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Experimental and numerical investigations in order to model the fire development and propagation for fire safety engineering studies

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ABSTRACT

Fire safety engineering plays an important role in achieving safety objectives in a building and is in way of generalization in all the countries of the world, especially for reaction to fire. It is based on the use of numerical models. However, numerical simulations used for this particular field has got some limitations, for example due to the size of the domains to simulate, the very large number and the complexity of the materials involved, the multitude of the geometric configurations… that do not allow the representation of all the processes. In consequence, reaction to fire cannot be treated accurately in engineering studies and flame ignition or propagation cannot be represented due to the time of calculation. Nevertheless, their description is of first order. In this context, this work gives a first approach on technical bases in order to represent ignition, fire growing and development and flame propagation in engineering study. This description requires an understanding of the different processes involved in both solid and gaseous phases as well as their interface. A means to represent small-scale phenomena with engineering model limitations (time to compute, size meshing) should be performed.

For this, a multiscale study both experimental and numerical is in progress on two types of polymers: a pine wood and PVC. This approach is conducted in order to identify relevant phenomena that drive fire growing and flame propagation for different configurations: vertical, horizontal, co-current and counter-current. The study should lead to the definition of new sub-models, of numerical model recommendations (size meshing, wall laws, etc.) in order to describe those phenomena at large scales without too large time consumption.

KEYWORDS

Reaction to fire; Fire Safety Engineering; Fire growing; Flame propagation; Multiscale approach; Experimental study; Numerical simulation; FDS.
CONTEXT AND OBJECTIVES

Fire safety engineering (FSE) is an increasingly important part in achieving the definition of fire objective in a building. It enters in the so-called performance based approach as it matches objectives with conditions of a given local. The CFD code Fire Dynamics Simulator [1] (FDS) is widely used in FSE to model the main elements accounted in a study building geometry, smoke extraction systems, detection systems, sprinkler system, main openings (doors, windows, outlets) and communications between volumes. Nowadays, FSE treats smoke removal and people evacuation studies, and is in way of development for reaction to fire. Reaction to fire is the fire behavior for a given material, including ignition, fire growing, propagation and extinction. It results in interactions between both the solid phase and the gaseous phase. It implies phenomena involved at larges scales as flow stream or thermal transport, but also at small scale, especially at the interface or in the reaction zone as mass and heat diffusion or chemical kinetic. Therefore, boundary layer flames features multi- physic phenomena, and these phenomena require specific near-wall model descriptions that so far have not been the focus of fundamental studies.

Gaseous phase [2][3] and solid phase [4][5] behavior are quite well understood separately, but the interaction between them isn’t really understood. Generally, solid phase is seen as a porous burner slab, like the recent work of Ren et al. [6]. They present LES simulations of buoyancy-driven turbulent vertical wall flames and illustrate the potential of LES for wall fire simulations. However, the simulation is wall-resolved, with a near-wall mesh size of millimeters order, and the pyrolysis of the solid phase is not treated. LES is sensitive to the accuracy of the physical models that treat near-wall turbulence, combustion, thermal radiation and soot formation. In addition, the LES performance is adversely impacted when the computational grid resolution is not sufficiently fine. In [6], a near-wall grid resolution from 10 mm is not sufficiently fine to resolve wall gradients. A grid with that resolution is impossible to use for fire safety engineering because of time to compute and large domain sizes; therefore, it is necessary to adapt near-wall model and to develop technical bases in order to represent gradients and to perform engineering studies to account for reaction to fire.

Previous works, using similar multiscale approach have been carried out in order to study the thermal decomposition of a material. The first one was those of Bustamante Valencia [7]. He studied experimentally and numerically the thermal decomposition of a polyether polyurethane foam at three scales. He started at the matter scale using a TGA apparatus in order to determine the decomposition mechanism and integrated it at small scale and at the product scale. This integration leads to understand which parameters are needed in order to perform thermal decomposition studies. It was pointed out that the decomposition mechanism of the foam remains unchanged independently of the scale analysed. Another similar study was performed by Marquis [8]. He studied a composite sandwich using the same methodology as Bustamante Valencia. The findings were that this methodology is still applicable for composite material. Camillo [9] focused on the fire behaviour of a seat and a wall panel from railway transport system. This study starts at the matter scale, up to the real scale with a quite good agreement for the comparison of the experimental and numerical heat release rate (HRR). All these studies lead to the evaluation of the mass loss rate and of the HRR for a given material. They were focused on the solid thermal decomposition kinetics, therefore fire growing and flame propagation weren’t pointed out by these studies.

In this context, the present work provides a new approach for technical bases in order to perform engineering studies including flame ignition development and propagation. It includes the study of the gaseous and the solid phases, with a specific attention at their interface. This study is focused on two materials in different configurations: vertical, horizontal co-current and counter-current. As numerous parameters and material properties are needed to model accurately the fire behavior at the material interface, the development of technical bases will include assessment of the relevant input parameters associated with the experimental tests needed. Numerical useful function and recommendation as wall laws or size meshing should be determined.

MATERIALS AND CONFIGURATIONS

The proposed methodology is applied on both a natural and a synthetic polymer that could be found in public buildings. The designated natural polymer is a cellulosic material, as pine wood. It will be considered as a partition panel, therefore in a vertical configuration. Wood exists through many varieties; its elementary composition is quite close from one to another. When heated, wood starts a pyrolysis process once the wood is reached. A carbonaceous layer appears at its surface, and constitutes the char. This layer plays an important role on wood decomposition as it becomes a heat shield for the virgin wood below its surface. In addition, the anisotropy of its properties makes it difficult to study experimentally and numerically. However, thermal decomposition of wood has been past studied in several sources [10][11]. Simple or detailed
decomposition models have already been proposed; also this current study is not focused on the development of thermal decomposition model.

The synthetic polymer is a polyvinyl chloride (PVC) coating that is usually found on floors in public buildings. PVC is the second most used plastic material and is composed of linear macromolecules with a general formula \([\text{CH}_2\text{CHCl}]_n\). The one studied is flexible and is used in floor application with a homogenous thickness with retardant added. We select a PVC floor coating with a Bfl-s2 reaction to fire ranking (Euroclasses). The support and the glue used must be taken into account to be as close as possible to real conditions. However, at small scale (matter scale and material scale) only the PVC is investigated. As the wood, its thermal decomposition has been past studied \([12][13]\) and it is assumed to occur in two steps: the first one relates to the dehydrochlorination, with release of few hydrocarbons, and the second one corresponds to scission reactions, with release of toluene.

Because airflow plays an important role when a flame is spreading along a surface, co-current and counter-current flow phenomena will be investigated to be accounted in the numerical simulation. The heat flux emitted from the flame to the unburnt material surface depends on the configuration. Thus, in a co-current flow, flame can propagate easily as the heat flux received on the virgin surface is important. Generally, radiation is the dominant mode of heat transfer, although convection is present close to the ignition region. The flow is turbulent, and chemical time is of secondary importance compared to the flow time. In a counter-current situation, the flame cannot spread quickly; the virgin material is heated up mainly by diffusion close to the ignition region. The radiative part incoming from the flame can be neglected.

All these phenomena, involved at different scales, are characterized in order to understand the flame behaviour for each case. The more important achievement of this study will result in the investigation of a pathway between small, intermediate and full scales, leading to a better representation in numerical simulations in the context of fire engineering studies.

**METHODOLOGY**

Flame propagation depends on the local and assembly effects, the fluid dynamics, the flame geometry, the chemical reactions and the mass and heat transport mechanisms for the gaseous phase. For the condensed phase, it depends on the mass loss rate, mainly driven by the pyrolysis kinetics and the heat flux incoming to the surface. The thermal loads depend on the radiative part of the flame, and the understanding of these complex phenomena is a big challenge. Moreover, the chemistry of the condensed phase can largely influence the quantity of energy transmitted to the fuel by the apparition of a carbonaceous layer on its surface. Therefore, the state of each phase is strongly dependent to one another: the flame depends on the amount of fuel released and the release depends on the amount of heat transmitted to the condensed phase. For this reason, this study is mainly focused on processes involved at the interface.

Owing to the multiscale processes, a multiscale methodology is performed that provides insight into important features at multiple times and lengths of a physical phenomenon. The strategies proposed attempt to experimentally capture inherently important properties at various scales of a system and to numerically correlate them accurately to the system’s macroscale properties by a multiscale validation. The numerical validation is admitted by comparison with experimental results: heat release rate, mass loss rate, spread rate, gas and solid temperature, etc. The proposed methodology is synthetized in the Fig. 1:
Fig. 1: Multiscale experimental and numerical methodology used.

Experimentally, the identification of relevant phenomena that must be modelled is performed at medium scale using radiant panel for the horizontal flame propagation of PVC, IMO-LIFT for lateral flame propagation, and a 1D vertical slab propagation (see Fig. 3) for wood. At this scale, all dependences on flame propagation described above are present; except the local and assembly effects. The processes of interest are mainly located at the interface of the solid. The instrumentation of the 1D vertical slab facility is shown in Fig. 2.

Similar instrumentation is used for the IMO-LIFT and radiant panel bench. Velocity and temperature measurements will be performed inside the reactive boundary layer. The average velocities (horizontal and vertical), as well as their fluctuations, will be measured thanks to the 'Particle Image Velocity' laser diagnostic and fine thermocouples (diameter: 0.1 mm) placed at different heights. Thus, two total and two radiative flux meters will be used at two different heights. This makes it possible to understand the phenomena controlling the
mixing of reactants (convection, turbulent diffusion, mass diffusion), as well as the role of convection on heat transfer at the interface. The evaluation of the residence time, as well as the gas analysis using a Fourier Transform Infrared (FTIR), will lead to the determination of the chemistry regime. In addition, fine thermocouples placed along the surface and into the thickness of the solid phase will allow to accurately mapping the evolution of the temperature inside the slab. This step allows to observe and to evaluate key phenomena driving the fire kinetic that must be modelled.

Tests at smaller scale are performed mainly in order to get input data for simulations. Results achieved for TGA apparatus, coupled with a particle swarm analysis should give the mechanism and kinetic of decomposition with the Arrhenius parameters of the solid phase. First experimental results are shown in Fig. 3. The numerical validation of the model with an increase in scale and in complexity is in progress.

The model of pyrolysis is validated at material scale using the cone calorimeter. At this scale, a 1D thermal and mass diffusion is assumed in the solid phase. In the gaseous phase, the cone calorimeter permits to study flame development, without propagation. Three thermocouples (for pine wood only), placed at the surface, in the middle of the thickness and at the back of the solid will permits to validate the mechanism of decomposition taking into account the gradient of temperature into the sample. Also, an analysis of gas emitted before ignition should allow the understanding on gas concentration and on which gas is the precursor for ignition, this analysis is performed by a GCMS apparatus. This apparatus measures gas production closed to the solid. It differs from the FTIR analyser, which has a measurement point far from the solid. Once the numerical model validated at the material scale, with a good estimation of the HRR, the model will be extrapolated and validated at the medium scale by the implementation of a pathway representing small-scale phenomena on coarser mesh. The validation will lead to identify pertinent numerical models and code recommendations.

Experimental investigations using single burning item (SBI) and room corner benches will allow the identification on modifications of relevant physics due to material assembly modes, as well as angle effects. These experiments will lead to the adaptation and validation of numerical models that finally will be used to predict fire behaviour and HRR at real scale using large calorimetric hood, in construction type facilities as stairs or corridor. Experiments performed at this scale should permit to validate the models and to identify the main parameters used in FSE (Heat release rate, calorific charge, etc.). All these steps could help to understand processes involved in fire propagation in different configurations. Unchanged processes involved from the medium scale to the real one should be identified and represented in numerical simulations taking into account code limitations. Therefore, a first step for technical bases can be proposed including relevant input parameters, experimental tests to perform at least to get them and model recommendation as mesh size.

CONCLUSION

To conclude, this beginning PhD work should give a first approach for reaction to fire in FSE. It will develops numerical models taking into account relevant phenomena driving the fire kinetic and relevant parameters with the way to assess them. This approach will allow FSE studies to estimate fire propagation of a given fire source and other secondary fire in order to define fire safety rules.
REFERENCES