Small scale simulation of artificial smoke optical properties

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Abstract. The use of numerical simulations in Fire Safety Engineering provides faster and more affordable ways of research and development, with the drawback that their use is often conditioned by available expertise and thorough validation. In this paper, the results of two small scale numerical simulations of artificially generated smoke are being validated by comparison of the smoke’s light extinction coefficient values and those of the visibility levels in the testing enclosures with the results obtained through experimental testing. The influence of grid size on simulation accuracy and computational time is evaluated by presenting the small gain in accuracy and the important increase in computational time for different sized meshes, showing that at least in numerical simulations dealing with artificial smoke, a larger grid size can produce fairly accurate results. A comparative evaluation of the effect that the positioning of the measuring devices inside the testing enclosure has on the results is also performed, both for the experimental setup and the numerical simulations.

1. Introduction

One of the lesser evident, but of paramount importance aspects that need to be considered when designing or improving a building has to be the safety it can provide in case of an extreme event like a fire. The safety of the building occupants and first responders in case of such an event has to be insured through the use of systems, structures and building materials specifically designed to react in a certain way in case of a fire, but not affect the design, comfort and use of the building in its normal state of affairs.

The use of building materials that produce a limited amount of smoke when exposed to high temperatures or flames is one way that can greatly impact the speed with which occupants can find an exit and travel to safety in case of a fire [1]. Building materials are evaluated as to their individual smoke emission and smoke optical properties with the use of a standardized test [2] that requires a significant amount of test samples. Innovative building materials in various stages of research and development may not be available in an appropriate amount for standard testing, therefore some kind of small-scale evaluation of their smoke emission properties, even if a comparative one, is of great importance.

Repetitive testing in the field of Fire Safety Engineering can be quite time and resources consuming, given the destructive nature of fire. One of the procedures that facilitate a greater repeatability in this domain is the use of numerical simulations, but the use of simulation software needs to be accompanied by the validation of the simulated phenomena through the use of experimental testing. Before simulating small scale smoke emission from building materials, the accuracy of the simulation software with regard to small scale smoke optical properties needs to be assessed.
This paper presents an accuracy assertion for small scale numerical simulations of artificial smoke optical properties. Two small scale experiments were reproduced virtually using a Fire Dynamics Simulator user interface named PyroSim. Based on the experimentally determined values of the light extinction coefficient of the smoke, the soot mass fraction that was injected in the simulated space was calculated and used as an input parameter.

2. Methodology

Both of the small-scale experiments were carried out by using an electrical resistance to heat up a certain amount of glycol-based smoke fluid in order to produce artificial smoke inside an acrylic enclosure of known dimensions. The enclosure was partially open, so the experiments were carried out at normal pressure. Timed, repetitive uses of the artificial smoke generating device were employed with the purpose of creating an incrementally smoke saturated environment. The light extinction coefficient of the smoke and loss of visibility were calculated by measuring the loss of intensity of a laser light source that travelled through the smoke for a certain known distance. Each of the experiments were repeated for each of the three measuring distances used to calculate the optical properties of smoke, with a total of six experiments. The light intensity measuring device was a UNI-T light meter, model UT383 BT, with a 0 to 9,999 lux measuring domain and a ±4% precision, which recorded the light intensity every two seconds.

In each of the simulations, the dimensions of the experimental enclosures were reproduced and devices that were predefined within the software library were placed at the appropriate distances in the simulated environment in order to record the path obscuration and smoke extinction coefficient of the simulated smoke. The smoke was represented by soot introduced in the simulation in timed, repetitive bursts that mimic the activation of the experimental smoke generating device. For each injection of soot, a new surface was defined, having a different soot to air mass fraction, calculated based on the light extinction coefficient (K) recorded in the experimental testing.

The formula used for calculating the soot density (S) is adapted from reference [3] and presented in equation (1).

\[ S = \frac{K}{K_m} \]  

For both of the experiments, K was calculated by using equation (2), adapted from the same reference cited above.

\[ \frac{I}{I_0} = e^{-K \cdot L} \]  

In equation (2), I represents the intensity of monochromatic light passing a distance L through the smoke, and \( I_0 \) is the intensity of monochromatic light at distance L from the source when there is no smoke. \( K_m \) is the mass specific extinction coefficient, having a predefined default value in the numerical simulation program of 8,700 m²/kg, corresponding to flame generated smoke [4]. In these specific simulations, the value for \( K_m \) used for calculating the soot density was 7,600 m²/kg, because the smoke used in the experiments was artificial, and not flame generated, with a lower expected \( K_m \) [5].

The soot mass fraction \( (Y_S) \) was calculated by dividing the soot density \( (S) \) to the density of air \( (\rho_{air} \approx 1.196 \text{ kg/m}^3) \), as per equation (3), adapted from reference [6].

\[ Y_S = \frac{S}{\rho_{air}} \]  

By combining equations (1) and (3), the soot mass fraction that was used in the simulations was determined taking into account the maximum light extinction coefficient recorded for each injection of the smoke for its calculation, according to equation (4).

\[ Y_S = \frac{S}{\rho_{air}} = \frac{K}{(K_m \cdot \rho_{air})} \]
The maximum value for the light extinction coefficient was used because each activation of the smoke generating device was followed by a timed pause in order for the atmosphere to settle. The artificial smoke loses its persistence in time, being diluted in the air, thus offsetting the average value for the light extinction coefficient calculated for that respective time interval.

The volume flow for the smoke generating device was calculated based on the specifications of a full-size smoke machine that uses the same kind of smoke fluid. The specifications stated that the full-size machine produced a volume flow of 128 m$^3$/min by using 72 ml/min of smoke fluid. Taking into account the approximate duration of one activation of the small scale smoke generating device and the amount of smoke fluid used during this time, a 0.0065 ml/s smoke fluid consumption was calculated. Assuming that the smoke fluid produces a constant amount of smoke per unit volume, the volume flow for the small scale smoke generating device would be about 0.011 m$^3$/s. This value was used in all of the simulations as the specified volume flow for the soot injecting surface.

For the first experiment, an acrylic enclosure having a length of 1 meter, width of 0.45 meters and height of 0.3 meters was filled with incremental amounts of smoke produced by 6.5 milliliters of smoke fluid. The light intensity measuring device was placed at 0.5 m, 0.75 m and 1 m respectively, and the experiment was repeated for each of the measuring distances. The experimental setup can be seen in figure 1.

![Figure 1. Experimental setup](image)

For the simulation of this experiment, the dimensions of the experimental enclosure were reproduced in the computational space, and the measuring devices for the smoke extinction coefficient and path obscuration were positioned at the appropriate distances, in order to record the smoke’s optical properties of interest. The path obscuration is recorded in percentage form by the simulation program, and the visibility is calculated as a difference between the value of 1 (one) and the path obscuration, as these parameters are reciprocal [7], in order to plot comparative charts between the simulation and experimental values. The virtual model for this first experimental setup can be viewed in figure 2.

In all of the simulations, the boundaries for the simulated testing space were defined as being inert, meaning that no mass transfer can occur through them and they maintain a constant ambient temperature of 20°C, and a small portion of space surrounding the soot injecting surfaces was defined as being open, meaning mass and heat can leave the computational space through them, in order to replicate the experimental conditions.
The 7th Conference of the Sustainable Solutions for Energy and Environment
IOP Conf. Series: Earth and Environmental Science 664 (2021) 012066
doi:10.1088/1755-1315/664/1/012066

Figure 2. Virtual model

The green squares in the image represent the surfaces that inject soot at the time of activation of the artificial smoke generating device, and the lines are the beam devices that record the path obscuration for the measuring distances used in the experimental testing.

For the 1:2 scale experiment, the main characteristics of the first experimental setup were reduced in half. The testing enclosure had a length of 0.5 m, a width of 0.225 m, and a height of 0.15 m, totaling an approximate volume equal to 1/8 the one of the first experiment testing enclosure. The distances from the light source to where the lux meter was placed were 0.25 m, 0.375 m and 0.5 m respectively, also representing of the first experiment distances. The amount of smoke fluid used was 3.25 ml, representing half the amount from the first experiment. The virtual model was adapted to the characteristics of the 1:2 experiment, with the dimensions being recalibrated, the measuring distances being reset and the soot mass fraction for the soot injecting surfaces were defined based on the values recorded in the 1:2 scale experiment. The experimental setup for this 1:2 scale experiment is presented in figure 3.

Figure 3. 1:2 scale experimental setup
The first run of the simulation for the 1:2 scale experiment was done using a mesh consisting of 512 cube shaped cells, having the dimensions of their sides of about 3 centimeters. The computational time for this run was about 24 minutes. The virtual model for the second experimental setup is presented in figure 4.

![Figure 4. 1:2 scale virtual model](image1)

For the second run of the simulation, the mesh was refined by a factor of two, resulting in about 5,000 cubic cells with the dimension of the side of about 1.5 cm. The computing time necessary for this simulation was about 96 minutes, and the refined mesh virtual model is presented in figure 5.

![Figure 5. 1:2 scale virtual model refined mesh](image2)

To evaluate the simulation program’s ability to accurately represent the optical properties of smoke even at small scales, after the successful simulation of the first experiment, the experimental setup was reduced to the 1:2 scale, and the virtual model was adapted to the new setup. The scale reduction consisted in linearly reducing the dimensions of the enclosure in order for the total volume in the 1:2 scale experiment to be 1/8 the first (as it would be if reducing each dimension in half), reducing the measuring distances in half and using half the amount of smoke fluid to produce the artificial smoke.
3. Results and discussion

The results of each of the simulations were compared with those obtained through experimental testing. Both the light extinction coefficient of the smoke and the visibility reduction in the testing compartment were analyzed and the average difference was calculated by identifying the average absolute difference between each of the values and then calculating it as a percent of the maximum value in the case of the light extinction coefficient of the smoke. In the case of visibility reduction, the mean average difference was used as a precision benchmark. The results presented in this paper pertain to the shortest measuring distances in both simulations, and experiments respectively, the other measuring distances producing similar results.

For the first simulation, the values of the light extinction coefficient present an average difference of about 8.93% for a maximum value of 2.58 m\(^{-1}\). The comparative chart for this optical property of the smoke is presented in figure 6.

![Figure 6. First simulation extinction coefficient comparison](image)

The average difference for the values recorded in the simulation and those recorded in the first experiment for visibility is about 5.46%. The comparative chart for the visibility values as measured at the shortest distance is presented in figure 7. With an accuracy between 5 and 10% for the representation of the optical properties of smoke, the simulation of the first experiment offers an acceptable level of precision.

![Figure 7. First simulation visibility comparison](image)
The values for the light extinction coefficient recorded for the intermediate measuring distance were used as a benchmark for determining how the positioning of the measuring devices affect the readings. In the first experiment, the values for the light intensity measured for the shortest distance differed from the ones in the intermediate distance by about 15.28%, while the ones measured at the longest distance from the light source differed by about 7.59%, for a maximum light extinction coefficient of 2.16 m⁻¹.

Some errors in measurement may be due to the fact that for each measuring distance, the experimental test was repeated. The comparative chart for the experimental values (noted with Ex) of the light extinction coefficient in the first experiment are presented in figure 8.

![Figure 8. First experiment measuring distances comparison](image)

The fact that within the simulation the values for the three measuring distances could be obtained simultaneously, without the need to repeat the simulations for each of the measuring distances, has led to a better accuracy between measuring distances, but there still was a 4.85% difference between the values for the light extinction coefficient measured from the shortest distance and the intermediate one, and 2.35% for the longest measuring distance, for a maximum light extinction coefficient of 2.58 m⁻¹. The comparative chart for the simulated values (noted with S) for the smoke extinction coefficient can be seen in figure 9.

![Figure 9. First simulation measuring comparison](image)
The values recorded for the light extinction coefficient in the simulation of the second experiment present a 6.72% difference from the ones recorded during the experiment, for a maximum light extinction coefficient of 4.27 m$^{-1}$. The comparative chart for this second simulation is presented in figure 10.

![Figure 10. Second simulation extinction coefficient comparison](image1.png)

For the visibility comparison between the second experiment and its simulation, the average recorded difference was of about 7.44%, the comparative chart being presented in figure 11.

![Figure 11. Second simulation visibility comparison](image2.png)

The difference in recorded values resulted from the positioning of the measuring device during the second experiment is about 9.65% for the shortest measuring distance and 11.68% for the longest,
relative to the intermediate one, for a maximum light extinction coefficient of 4.08 m$^{-1}$. The comparative chart for the measuring distances in the second experiment can be viewed in figure 12.

![Figure 12. Second experiment measuring comparison](image)

The smaller differences may be due to the fact that the distance that each of the measuring points was offset from the other by half the distance used in the first experiment, as the scale would dictate. In the case of the second simulation, the differences were about 4.85% for the shortest measuring distance and 2.35% for the longest, relative to the intermediate one, for a maximum light extinction coefficient of 2.58 m$^{-1}$.

The fact that the second simulation has dealt with such short distances, and that the simulation program was designed to reproduce full scale fire phenomena, the Large Eddy Simulation has omitted the calculation of the small turbulence effects, thus resulting in a smoother chart, with plateaus instead of the small oscillations visible in the experimental data. The increase of the number of cells in the second run of the second simulation has only resulted in a precision of 6.52% (0.2 % improvement) for the light extinction coefficient and 6.22% (1.22% improvement) for the visibility. The comparative chart for the light extinction coefficient for the two runs is shown in figure 13.

![Figure 13. Second simulation grid size influence](image)
4. Conclusions
By comparing the values of artificially generated smoke’s optical properties obtained in testing compartments to the results of Computational Fluid Dynamics simulations, the fidelity of the small-scale numerical simulation of the smoke’s optical properties could be evaluated. Numerical simulations can provide an acceptable level of accuracy in representing the optical properties of smoke, with differences in the 5 to 10% interval between the values obtained through simulation and those measured experimentally. The advantages of repeatability and relatively low cost of the numerical simulation approach compared with experimental testing can provide a faster and more targeted development in the Fire Safety Engineering field, although in order to ensure proper validation of the simulations, a certain degree of expertise and familiarity with the software is required.

The positioning of the measuring device had greater influence on the values of the smoke extinction coefficient in the experiments than in the simulations. This is due to the fact that for each different measuring distance, the experiments had to be repeated, because only one lux meter was available. The differences between the values calculated based on the measurements recorded at different distances from the light source varied between 8 and 16%. In the case of the simulations, the values for the smoke extinction coefficient were simultaneously recorded in the same simulation, by using virtual devices available in the software library, thus providing differences between 2 and 5%.

Regarding the computational cell size influence on the simulation’s precision, the small gain in accuracy obtained by using a more refined mesh had a great influence on the time needed to run the simulation in similar conditions. By using 10 times the number of cells distributed in the same computational domain, the time needed to run the refined mesh simulation has been about four times greater than that of the coarser mesh simulation (from 24 to 96 minutes) and the increase in precision was almost negligible (0.2% in the case of the smoke extinction coefficient and 1.22% in the case of visibility levels in the testing enclosure).

Future research can pursue the validation of small and natural scale simulations of the optical properties of smoke generated through the burning of different types of building materials. Furthermore, the adequacy of scale reduction in numerical simulations dealing with the optical properties of smoke can be evaluated by comparison with the experimental scale reduction, to see if computational fluid dynamics simulations can provide meaningful insight on small scale smoke emission.

Acknowledgements
This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI - UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0350/38PCCDI within PNCDI III.

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