CHARACTERIZATION AND MODELLING OF SELF-SUSTANINING SMOLDERING OF WOOD INDUSTRIAL PRODUCTS

CARACTERIZACIÓN Y MODELIZACIÓN DE LA COMBUSTIÓN LATENTE AUTOSUSTENTADA DE PRODUCTOS INDUSTRIALES DE MADERA

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Abstract

Multiple wood industrial products such as wood-fiber insulation boards are susceptible to smolder. This special type of slow and flameless thermal degradation is very dangerous because it can easily go unnoticed until catastrophic damages are produced. For this reason, the utilization of wood-based insulation materials, which is much more environmentally-sustainable than classical polymeric-based insulations, is not permitted beyond mid-rise buildings in many countries worldwide. The objective of this investigation was to characterize such a smoldering combustion and create a theoretical model that can predict this phenomenon. The experimental characterization involved a suite of experimental methods such as thermogravimetric analysis (TGA), differential scanning calorimetry (DSC) and cone calorimeter tests. The core of the numerical model entailed 6 governing equations describing the heat, the mass, the linear momentum and the species conservation of the wood panel that were solved via Finite Volume Method (FVM). The model could successfully simulate a 25-minute cone calorimeter experiment without any external radiation. To the best knowledge of the authors, this is the first model that can simulate the self-sustaining smoldering of wood industrial products, so it is expected to contribute on the development of future fire retardant compounds of timber structures.

Keywords: smoldering; finite volume method; computational fluid dynamics; cone calorimeter; wood fiber panel; fire retardant

Resumen

Múltiples productos industriales de madera tales como paneles aislantes de fibras de madera son susceptibles de sufrir combustión latente. Este es un tipo especial de degradación térmica que se caracteriza por ser muy lento y carecer de llama, lo cual lo convierte en un fenómeno peligroso pues puede pasar fácilmente desapercibido hasta que se producen daños catastróficos. Por esta razón, la utilización de materiales aislantes derivados de la madera y afines no está permitida en edificios de cierta altura en muchos países del mundo. El objetivo de esta investigación fue el de caracterizar dicha combustión latente, y crear un modelo teórico que pudiese predecir este fenómeno. La caracterización experimental comprendió una serie de métodos tales como análisis termogravimétrico (TGA), escaneado por calorimetría diferencial (DSC) y ensayos en cono calorimétrico. El núcleo del modelo numérico se compone de 6 ecuaciones de gobierno que describen la conservación de calor, masa, momento linear y especies la cuales fueros resueltas via método de los volúmenes finitos (FVM). El modelo pudo similar satisfactoriamente 25 minutos de un experiment de cono calorimétrico sin radiación externa. Según el conocimiento de los autores, esta es la primera vez que se puede similar la combustión latente autosustentada de un producto industrial de la madera y por tanto se espera que pueda contribuir al desarrollo de futuros compuestos retardantes para estructuras de madera.

***Palabras clave**: combustión latente; método de los volúmenes finitos; dinámica de fluidos computacional; cono calorimétrico; paneles de fibra de madera; retardante de fuego*

1. INTRODUCTION

Wood fiber smoldering is the central problem hampering the spread of wood as insulator material for mid and high-rise buildings. In some countries as Germany, the utilization of wood fiber insulation panels (WIP) is limited to only 7-meter-high buildings due to smolder risk. Smoldering can indeed be dangerous because, as opposed to a conventional fire scenario, it is a flameless and surprisingly slow thermal degradation process so that it can last unnoticed several hours until either irreversible structural damages or critical smoke levels inside buildings are reached. Apart from this smoldering phenomenon, WIP is an outstanding insulator material with a dry thermal conductivity of about 0.04 W/m^2K. Also, the ecological benefits of using WIP are especially remarkable because of the wide spread of petroleum-based competitors.

Remediating the smoldering problem is thus the key target for WIP manufacturers since decades and as such has been extensively investigated. Uncountable experiments and fire-retardant treatments have been developed aiming at stopping the smoldering or at least test improve our understanding of the process. However, the results of those efforts have been rather unsatisfactory [1] - the smoldering could not be stopped yet and we only could gather a few certainties: the only stopping chance is to completely remove the oxygen, and some parameters such as density, porosity, particle size and air flow have a clear influence on the speed of the degradation.

In views of the little experimental outputs also some theoretical models have been developed in the past [2-4]. Those models were typically based on Computational Fluid Dynamics (CFD) methods such that the smoldering simulation is based on the conservation of the mass, momentum and energy of the wooden panel. Several of those models have been successfully validated with experiments (mainly cone calorimeter) serving thus to improve the understanding of the process. However, previous models have always been constructed and validated using an external heater, i.e. a constant radiating source was heating the wood. In reality however, there is not such a boundary condition and the wood is consumed without any external ‘aid’ in a very slow fashion, i.e. it suffers self-sustaining smoldering, and to the best of our knowledge this has never been modelled for wood products before.

The aim of this investigation was characterizing the smoldering process and create a numerical model that is able to simulate the self-sustaining smoldering of wood products. The paper is devoted to present the model as well as the experiments needed for its construction.

2. 0D EXPERIMENTS: TGA AND DSC

The reactions, solid species and gas species of the model are presented in the Figure 1. As it is shown in the figure, four reactions are considered. The first reaction involves the moisture evaporation from the wet WIP to the dry WIP (highly endothermic, peak of about 100°C). The second is the inert pyrolysis that converts the dry WIP into pyrolysates and char (endothermic, peak about 300-350°C). This reaction actually concerns the degradation of hemicellulose, cellulose and lignin and therefore normally shows different peaks as each polymer is degraded at different temperatures. The third is the oxidative pyrolysis. This reaction is similar to the inert pyrolysis except that it requires oxygen, is normally produced at slightly higher temperatures, is exothermic and does not generate pyrolysates but products. The last is the char oxidation (highly exothermic, peak about 420°C) and concerns the degradation of char using oxygen to produce ash and additional gas products. The nitrogen is also present in the atmosphere but it is assumed not to take part in any of the reactions. Note that all the reactions involve the production of one gas species, progressively reduce the density of the solid material, and involve a reduction of the thickness (shrinking).

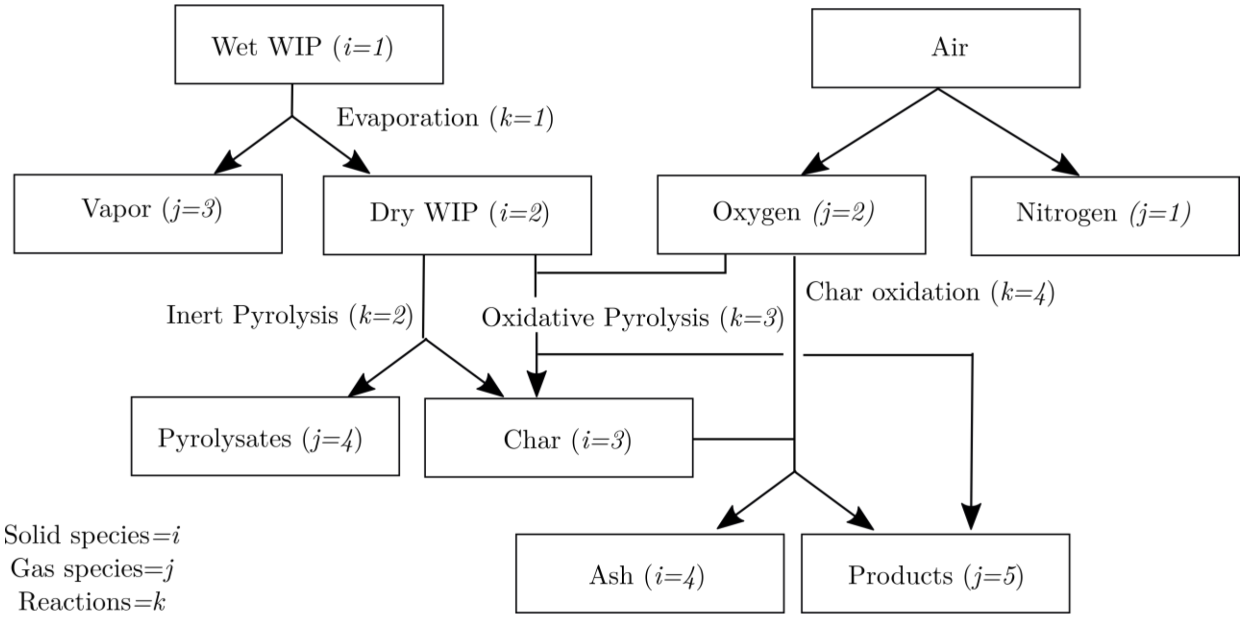

Figure 1: Reactions, solid species and gas species considered in the model

As it will be presented later, all each of those reactions are accounted for by the model by means of a specific Arrhenius-type equation. There are many kinds of Arrhenius expressions but they share the common feature that assume the mass of a solid substance decreases according to the natural algorithm of the temperature. The most common approach to find out the exact parameters that describe such a mass-temperature relationship is to perform a thermogravimetric analysis (TGA) in where the mass decrease is finely measured at a fixed heating rates. In addition, these mass is usually very small, only weights about few milligrams, so that it can be assumed that all stands at the same temperature. This procedure serves to find out the pre-exponential factor, the activation energy and the order of the reaction (assuming one considers a conventional n-order reaction model). Accordingly, during this investigation we performed several TGA experiments at different heating rates and oxygen concentrations in order to find out the parameters of the above four reactions. Although there exist several methods to directly calculate the reaction parameters out of the experiments, we obtained these values by reverse engineering, i.e. we simulated the four reactions with different values until the experimental mass loss and mass loss rate was obtained at different heating rates and oxygen concentrations, see an illustration on the Figure 2 and Figure 3, respectively.

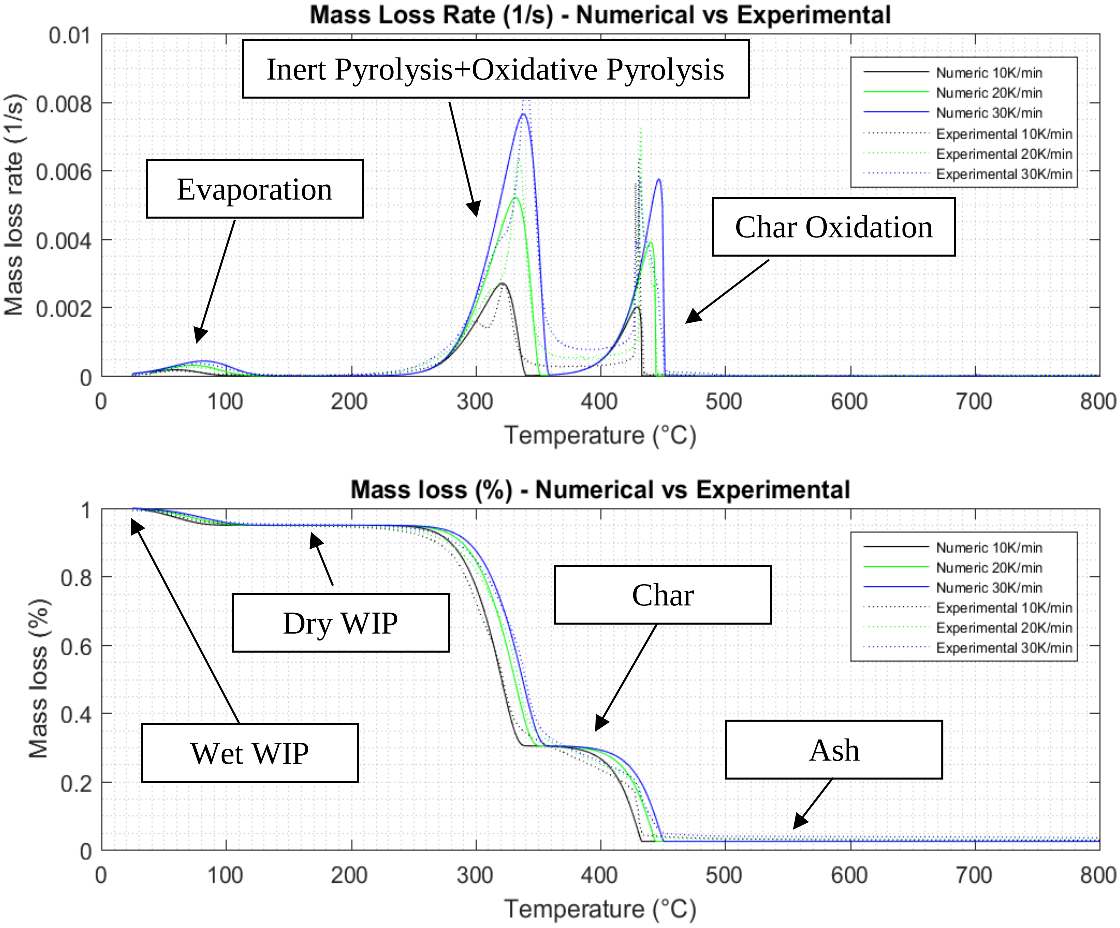

Figure 2: Comparison of modelling and measured reactions at different heating rates

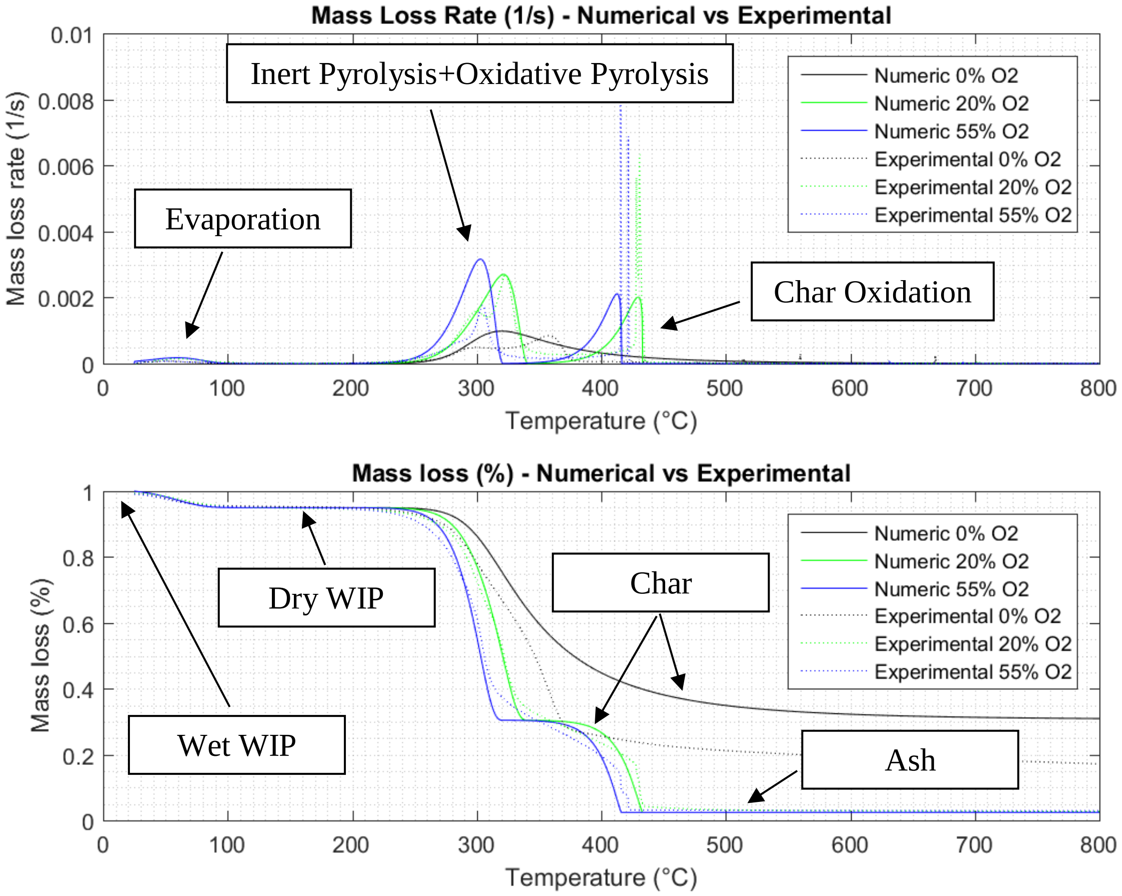

Figure 3: Comparison of modelling and measured reactions at different oxygen concentrations

As shown in the Figure 2 and Figure 3 the modeling of the 4 reactions could be reasonably achieved by using Arrhenius equations, nevertheless, the obtained values were modified afterwards as they were not suitable for modelling larger pieces of WIP as presented later. Some additional information that can be seen out of the above figures is that moisture content of the WIP was about 5% in mass, yield of char was about 20% and yield of ash was about 4%. In addition, the char oxidation seems a very fast reaction that only occurs with oxygen and is less sensitive to oxygen concentration than the oxidative pyrolysis. As presented later, the oxidative pyrolysis is actually the dominating reaction allowing for self-sustaining smoldering. However, in reality this reaction occurs very slowly because it basically depends on oxygen diffusion.

In addition to the TGA experiments, we performed a series of digital scanning calorimetry (DSC) experiments in where one can measure the heat absorbed by a very small sample when heated and thus we could determine the heat capacity of the WIP. The measuring of the heat transfer coefficient was measured via transient hot bridge.

3. 1D EXPERIMENTS: CONE CALORIMETER

In addition to the experiments in small particles, we performed a cone calorimeter experiment of a 100×100×50mm and 213 kg/m3 WIP sample. The cone calorimeter is an extremely precise experiment in where heat release, gas products, oxygen consumption and mass loss of a sample are measured when subjected to a controlled constant radiation source. The experiment we performed was however a non-standard test. After the initial ignition (which occurs just some seconds after experiment starts) we switched off the radiation source so that the sample was actually burning by itself (see Figure 4c). Also 4 thermocouples were inserted at 10, 20, 30 and 40 mm depth inside the sample. See an illustration of the experiment in the Figure 4.

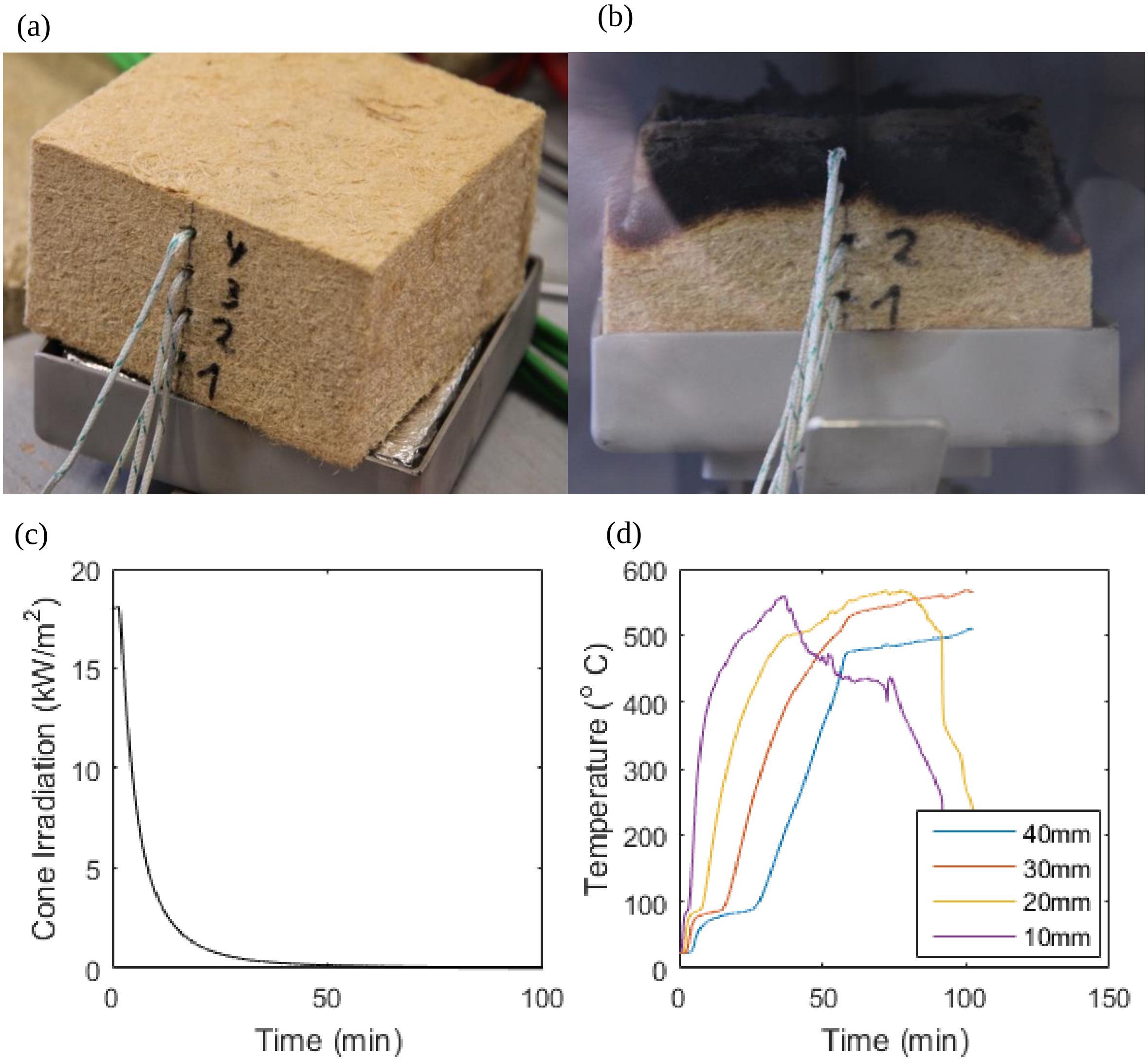

Figure 4: WIP cone calorimeter experiment: (a) sample with 4 thermocouples ready for testing; (b) self-sustaining smoldering of the sample during testing; (c) cone irradiation during test; (d) measurement of temperature at different thicknesses.

This experimented served us to build up our model for self-sustaining smoldering of WIP.

4. NUMERICAL MODEL

A 1D model was constructed to simulate the self-sustaining smoldering experiment presented in the previous section. The main equations of the model are presented in the following. Note however, that for the sake of brevity and simplicity, only the main ideas behind each equation are explained, but not the meaning of all components of the equations. The conservation equations are presented in Table 1, the heat sources in Table 2, and the formation and destruction of the different species and gas in Table 3.

Table 1: Conservation equations

Conserved Quantity	Equation	Explanation
Solid phase conservation	$\frac{\partial \bar{\rho}}{\partial t} = -\dot{\omega}'''_{fg}$	*Δ WIP = – formation of gases*
Mass phase conservation	$\frac{\partial (\rho_g \bar{\psi})}{\partial t} + \frac{\partial \dot{m}''}{\partial z} = \dot{\omega}'''_{fg}$	*Δ gas + gas convection = formation of gases*
Condensed phase species conservation	$\frac{\partial (\bar{\rho} Y_i)}{\partial t} = \dot{\omega}'''_{fi} - \dot{\omega}'''_{di}$	*Δ solid sp. = formation solid sp. – destruction solid sp.*
Gas species conservation	$\frac{\partial (\rho_g \bar{\psi} Y_j)}{\partial t} + \frac{\partial (\dot{m}'' Y_j)}{\partial z} = -\frac{\partial \dot{j}''_j}{\partial z} + \dot{\omega}'''_{fj} - \dot{\omega}'''_{dj}$	*Δ gas sp. + gas sp. convection = gas sp. diffusion – formation gas sp. – destruction gas sp.*
Energy conservation	$\frac{\partial (\bar{\rho} \bar{h})}{\partial t} = -\frac{\partial \dot{q}''}{\partial z} - \dot{m}'' c_{pg} \frac{\partial T}{\partial z} + \sum_{k=1}^{4} \dot{Q}'''_k + \sum_{i=1}^{4} (\dot{\omega}'''_{fi} - \dot{\omega}'''_{di}) h_i$	*Δ enthalpy = - conduction – exchange with gas + reactions sources + change of sensible enthalpy due to formation and destruction of the solid species*
Gas phase momentum (pressure evolution)	$\frac{\partial}{\partial t}\left(\frac{P\bar{M}}{RT}\bar{\psi}\right) = \frac{\partial}{\partial z}\left(\frac{\bar{K}}{\nu}\frac{\partial P}{\partial z}\right) + \dot{\omega}'''_{fg} - g\frac{\partial}{\partial z}\left(\frac{\bar{K}}{\nu}\rho_g\right)$	*Δ gas density = variation due to pressure change + formation of gases – variation due to gravity force*

Table 2: Heat Sources

Heat Source	Equation
Evaporation	$\dot{Q}'''_{ev} = -\dot{\omega}'''_{fvap} \Delta H_{ev}$
Inert pyrolysis	$\dot{Q}'''_{pyri} = -\dot{\omega}'''_{fpgas} \Delta H_{pyr} i$
Oxidative pyrolysis	$\dot{Q}'''_{pyro} = -1.41 \cdot \dot{\omega}'''_{dwo} \left(1 - \frac{\rho_{ch_0}}{\rho_{w_0}}\right) \Delta H_{pyro}$
Char oxidation	$\dot{Q}'''_{chox} = -\dot{\omega}'''_{d_{O_2}} \Delta H_{chox}$

The only boundary condition of the model was setting a decreasing radiation as shown in Figure 4 as well as the cooling by convection and radiation to the ambient. The initial conditions included T_{amb}=298K, P_{amb}=101300Pa, Y_{N2}=0.77, Y_{O2}=0.23 and Y_m=1.The thermal material parameters and the kinetic values used for the different species and reactions were those measured in the TGA and DSC experiments, and for the rest unknown values, the values reported for wood and cellulose were considered instead [5,6]. The model was implemented in the research software GPyro [6], that is based in the control or finite volume element method (FVM) [7] and uses a tridiagonal matrix algorithm for the numerical solution procedure. Note that the partial differential equations have a very strong dominance of the source term, so that the decomposition is mandatory and the FVM is much more convenient than FEM. In addition, the FVM is very strong to ensure conserved quantities throughout each element. The size of the mesh was set to 0.25 mm and initial time step to 0.05

seconds. Finally, we also considered an overall shrinking (mesh reduction) of about 30% after WIP was consumed.

Table 3: Formation and destruction of species and gas

Species	Formation	Destruction
Wet WIP	–	$\dot{\omega}'''_{dm} = \bar{\rho} Y_m A_{ev} \exp\left(-\frac{E_{ev}}{RT}\right)$
Dry WIP	$\dot{\omega}'''_{fw} = \dot{\omega}'''_{dm} \frac{\rho_{w_0}}{\rho_{m_0}}$	$\dot{\omega}'''_{dwi} = \bar{\rho} Y_w A_{inpyr} \exp\left(-\frac{E_{inpyr}}{RT}\right)^{n_{inpyr}}$ $\dot{\omega}'''_{dwo} = \bar{\rho} Y_w A_{oxpyr} \exp\left(-\frac{E_{oxpyr}}{RT}\right)^{n_{oxpyr}} Y_{O_2}^{n_{O_2,k}}$
Vapor	$\dot{\omega}'''_{fv} = \dot{\omega}'''_{dm}\left(1-\frac{\rho_{w_0}}{\rho_{m_0}}\right)$	–
Char	$\dot{\omega}'''_{fch} = \dot{\omega}'''_{dw} \frac{\rho_{ch_0}}{\rho_{w_0}}$	$\dot{\omega}'''_{dch} = f\left(\alpha_{A_k}\right)\bar{\rho} Y_{ch} A_{chox} \exp\left(-\frac{E_{chox}}{RT}\right) Y_{O_2}^{n_{O_2,k}}$ Where $f\left(\alpha_{A_k}\right) = \frac{3/2}{\left(1-\alpha_{A_k}\right)^{-1/3}-1}$
Pyrolysates	$\dot{\omega}'''_{fpgas} = \dot{\omega}'''_{dwi}\left(1-\frac{\rho_{ch_0}}{\rho_{w_0}}\right)$	–
Ash	$\dot{\omega}'''_{fash} = \dot{\omega}'''_{dch} \frac{\rho_{ash_0}}{\rho_{ch_0}}$	–
Products	$\dot{\omega}'''_{fprod} = 1.41 \cdot \dot{\omega}'''_{dwo}\left(1-\frac{\rho_{ch_0}}{\rho_{w_0}}\right) +$ $3 \cdot \dot{\omega}'''_{dch}\left(1-\frac{\rho_{ash_0}}{\rho_{ch_0}}\right)$	–
Oxygen	-	$\dot{\omega}'''_{dO_2} = 0.41 \cdot \dot{\omega}'''_{dwo} + 2 \cdot \dot{\omega}'''_{dch}$
Total gas	$\dot{\omega}'''_{fgas} = \dot{\omega}'''_{fv} + \dot{\omega}'''_{fpgas} + \dot{\omega}'''_{fprod} - \dot{\omega}'''_{dO_2}$	$\dot{\omega}'''_{dgas} = \dot{\omega}'''_{dO_2}$

5. MODELLING THE SELF-SUNTAINING SMOLDERING OF WIP

The modelling with the values obtained from the 0D experiments, and those from literature did not succeed on modelling the self-sustained smoldering of WIP. The smoldering was stopping after radiation was removed, so it seemed rather impossible to achieve a self-sustaining process without any external heat source. Thus, we decided to use the suite of measured and reported values as initial guess, and performed an optimization analysis to find out whether it was possible to simulate to simulate self-sustaining smoldering of WIP or not. After about 3000 simulations with genetic and latin hypercube algorithms we achieved a relatively good approximation using reasonable material parameters, see Figure 5. Note we only compared the first 25 minutes of the test (Figue 4d) as reference, because after that point the material at the top was very degraded and the thermocouples started sliding, so the measurements were not reliable anymore.

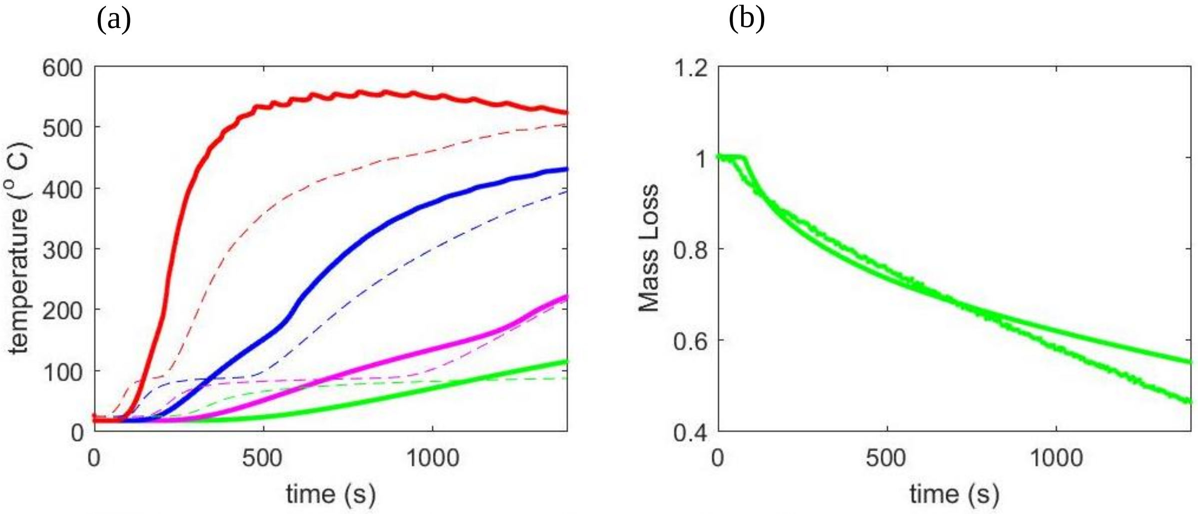

Figure 5: Simulation of self-sustaining smoldering of WIP (a) comparison of experimental (dashed) and simulated (continuous) temperatures, and (b) experimental (noisy) and numerical (continuous) mass loss.

6. CONCLUSION

In this research we aimed at modelling the self-sustaining smoldering of wood insulation products in order to develop more efficient wood protective treatments and spread the utilization of the wood as an insulation material. For the best knowledge of the authors, previous similar models always tried to simulate the smoldering of wood using an external heat source, thus this problem was not modeled before.

In order to develop such a model, a suite of TGA and DSC experiments to determine the material parameters was performed and the remaining not measured values were obtained from the literature. The self-sustaining smoldering was tested by conducting a non-standard cone calorimeter experiment of a 100x100x50mm WIP sample in where the radiation of the cone was switched off after about 4 minutes after test started. Thus, the wood was degraded in a very slow fashion for about two hours, as it happens in reality, and this result was used as a reference. The model accounted for the conservation of mass, momentum, energy and species of the wood as well as the vaporization, inert pyrolysis, oxidative pyrolysis and char oxidation reactions. The oxygen consumption and its flow, as well as the wood shrinking were also taken into account.

First results did not succeed in modelling the self-sustaining smoldering but we use the initial material parameters as the initial guess of an optimization process based on genetic and latin hypercube algorithms. After about 3000 simulations in where we searched the material parameters within realistic ranges, the self-sustaining smoldering was achieved obtaining similar temperatures and mass loss ratios as those measured in the experiment.

The results of the model open the door to a new understanding of the process that eventually could contribute to solve this long standing smoldering problem. It is remarkable that if one performs a smoldering experiment the chance to stop the process is virtually zero. However, we needed almost 3000 simulations until self-sustaining smoldering without external heat sources could be achieved. This, and also our observations during the modelling process, suggest that the smoldering is given by an extremely delicate equilibrium between the oxygen consumption, oxygen flow/flux and reactions, it appears however very hard to brake such extremely fine balance in nature. This is also evidenced by the fact that the heat of the char oxidation reaction is extremely large and in principle would be sufficient to trigger a very fast degradation of the wood. The process is however extremely slow which indicates that the oxygen, which mostly penetrates by diffusion, is being consumed according to the finest equilibrium.

REFERENCES

[1] Kolb, T., Neumann, M., Rüther, N. and Guindos, P. 'Glimmbeschleunigung als neuer Materialkennwert', *Holztechnologie* (in press).

[2] Moallemi, M. K., Zhang, H. and Kumar, S. 'Numerical modeling of two-dimensional smoldering processes' *Combustion and Flame* 95(1) (1993) 170-182.

[3] Das, O. 'Modelltheoretische Untersuchungen von Schwel- und Glimmbränden in Dämmschichten, Simulation von Schwel- und Glimmbränden in Cellulose' Fortschritt-Berichte VDI Nr. 154. VDI Verlag (1999) Düsseldorf.

[4] De Souza Costa, F. and Sandberg, D. 'Mathematical model of a smoldering log' *Combustion and Flame* 139(3) (2004) 227-238.

[5] Kashiwagi, T., & Nambu, H. 'Global kinetic constants for thermal oxidative degradation of a cellulosic paper' *Combustion and Flame* 88(3-4) (1992) 345-368.

[6] Lautenberger, C. and Fernandez-Pello, C. 'Generalized pyrolysis model for combustible solids' *Fire Safety Journal* 44(6) (2009) 819-839.

[7] Patankar, S. 'Numerical heat transfer and fluid flow' (1980) CRC press.