Parametric analysis of input data on the CFD fire simulation

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Abstract. During the last decades the CFD computer modelling of fire has increased significantly. The CFD fire simulator has been purposely developed and optimized for fire protection; nowadays they have a high reliability and ample perspectives of further development. The main drawbacks of CFD fire simulators are mainly due to the complexity of its setting. They are not user friendly and require a good competence on fires and fair competence in computing. To be able to estimate how the simulation outcome is influenced by model assumptions and simplifications, the user has to evaluate the dominating physical processes and involved empirical parameter that has an essential influence on the specific fire scenario. In this paper the Thermo-gravimetric (TGA) and Cone-calorimetric tests will be used to show in which ranges the input parameters such as reference temperature (i.e. the temperature of the released mass rate peak), thermal conductivity, pyrolysis range, specific heat, in a fire simulation with the "Fire Dynamics Simulator”, will vary based on the measurement errors, measurement uncertainty, or misinterpretation of the user. Fire simulation validated on experimental tests are used to evaluate the impact of those variant input data on the simulation. A parametric analysis has been carried out and the results are evaluated and discussed.

1. Introduction
Over the years, thanks to the progress of Computational technique of Fluid Dynamics (CFD), the fire protection has been continuously evolving, shifting from a ‘prescriptive-based’ to a ‘performance-based’ design. The method based on prescriptive procedures even if simpler to use, is not free of design limitations. Instead, the performance-based design allows more flexibility than prescriptive regulations in order to satisfy the fire protection needs of modern buildings. Nevertheless, there are essential prerequisites to computer simulations to achieve representative realistic fire conditions of high quality and reliability i.e. the evaluation of the dominating physical processes and the involved empirical parameters that have an essential influence on the specific fire scenario, such as chemical and thermal material properties, ignition temperature, reaction rate, pyrolysis range, heating rate, etc. The latter aspect is to evaluate them accurately and the subsequently transfer them to the CFD code adequately. This task is crucial to obtain representative realistic fire evolution. In fact, very often the ‘quality’ of CFD simulations depends more on this task than on the capabilities of the CFD code itself[1-3]. In fact, FDS is used to study the influence of different parameters on the results of the simulation [4-6] in order to have useful indication, sometimes on specific aspects as the gasification performance [7], the auto-ignition [8], the carbon monoxide concentration distribution [9]; other times to mark the influence of the CFD models and settings on the ability of FDS to correctly simulate the real processes [8,10,11].
Usually, the input parameters are validated by modeling the laboratory scale experiments, like the cone calorimeter or thermogravimetric analysis. Afterwards the input parameters are transferred into the real scale scenario or user specific fire scenario. Different authors show the challenge of modeling [12-14] and reproducing a real experiment with FDS [15]. The approach to implement data from laboratory scale experiments requires the knowledge about the fire behavior of the used materials and about the transferability of the experiments to the considered fire scenario.

To be able to estimate how the simulation outcome is influenced by model assumptions and simplifications, the user has to evaluate the dominating physical processes and involved empirical parameters that have an essential influence on the specific fire scenario.

In this work the Thermo-gravimetric (TGA) and Cone-calorimetric tests will be used to show in which ranges the input parameters such as reference temperature (i.e. the temperature of the released mass rate peak), reaction rate, pyrolysis range, heating rate, in a fire simulation with the "Fire Dynamics Simulator", will vary based on the measurement errors, measurement uncertainty, or misinterpretation of the user. Fire simulation validated on experimental tests has been used to evaluate the impact of those variant input data on the simulation. A parametric analysis is carried out and the results are evaluated and discussed.

2. Experimental tests

To validate fire spreading with the pyrolysis model of FDS, thermogravimetric and cone-calorimetric analyses on chipboard were conducted.

2.1. TGA analysis

TGA measurements provided the pyrolysis rates and mechanisms and char yield in nitrogen from 30 to 900 °C; the latter corresponds to a heating rate of a material in the cone calorimeter and in real fires for some cases.

Thermogravimetric analysis was carried out on 4.5 mg of low-cost board sample shavings using a Perkin Elmer Pyres 1 TGA system. This analysis was useful in determining the amount of sample mass lost during heating and in assessing the percentage of glass fiber in the tested sample. The test was performed in the presence of an air flow of 150 ml/min, starting from 30 °C up to 900 °C with a heating ramp of 5 K/min. The test is reported in the figure 1, where two mass release peaks at two different temperatures at approximately 80 °C and 350 °C are shown.

![Figure 1. Thermogravimetric analysis](image-url)
In particular, the pyrolysis interval value represents the range in which the specimen burns. As shown in the figure 2, the weight loss starts at 220 °C and ends at 320 °C. The mass loss, before the 220 °C, is due to the evaporation of humidity (peak at 100 °C) and other substances. The pyrolysis interval is one of most important parameters to set FDS pyrolysis and was reported in table 2.

2.2. Cone Calorimeter analysis

Most of the key flammability properties, as thermal properties of the original material (conductivity, density, specific heat), ignition temperature, heat of pyrolysis or gasification of the solid, thermal properties of char, extinction properties etc., to assess fire spread and fire growth of chipboard material can be obtained by experiments conducted in a cone calorimeter in according to standard. The test specimens are 88.4 cm² and 2 cm thick, while their mass is m=0.130 kg. The Cone Calorimeter test was repeated 3 times with a heat flux of 50 kW/m². The results of the test are shown in the table 1, with the corresponding measurement extended uncertainties, and in the figure 2.

| Table 1. Cone Calorimeter test results |
|----------------------------------------|
| Test end time | First test | Second test | Third test | Mean value | Uncertainty |
| Ignition time | s  | 1920 | 1920 | 1920 | 1920 | 37.41 |
| Average values for the first 180 s after ignition | kW/m² | 136.2 | 137.9 | 133.5 | 135.9 | 3.74 |
| Average values for the first 300 s after ignition | kW/m² | 117.7 | 124.7 | 117.1 | 119.8 | 7.12 |
| Heat released for unit of surface (HRUS) | MJ/m² | 143 | 159.8 | 148.1 | 150.3 | 14.52 |
| Heat release rate peak | kW/m² | 294.9 (88 s) | 247.6 (58 s) | 276.2 (66 s) | 272.9 (70 s) | 40.16 |
| Average Heat Release Rate | kW/m² | 93.9 | 102.9 | 95.1 | 97.2 | 8.24 |
| Mass remaining after the test | g | 34.6 | 34.4 | 35.6 | 34.9 | 1.08 |
| Sample mass loss | g/sm² | 8.38 | 8.60 | 8.54 | 8.51 | 0.19 |

The results of the test at the Cone Calorimeter show that during the whole test the spacerman does not flame out until the end of the test (figure 2) and the time to ignition is on average 48 s with a heat release rate peak of about 272 kW/m² on average at 70 s (see table 1).

The measurement reported in table 1 was used to calculate the setting parameters for FDS reported in the table 2. From the Heat Release for unit of surface (HRUS) by specimen during Cone Calorimeter tests, it was been possible to evaluate the average Lower Heating Value (LHV) of the material, as:

Total Heat Release=HRUS A= 150.388.4 10⁻⁴=1328.65 kJ

where A is the specimen surface

LHV=THR/m= 1328.65/0.130=13971 kJ / kg

with 0.095 kg the mass of the specimen and where THR is the Total Heat Released

The relative vapor fuel vapor and char were calculated from the residual mass (RM) after the combustion process:

Char=Rm/m=0.035/0.130=0.3

Vapor Fuel = Bm/m=0.095/0.130=0.7

where Bm is the mass burned and Rm the residual mass.
3. Numerical simulation

The Computational Fluid Dynamics technique is applied in order to solve a set of non-linear partial differential equations derived from basic laws of nature. They solve numerically the equation of continuity, the conservation of momentum and energy as a system of partial differential equations, relying on few sub models to take into consideration particular aspects. In the case of fire simulation, a combustion model is used to simulate the evolution of combustion, a turbulence model has to be included for the prediction of the buoyancy driven turbulent flow as well as a radiation model is needed to simulate the thermal radiation. Moreover, reaction kinetics, radiation transport and pyrolysis have to be considered [16]. The CFD code allows to simulate the entire development of fire [17]. For momentum conservation, FDS solves the Navier–Stokes equations using large eddy simulation (LES) to account for sub grid turbulence, and for the combustion reactions, it uses the mixture fraction model. Heat transfer to solid surfaces and convection within the fluid are taken into account. Moreover, the radiative transport equation for an absorbing/emitting and scattering medium is also solved.

Charring materials produce a barrier between the pyrolysis zone and the exposed surface. The process of decomposition is reduced depending on the properties of the material, the char and heat source. The user of FDS should implement the residue of the charring and needs to be aware, that breaking the char layer during the decomposition cannot be modeled; it is impossible with FDS because the user needs to characterize liquid properties (e.g. boiling temperature) for the sample, although the initial state is solid. Considering additionally layers for modeling the producing and breaking of char layers helps to take into account the effects of the combustion.

3.1. FDS simulation for the determination of chipboard combustion parameters

Thanks to the results of the tests to the cone calorimeter the thermal quantities and the pyrolysis parameters necessary for the thermo-fluid dynamics simulation have been obtained. In particular, the parameters obtained from the pyrolysis tests have been set directly as shown in table 2, while for the parameters of thermal conductivity and specific heat, various simulations have been carried out by varying these parameters in the intervals shown in table 3. Figure 3 shows the simulation model in FDS that reproduces the test at the cone calorimeter in order to evaluate the correctness of the combustion parameters and the properties of the material to be set in the code for the simulations of the fire scenarios. The boundary conditions that reproduce the test at the cone calorimeter were imposed; in particular, a thermal flow of 50 kW/m² was imposed on the chipboard surface. Comparison between the CFD and cone calorimeter test results is shown in the figure 4. The validated FDS simulation, on experimental test results, has been used to evaluate the impact of those variant input data on the simulation.
**Table 2.** Material properties of chipboard obtained from Cone Calorimetric and Thermogravimetric Tests

| Property                              | Value         |
|---------------------------------------|---------------|
| Temperature of maximum heat release rate | 430 °C        |
| Heating rate                          | 5 K/min       |
| Pyrolysis interval                    | 100 °C        |
| Heat of reaction                      | 800 kJ/kg     |
| LHV                                   | 13895 kJ/kg   |
| Density                               | 720 kg/m$^3$  |
| Fuel vapor                            | 0.7 -         |
| Residual                              | 0.3 -         |

**Table 3.** Material properties of chipboard obtained from literature

| Property          | Residual | Chipboard |
|-------------------|----------|-----------|
| Density           | kg/m$^3$ | 36        | 720      |
| Specific heat     | kJ/kgK   | 0.3÷0.50  | 2÷4      |
| Thermal conductivity | W/mK   | 0.1÷0.2  | 0.1÷0.2  |
| Emissivity        | -        | 0.0       | 0.9      |
| Absorption thickness | 1/m    | 50000     | 50000    |

**Figure 3.** Cone Calorimeter test: FDS simulation model
3.2. FDS results and parametric analysis

The figures from 5 to 11 show the parametric analysis carried out for different thermal and combustion parameters.

In particular, the figure 5 shows the influence of thermal conductivity on HRR-time curve, for fixed k=1.9 W/mK, for variation of the thermal conductivity values: -20%, -10%, -5%, +5%, +10%, +20% with respect of its imposed value. It is noted that a -20% error on the correct value (k=1.5 W/mK) of the thermal conductivity, involves a decrease in the time of about 15 s with a first heat release rate peak of about 235 kW/m² (see figure 6). Vice versa, an error of +20% (k=2.3 W/mK) involves a delay of about 12 s of the first heat release rate peak, with an HRR value equal to about 229 kW/m². Moreover, in figure 5, for a +20% error, the time of maximum mass loss, compared to the base case, is reduced by about 100 s, while for a -20% error, the time increases by about 120 s. The value of the HRR, at the second peak, decreases as the thermal conductivity decreases from 157 kW/m² to about 110 kW/m².

With regards to the influence of heat specific capacity on HRR-time curve, as shown in the figures 7 and 8, considering the same errors used for the conductivity, it is possible to note that, for fixed cp=2.8 kJ/kgK, an error equal to -20% (cp=2.2 kJ/kgk) on the correct value of the heat specific capacity, involves a decrease in the time of 15 s at which the first peak of combustion is obtained with a value about 315 kW/m². An error equal to +20% (cp=3.4 kJ/kgK) involves a delay of about 64 s of the first heat release rate peak with a value about 170 kW/m². Moreover, in figure 7, for a -20% error, the time of maximum mass loss, compared to the base case, is reduced at about 285 s, while for a +20% error, the time increases by about 300 s. The value of the HRR, at the second peak, decreases as heat specific capacity increases from 195 kW/m² to about 100 kW/m².

With regards to the influence of reference temperature on HRR-time curve, as shown in the figures 9 and 10, considering the same errors, it is possible to note that, for fixed T_ref=380 °C, an error equal to -20% (T_ref=304 °C) on the correct value of the reference temperature, involves a decrease in the time (35 s) at which the first peak of combustion is obtained with a value of HRR of about 420 kW/m². An error equal to +20% (T_ref=465 °C) involves a delay of about 70 s of the first heat release rate peak with a value of about 180 kW/m². Moreover, in figure 9, for a -20% error, the time of maximum mass loss, compared to the base case, is reduced by about 540 s, while for a +20% error, the time increases about 500 s. The value of the HRR, at the second peak, decreases as reference temperature increases from 308 kW/m² to about 55 kW/m².

![Figure 4. Comparison between the CFD and cone calorimeter test results](image-url)
With regards to the influence of pyrolysis range on HRR-time curve, as shown in the figures 11 and 12, considering the same errors, it is possible to note that, for fixed pyrolysis range =120 °C, an error equal to -20% (pyrolysis range =96 °C) on the correct value of the reference temperature, involves a decrease in the time (10 s) at which the first peak of combustion is obtained with a value about 407 kW/m² and an error equal to +20% (pyrolysis range =144 °C) involves a delay of about 60 s of the first heat release rate peak with a value about 123 kW/m². Moreover, in figure 11, the influence due to the pyrolysis range variation is negligible for both time and HRR pick values.
4. CONCLUSION
The main drawbacks of CFD fire simulators are due to the not user friendly and require a good competence on fires and fair competence in computing. To estimate accurately the influence of the model assumptions and simplifications on the simulation outcome, it should know the dominating physical processes and involved empirical parameters that have an essential influence on the specific fire scenario.

In the present paper, a parametric analysis was carried out to evaluate the influence of the main thermal and combustion parameters on goodness of CFD simulation. The results showed that the variation of ±20% of these parameters, such as thermal conductivity, heat capacity, reference temperature and pyrolysis range, with respect to their nominal values, implies, in some cases, an important variation in terms of HRR peak and combustion time. For example, in the case of reference temperature, its variation of +20% with respect to the fixed base value, implies an advance of the combustion peak of about 8 min with a reduction of combustion time of about 10 min. This variation could be significantly important for fire risk analysis. Furthermore, the value of the HRR, at the second peak, decreases as reference temperature increases from 308 kW/m² to about 55 kW/m². Therefore, an accurate parametric a-priori analysis is necessary in order to obtain reliable results for a subsequent fire risk analysis. The sensitivity
of the error in the setting of some parameters is very high and would lead to completely incorrect evaluations.

Figure 9. Influence of reference temperature on HRR-time curve, fixed $T_{\text{ref}}=380$ °C

Figure 10. Particular of influence of reference temperature on the first peak of HRR-time curve

Figure 11. Influence of pyrolysis range on HRR-time curve, fixed pyrolysis range equal to 120°C
Figure 12. Particular of the influence of pyrolysis range on the first peak of HRR-time curve

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