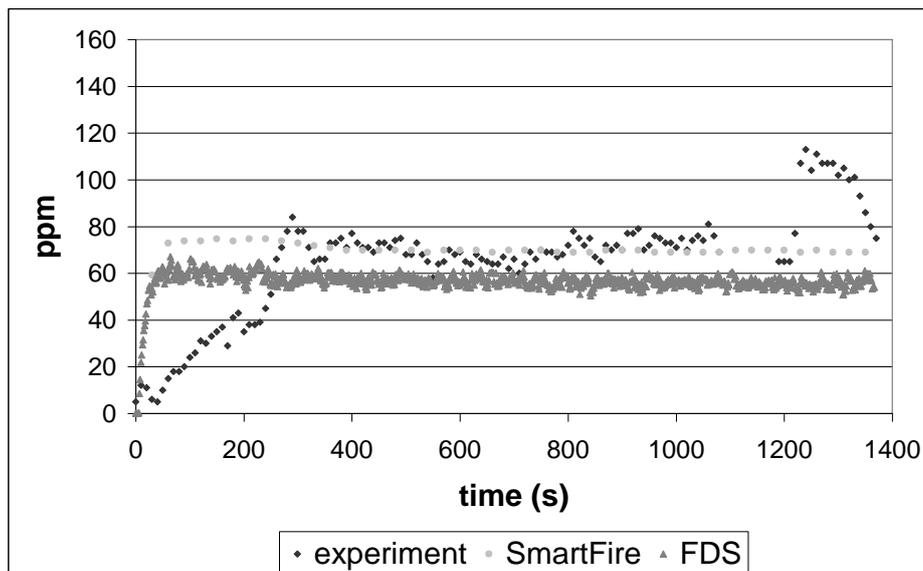
Fig 4: Heptane, the content of CO

5. Conclusion

Both SmartFire and FDS showed reasonable qualitative agreement with the experimental data in overall trends of the vertical temperature distribution, although SmartFire predicted higher temperature in the upper positions. The main issue in

SmartFire simulation is how to estimate the appropriate value of combustion efficiency, which has to be set by a user. If the combustion efficiency was considered equal to 1, the obtained temperatures could be used as the estimation of maximum temperatures. The prediction of carbon monoxide concentration plays an important role in fire safety engineering and assessing the risks for people during compartment fires. Both FDS and SmartFire showed good agreement between measured and calculated values if a variance of measured data is taken into account.

Acknowledgements

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