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The determination and numerical simulation of the optical properties of smoke generated in fires

DOCTORATE THESIS SUMMARY

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1. Introduction

The technological advancement, the sustained development rhythm of the new construction buildings and the need for ensuring the fire safety engineering of modern buildings, and improving this performance criterion for old building leads to the use of new building materials, that are obtained through up until now inaccessible means, like the modification of the constituent ratio of building materials used in modern buildings. One of the main elements that ca influence the development of a fire, the evacuation process of the users of a building in case of a fire, as well as the way in which professional emergency situations services intervene in case of a fire is the quantity of smoke that is produced during a fire, as well as its properties. From the viewpoint of heat transfer from the fire bed to other parts of the building, the toxic, irritating or asphyxiating effect, as well as its capacity of obscuring the evacuation routes and the signs that point towards them, the smoke that is generated during fires is an element that leads to deaths and serious property loss. Because of this, the reduction of smoke emission of the building materials that are used in the building manufacturing is an important area that can boost the fire safety of buildings.

2. General conclusions

This doctorate thesis has presented the importance of numerical simulation use in the fire safety engineering area in order to ensure an evidence based framework for the adoption of the best solutions in the choice of building materials that have a low smoke emission in case of a fire. In the first chapter the current process used to label building materials based on their fire reaction class was presented, along with the standard testing methods and the shortcomings of this process, mainly referring to the large quantities of materials that are needed for testing and the destructive nature of these tests. Together, these characteristics of the standardized experimental tests used to determine the smoke emission of building materials can lead to significant costs and long durations of the research and development processes of modern building materials. Given the significant negative effect that smoke generated by construction materials involved in a fire can have on the evacuation of victims, the development and spread of fire, the difficulty of interventions by professional emergency services, and the shortcomings that prevent the use of standardized tests in phases of research and development of new construction materials, this paper proposes a methodology for estimating the smoke emission of construction materials by using numerical simulations developed based on the results of small-scale experimental tests.

For the experimental determination of the optical properties of the smolder generated smoke of some common construction materials, the principle of light intensity attenuation was used, the same principle underlying the determination of smoke emission of construction materials through standardized experimental testing. Thus, a total of 24 experimental tests were developed in this research program, of which 12 with artificial smoke and 12 with smoke generated by the smoldering of some common construction materials. The 12 experimental tests with artificial smoke were developed to demonstrate the applicability of the methodology for determining the optical properties of smoke by using the principle of attenuation of light intensity of a laser beam passing through the smoke layer created in a test chamber. The first three of these artificial smoke experiments were on a full scale, one for each of the three measuring distances of 5, 7.5 and 10 meters between the light source and the luxmeter. These three experiments were performed in both natural light and dark room conditions. By using artificial smoke, three more experiments were then developed at a scale of 1:10, one for each of the three measuring distances of 50, 75 and 100 centimeters between the light source and luxmeter and three other experiments at a scale of 1:20, one for each of the three measuring distances of 25, 37.5 and 50 centimeters between the light source and the luxmeter.

The 12 experimental tests with smoke generated by the smoldering combustion of construction materials were composed of three sets of tests, one on a full scale, one on a 1:10 scale and one on a 1:20 scale for each of the four types of materials that are representative for the current built environment, namely wood chipboard (PAL), gypsum board (GC), expanded polystyrene (PST) and polyvinyl chloride (PVC). Small-scale experimental tests to determine the optical properties of smoke generated by smoldering of building materials were used to determine parameters used as input data in the numerical simulation program to virtually reproduce the smoke emission of these materials. Experimental full-scale tests for each of these materials were used as a comparison standard for validating simulations of the natural-scale smoke emission of construction materials developed on the basis of small-scale determined smoke properties, and for assessing the accuracy of these numerical simulations, in order to determine the extent to which they can be used to approximate the real, natural-scale optical properties of the smoke produced by the analyzed building materials.

For each of the experimental tests presented in this paper, a validated numerical simulation was developed based on the results obtained by experimental testing, stating that for repeated experimental tests, for different measuring distances between the light source and luxmeter, only one numerical simulation was developed, in which three measuring devices were used simultaneously, positioned at the corresponding distances. Numerical simulations of the optical properties of artificially generated smoke were used to demonstrate the possibility of using numerical simulations to recreate the emission of smoke characterized by optical properties comparable to those obtained experimentally, both on a full scale and on small scales. After demonstrating this way of using numerical simulations and obtaining favorable results in terms of simulating the optical properties of artificially generated smoke, both on a full scale and on a small scale, the same principle was used to develop and validate numerical simulations of smoke emissions for the construction materials, at a scale of 1:10, respectively at a scale of 1:20, to demonstrate the applicability of the simulation methodology in the case of smoke generated by the smoldering combustion of construction materials.

For each of the four construction materials, natural-scale simulations of their smoke emissions were developed based on the results of small-scale experimental tests. The results regarding the optical properties of smoke of the full scale simulations thus developed were compared with those obtained by experimental testing on a full scale, presenting a percentage of similarity around 89%, a favorable result composed of comparing parameters such as the average percentage difference between the simulated and experimental optical smoke extinction coefficient, the percentage difference between the maximum simulated and experimental optical smoke extinction coefficient, the average of the differences between the recorded values of simulated and experimental visibility levels and the difference between the minimum values of simulated and experimental visibility levels. These parameters were chosen to illustrate the ability to approximate by numerical simulation both the evolution over time of the monitored parameters and in terms of the final state of the optical properties of smoke achieved at the end of the experimental tests and numerical simulations for the smoldering combustion of building materials.

Chapter II presents the theoretical elements that formed the basis of the research efforts presented in this paper, the definitions of the terms used in fire safety engineering to describe the phenomena related to the smoke emission of materials and the optical properties of this smoke are presented. The role of smoke emission in the classification of construction materials and products into reaction to fire classes based on standardized experimental tests is also presented. The reaction to fire classes, how they are represented on the label of construction materials and products, as well as the meaning of the symbols that accompany this labeling are presented. The equations used to determine the smoke emission of construction materials by standardized testing and the criteria leading to the characterization of the smoke emission of a construction material as significant, medium or low are presented. The configuration of the test stand for the standardized experimental test most often used to determine the smoke emission of construction materials is also presented. Also, in this chapter the numerical simulation model that was used is presented, that of computational fluid dynamics (CFD), the approach being that of LES - Large Eddy Simulation. The conservation equations of mass, momentum and energy underlying the simulation program used are presented, as well as some of the results that can be obtained through such a simulation. The simulation program used, Fire Dynamics Simulator, is presented, as well as the result visualization program that accompanies it - Smokeview. Also, due to the fact that the input data for this simulation program is entered in the form of lines of code, its use is conditioned by the user's knowledge of the programming language used in this simulation program. Thus, in order to avoid this impediment, as well as for an easy development of the virtual simulation environment through a graphical user interface, the PyroSim program was used for the numerical simulations within this research program.

Considering the particular case of the smoke emission of construction materials addressed by this scientific research program, in the same chapter are presented aspects related to smoke numerical simulation, as well as predefined values for certain parameters that influence the simulation of the emission of smoke and the visualization of the results. Considering the need to define a certain smoke emission capacity for the construction materials represented in the simulation program, the equations underlying the experimental determination of the material parameters necessary for the reproduction in the virtual environment of their smoke emission were presented.

The smoke emission of construction materials is conditioned in intensity and duration by the way the analyzed materials react to exposure to high temperatures, so this reaction had to be defined for each material in the numerical simulation program based on small scale tests of thermogravimetry and microcalorimetry, which provided the parameters necessary to define the pyrolysis reaction, respectively the combustion reaction of the used materials. The capacity of the numerical simulation program to virtually reproduce these two types of tests was used to validate the virtual models of the analyzed construction materials with degrees of similarity between about 83% and 96%, the maximum degree of similarity being reached in the case of plasterboard, which has a low reaction to exposure to high temperatures, and the minimum for polyvinyl chloride, that undergoes multiple transformations by exposure to high temperatures, including melting and burning, which makes high-precision numerical simulation of the behavior of this material to exposure to high temperatures more difficult.

Chapter III of this paper presents the state of the art at a national and international level in the field of smoke emission research of construction materials using the principles of fire safety engineering. The two current international approaches to ensuring the fire safety of buildings are presented, the prescriptive and the performance-based one. International studies that highlight the factors that influence human behavior in the event of a fire are also presented, from warning users in a building about the existence of a fire, to their behavior in response to exposure to certain characteristics of fires. This chapter presents how the smoke emitted in the event of a fire can have an impact on the users of a burning building, as well as thresholds of human tolerability to exposure to smoke, established through scientific research and legislative recommendations at the international level. The experimental determination methodologies for the optical properties of smoke, as well as of its gaseous composition used to provide information regarding its toxicity are briefly presented. Some models of numerical simulation of fires currently used internationally are also presented in this chapter.

Chapter IV presents the experimental framework used for this scientific research project for each of the 24 experimental tests and the development of the corresponding numerical simulations. For the experimental testing of the artificial smoke at a full scale, the devices used, such as the smoke machine, the light intensity measuring device, the light source, the test enclosure and their positioning within the experimental enclosure, the duration of each experiment and the intended purpose are presented. Next, the numerical simulation of this full scale experimental is developed based on the experimental configuration of the tests performed, as well as multiple iterations of the simulations in order to determine the optimal mesh size to produce accurate results within an acceptable amount of time. The methodology used to determine the parameters necessary to define artificial smoke in the simulation is presented along with the benchmarks used to compare the results obtained by numerical simulation and those obtained by experimental testing.

The next experiments presented in this chapter are those for determining the optical properties of small-scale artificial smoke. The methodology used for the scaling of the experimental configuration, that included the test chamber, the smoke generating device and the light intensity measuring device is presented. The smoke extinction area parameter was used for comparing the experimental and simulation results when using artificial smoke, and was presented in this part of the paper.

These small-scale experiments were then duplicated in the virtual environment by the development of numerical simulations of the experimental tests at the 1:10 and 1:20 scales that reproduced both statically and dynamically the small-scale experiments. A different approach to reproducing the optical properties of artificial smoke was also used in these numerical simulations. In the case of the numerical simulations based on experimental full scale testing of artificial smoke, a repetitive adjustment approach of the input parameters was used for numerical simulation until a high degree of accuracy of the results was reached, starting from a theoretical value of the smoke parameters calculated from the smoke machine manufacturer's specifications. In the case of the numerical simulation of the small-scale experimental tests of the artificially generated smoke, the ratio of the mass of soot to air introduced in the simulation was determined by calculation, based on the optical extinction coefficient of the smoke within the experimental tests for each activation period of the artificial smoke generating device.

After achieving promising results by using artificially generated smoke led to the attempt to apply the testing and simulation methodology for smoke generated by smoldering of construction materials, so that the continuation of this chapter presents the experimental configuration used to determine the optical properties of the smoke emitted by the analyzed construction materials. The test chamber, the materials used, the burner and the exposure of these materials to a sufficiently high heat flux to determine the smoke emission are presented, as well as images of the tested samples before and after each experiment. Next, the down scaling methodology to 1:10 and 1:20 scales is presented, along with the full scale construction materials smoke emission experiment used to determine the optical properties of the smoke generated by the smoldering construction materials. The dimensions of the test chamber, the quantity of material used and the intensity of the heat flux to which the material was exposed are also presented. The materials tested in the small scale experiments were weighed before and after the experiments, in order to determine the amount of material consumed by burning, which caused the emission of smoke. As a simplifying hypothesis, it was considered that the entire mass of material lost by smoldering was transformed to soot particles, i.e. smoke, which in turn caused the reduction of the light intensity of the light ray that passed through the smoke layer thus formed, recorded by the measuring instrument during the experiments.

Based on the experimental configuration used to determine the optical properties of the smoke emitted by the smoldering of building materials, as well as based on the virtual models of building materials developed using the results of the thermogravimetry and microcalorimetry laboratory tests, the 1:10 and 1:20 scale simulations were developed. These were validated by the comparison of the results obtained by numerical simulation with those obtained by experimental small-scale testing of the smoke emission of construction materials.

Given the promising results obtained by the numerical simulation of the optical properties of smoke generated by smoldering of building materials, numerical simulations of the full scale experiments were developed based on the experimental configuration of full-scale tests, the results of small-scale experimental tests and virtual models of the analyzed materials. These simulations also used information such as the dimensions of the calculation cells needed to obtain high-precision results, but large enough not to make it difficult to calculate the simulation in exchange for a modest advantage in terms of the level of accuracy.

Chapter V of this paper presents the results of the conducted research for each of the 24 experimental tests and their numerical simulations. The results are generally presented in the form of comparative graphs of the evolution over time of the various parameters taken into account to determine the degree of similarity of the results obtained by numerical simulation and those obtained by experimental testing. In the case of the experimental testing on a natural scale to determine the optical properties of artificially generated smoke, the influence of the lighting level in the compartment was taken into account. In this sense, comparative graphs of the results obtained under natural lighting and darkness were plotted and the values obtained after each activation of the smoke machine for the optical smoke extinction coefficient and the level of visibility in the compartment, for each of the three measuring distances and for each lighting condition are also shown. The influence of the lighting levels of the test compartment on the results was not identified as major, the differences between the two sets of values being on average about 6%, but the optical properties of the smoke evaluated by experimental testing were determined based on the initial light level in the test chamber for each of the experimental tests, so that the light level in the test chamber does not affect the results obtained nor does it affect the possibility of comparing the results obtained in experimental tests with different light levels.

In the case of simulating the optical properties of artificial smoke in a natural scale, the evolution over time of the visibility level was reported as a percentage of 30 meters, considered the maximum visibility distance in the numerical simulation program, given that the purpose of this program is the simulation compartment fires. The level of visibility in the compartment was recorded in these simulations in the form of meters visible on the path of the ray drawn in the numerical domain by means of a simulated device. Also, these simulations exemplified the use of the results viewer to change the smoke display properties based on the images captured during experimental tests in order to display a smoke color similar to that of the artificial smoke used in the experiment. The average degree of similarity for the optical smoke extinction coefficient and the level of visibility in the compartment between the results obtained by experimental testing and those obtained by numerical simulation for the full scale experiments and numerical simulations in the case of artificial smoke ranged from about 88% to 94%, indicating the fact that numerical simulation can be successfully used for the virtual reproduction of the optical properties of artificial smoke.

Following the promising results obtained both for experimental testing on a natural scale and for the numerical simulations, the results of experimental small-scale testing of artificially generated smoke and the use of the smoke extinction area as a comparative parameter for evaluating the efficiency of scale reduction are presented. With a degree of similarity between the values that characterize the evolution over time of the smoke extinction area obtained by natural scale testing and those obtained on reduced scales located in the range of about 84% to 94%, the methodology of down scaling the experimental framework for determining the optical properties of artificially generated smoke proved to be suitable for this type of application. In the small scale experimental tests on the optical properties of artificially generated smoke, the impact that the positioning of the measuring device in the test compartment may have on the recorded results was also evaluated, revealing differences in the percentage range of about 8% up to 15%. These relatively high values were obtained due in part to the need to repeat each experiment after repositioning the luxmeter at the appropriate distance from the light source to perform a new experiment. To demonstrate the possibility of using numerical simulation to reproduce via numerical simulation the optical properties of artificially generated smoke determined by small-scale experimental testing, the values characterizing the evolution over time of the optical smoke extinction coefficient and the visibility level in the test compartment were compared. The similarities were in the percentage range of 90% to 95%, thus demonstrating the applicability of the numerical simulation methodology of the optical properties of artificially generated smoke at a small scale. Also, due to the fact that the values for the three measuring distances could be obtained simultaneously in the numerical simulations by using three virtual measuring devices in the same simulation, the differences in the values recorded by the three devices were in the range between 2% and 5%.

Once the research phase in which artificially generated smoke was used to demonstrate the applicability of the experimental testing methodology and numerical simulation on both natural and small scale was completed, the optical properties of real smoke were determined in full scale experiments. In this chapter, the results regarding the evolution of the light intensity of the light ray passing through the smoke layer during the experiment were presented, along with the level of visibility in the test compartment, as well as of the optical smoke extinction coefficient generated by the smoldering of the construction materials. For each material, it was considered that the minimum value of the light intensity of the light ray passing through the smoke layer coincides with the end of the smoke emission, at which point the material stopped producing smoke either due to its consumption or the formation of a carbonized layer on the interface between the contact surfaces and the support through which the heat exchange took place. The results presented in that section of the mentioned chapter were used as a benchmark for the evaluation of full scale numerical simulations developed on the basis of small scale experimental results. Small-scale experimental testing of the smoke emission of construction materials produced results that pertained to the decrease of the light intensity of the light ray passing through the smoke layer, the decrease of the visibility level in the test compartment, as well as the increase of the optical smoke extinction coefficient, to the mass of material consumed by smoldering combustion during experiments.

Based on this information, as well as on the average smoke extinction coefficient recorded during the small-scale experiments for each of the analyzed materials, the mass of soot produced by the amount of material consumed by smoldering combustion for each material was calculated, for each of the small-scale experiments. The mass of suspended soot produced by the material by smoldering combustion should theoretically be a material constant, and this was highlighted by differences between the values of this parameter determined by experimental testing at 1:10 scale and experimental testing at 1:20 scale for the same material in the percentage range between about 4% and 18%, the significant differences being registered in the case of plasterboard, a material that has a low smoke emission, which negatively influences these differences by offering low values for the differences to be calculated against.

The numerical simulation of the optical properties of the smoke generated by the smoldering of construction materials led to the achievement of degrees of similarity between 82.44% and 95.59% for the evolution over time of the optical smoke extinction coefficient and from 96.16% to 99.24% for the evolution over time of the visibility level in the test compartment, compared to the values of these parameters determined by small scale experimental testing. These levels of similarity lead to the conclusion that the virtual models of the construction materials, together with the burning reaction parameters used, determined on the basis of small scale laboratory experimental tests provide a suitable representation of the smoke emission of these small-scale materials. These virtual models of the building materials, as well as their associated combustion reactions, have been used to develop the numerical simulations of full scale smoke emission of the building materials. The results of these simulations were validated by comparison with those obtained by full scale experimental testing of these materials, by establishing four types of parameters to assess the similarity both in terms of evolution over time of the smoke emission of materials, and from the point of view of the final state of the atmosphere in the test compartment, at the end of the smoke emission of the construction materials. The degree of similarity that characterizes all the parameters used, for all the construction materials, for the numerical simulation on a natural scale developed based on the experimental results at 1:10 scale was about 89.87%, and for the numerical simulation of the experiment developed on the basis of the experimental results at 1:20 scale was about 89.10%.

Such results regarding the level of similarity between the results obtained by natural scale experimental testing and those obtained by numerical simulation developed on the basis of small-scale experimental tests offer a promising perspective on the possibility of using small-scale experimental testing and the numerical simulation capability of the specialized programs currently used in this field of study for obtaining information on the emission of smoke from construction materials, without the need for the said materials to be subjected to standardized tests.

3. Original contributions

The classification of the reaction to fire performance, and thus the emission of smoke of a construction material is impossible when small amounts of material are available. For this reason, this paper proposes a methodology for small-scale experimental testing of common building materials in order to determine the optical properties of the smoke generated by them and the use of these properties as input parameters for the development of numerical simulations of the smoke emission without the use of significant amounts of material, with acceptable levels of accuracy. Among the original contributions presented in this doctoral thesis is the demonstration of the possibility of applying the principle of attenuation of light intensity to determine the optical properties of smoke over longer distances (of the order of meters) than those used in standardized testing of construction materials for their inclusion in performance classes based on their reaction to fire (of the order of centimeters) by means of full scale artificial smoke experimental tests.

Through small-scale experimental tests with artificial smoke was demonstrated the possibility of using a theoretical parameter called the smoke extinction area to correlate the data obtained by testing at different experimental scales. This correlation of data on the optical properties of smoke obtained at different experimental scales is mentioned in scientific literature as being only theoretically possible by using the smoke extinction area. Thus, through the research efforts within this doctoral thesis, it was possible to demonstrate the use of this parameter in an experimental framework.

The numerical simulation of the smoke emission of construction materials developed based on the optical properties of smoke determined experimentally on a small scale demonstrated the possibility of using experimental tests to determine the amount of suspended soot produced by mass unit of burned material, to be used as a input parameter for the numerical simulation of the smoke emission of these materials with a reasonable level of accuracy. Thus, in this research program it was possible to numerically simulate the full scale smoke emission of some common construction materials based on the small scale experimental determination of the optical properties of the smoke created by their smoldering. The amount of suspended soot generated by the mass unit of burned material was the key parameter used in the numerical simulation of the smoke emission of construction materials. This parameter was determined on the basis of the optical smoke extinction coefficient, obtained by the experimental use of the principle of light intensity attenuation, on the basis of the optical mass extinction coefficient, a parameter taken from the scientific literature for smoke generated by smoldering and based on the amount of material consumed by combustion in the experimental test, determined by weighing the sample of material before and after the experiment. The use of the amount of suspended soot produced by the unit mass of burned material as an alternative to specifying the parameters of the chemical combustion reaction in the numerical simulation program is an innovative approach in the numerical simulation of the smoke emission of construction materials. The method of experimental determination of this parameter, as well as the use of it as an input parameter specified by the user in the numerical simulation program are original contributions of this doctoral thesis in the field of fire safety engineering. Thus, by using small-scale experimental laboratory tests of thermogravimetry, microcalorimetry and the determination of the amount of suspended soot generated by the unit mass of burned material, numerical simulations with an acceptable level of accuracy for the smoke emission of a given construction material can be obtained.

In conclusion, the main original contribution of this doctoral thesis is the development of a methodology for small scale determination of the optical properties of smoke generated by smoldering of common building materials and their use for the development of numerical simulations with an acceptable level of accuracy of full scale smoke emission for the analyzed construction materials.

4. Articles that were published during the research program

Most of the results obtained through this research effort were disseminated through presentation at conferences with national and international participation, by publishing in the volumes of these conferences, as well as by publishing articles in non-indexed journals. Thus, the conferences with international participation in which papers were presented and in which the results of this research program were disseminated are CIEM 2019 – 9th International Conference on ENERGY and ENVIRONMENT, the article that was published in this conference’s volume being presented in reference [1], at the moment of publishing, in the year 2020, the editor IEEE Xplore having an impact factor of 5.24. Other articles have been presented and published at the 2nd Conference of the UTCB Doctoral School 2019, the article that was published in this conference’s proceedings being presented in reference [2], at the EENVIRO 2020 Sustainable Solutions for Energy and Environment, 7th edition conference, the article that was published in this conference’s proceedings being presented in reference [3] and the 3rd Conference of the UTCB Doctoral School 2020, the article published in this conference’s proceedings being presented in reference [4]. At the time of publishing of these three articles, in the year 2021, the editor IOP Conference Series had an impact factor of 0.41.

Furthermore, part of the results of this research program have been presented in the International Conference on Hydraulics and Pneumatics HERVEX 2019, the article that was published in this conference’s proceedings being presented in reference [5], and the journals that were used to present some of the results of this research program were Buletinul de Informare și Documentare al Ministerului Afacerilor Interne [6] and Buletinul Pompierilor [7].

In total, the results of this research program were presented in four international conferences, the publishing of four Web of Science (WoS) indexed articles, one international databases indexed article (EBSCO, Google scholar, TIB Leibniz Information Centre for science and technology university library), and two articles in national un-indexed journals.

5. Closing remarks

The continuous improvement of the production and testing processes of construction materials with improved fire properties can lead to a safe built environment for users and emergency response teams in the event of a fire emergency. Also, the freedom to choose their own technical solutions by designers and builders in order to meet performance-based legislative requirements in the field of fire safety of buildings can facilitate the use of innovative construction products and original technical solutions. For these reasons, the numerical simulation of the fire behavior of building materials based on reliable results of low-cost experimental tests, such as small-scale ones, can be the engine of the development of new types of building materials, as well as the basis for the argumentation of their use in functionally, aesthetically and economically appropriate technical solutions that ensure adequate fire safety for the buildings of the future.

6. Bibliography

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