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A pyrolysis model for steel-insulation sandwich building façade systems under fire

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Abstract

Sandwich panels consist of two thin-walled steel faces plus an insulation core. For this core, materials are selected that provide high (shear) stiffness and high thermal resistance. When the panels are subject to fire, the (a) temperature-dependent behaviour of the steel faces and (b) the possible chemical reactions of the insulation core should both be considered, to accurately predict the structural behaviour. Provisions in Eurocode EN 1993-1-2 can be used for (a). Regarding (b), this paper adds a verified pyrolysis model to Heat Transfer (HT) analyses, and obtained results are transferred to a Structural Response (SR) analysis. Then, the HT and SR analyses are demonstrated in so-called One-Way Coupled (OWC) and Two-Way Coupled (TWC) fire-structure simulations, the latter including the effects of structural failure on the fire behaviour. For the cases studied, structural behaviour for OWC and TWC simulations is very similar, which indicates that the structural (failure) behaviour does not significantly influence the fire behaviour. Differently, the difference in failure time between simulations with and without pyrolysis is more than 15%, due to endothermic effects. As such, for the cases studied, modelling of pyrolysis is more important than the effect of structural failures, and this modelling can be included as demonstrated in this paper.

Keywords

Heat transfer analysis, Structural response analysis, Pyrolysis, Coupled fire-structure simulation, Sandwich panel

1 Introduction

Buildings façades can be made with sandwich panels, which consist of two thin-walled plates (faces) and a core. Traditionally, materials like stone wool, PUR (polyurethane), PIR (polyisocyanurate), EPS (expanded polystyrene), and XPS (extruded polystyrene) have been used for the core. The flammability of these materials has been investigated by researchers such as Giunta d'Albani et al. [1]. However, with advancements in material science, also polymer composites are used for the core, for example, to increase stiffness [2,3]. While most research has focused on the mechanical behaviour of such novel sandwich panels to overcome traditional panel problems [4], composite materials may increase fire risks. For instance, Khan et al. found that typical flame-retardant aluminium composite panels could ignite at a lower heat flux than traditional panels [5]. Birman et al. concluded that it is necessary to account for the process of resin decomposition in sandwich panels (including composites), as this may significantly affect panel deformations [6]. This is due to chemical reactions that take place when composite materials are exposed to fire, and the resin degrades, partly becoming a gaseous product, changing thermal and mechanical properties.

When a sandwich panel with an insulation core is exposed to fire, simulations may help to understand the panel's behaviour. These simulations include thermodynamic and thermomechanical aspects. Firstly, using a Heat Transfer (HT) analysis, the temperature distribution within the structure is predicted. The thermal boundary conditions for the HT model may come from a fire dynamics simulation, using the concept of the Adiabatic Surface Temperature (AST) [7]. Next, the thermal data from the HT model is transferred to a Structural Response (SR) model to analyse the mechanical behaviour. By following these procedures, including a fire dynamics simulation, a so-called One-Way Coupled (OWC) fire-structure simulation is conducted. Additionally, if structural behaviour (e.g. the failure of a panel) influences the fire development, this structural behaviour can be coupled back to the fire dynamics simulation. This is called a Two-Way Coupled (TWC) simulation, demonstrated by Feenstra et al. and De Boer et al. [8,9].

This paper introduces the concept of including a pyrolysis model in OWC and TWC fire-structure simulations. Section 2 provides the theory and finite element implementation of the pyrolysis model. Then, in Section 3, the implementation is verified, whereafter in Section 4 it is demonstrated for OWC and TWC simulations. In that section, also the importance of pyrolysis phenomena in relation to the inclusion of structure-to-fire effects is discussed. Finally, conclusions and recommendations for future research are given in Section 5.

2 Pyrolysis model: governing equations and implementation

The pyrolysis model used in this paper is based on the work of Henderson et al. [10] and further developments by Zhang [11]. A brief review of the governing 1D equations is provided here. Combustion is not modelled, and the model has the following assumptions: (a) there is no thermo-chemical expansion in the solid phase; (b) there is no accumulation of decomposition gases in the solid phase; (c) thermal equilibrium (i.e., equal temperatures) exists between these gases and the solid material. Under these assumptions, the three governing Eqs. (1) to (3) need to be solved simultaneously. Firstly, the one-dimensional heat transfer equation considering the pyrolysis behaviour in the x-direction is given by:

$$\frac{\partial}{\partial t}(\rho h) = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) - \frac{\partial}{\partial x}(\dot{m}_g h_g) - Q\frac{\partial \rho}{\partial t} \quad (1)$$

where ρ is the instantaneous density of the solid material [kg/m^3], t is the time [s], T is the temperature [K], x is the location [m], k is the thermal conductivity of the solid material in x-direction [W/(mK)], h and h_g are enthalpies of the solid material and gas [J/kg] respectively. Variable $\dot{m}_g$ is the mass flux of the gas (as a product of the pyrolysis reaction) [kg/(m^{2}s)], and Q is the so-called heat of decomposition [J/kg]. With decreasing density, if Q has a negative value, the material enthalpy will decrease, so an endothermic reaction takes place.

Secondly, the decomposition of the pyrolyzing material is given by the Arrhenius Equation. For an n-th order reaction:

$$\frac{\partial m}{\partial t} = -A(m_v - m_c)\left(\frac{m-m_c}{m_v-m_c}\right)^n e^{-\frac{E}{RT}} \quad (2)$$

where m, m_v, and m_c are the instantaneous mass, the virgin (unpyrolyzed) material's mass, and the char (e.g. fully pyrolyzed) material's mass [kg]. Symbol A is the pre-exponential factor [s^{-1}], symbol n is the order of reaction, E is the activation energy [J/mol], and R is the universal gas constant: 8.314 [J/(Kmol)].

Thirdly, if the accumulation of gases over the total material thickness l [m] is ignored, the mass flux of the gas at an arbitrary location x can be expressed by the conservation of mass as:

$$\dot{m}_g = -\int_l^x \frac{\partial \rho}{\partial t} dx \quad (3)$$

Expanding the left part of the 1D heat transfer Eq. (1) by the chain rule, defining the specific heat of the solid and gas by C_s and C_g, and combining this with 3D heat transfer equations yields:

$$C_s = \frac{\partial h}{\partial T},\ C_g = \frac{\partial h_g}{\partial T} \quad (4)$$

$$\rho C_s \frac{\partial T}{\partial t} - \nabla\left(k_1\frac{\partial T}{\partial x}\mathbf{i} + k_2\frac{\partial T}{\partial x}\mathbf{j} + k_3\frac{\partial T}{\partial x}\mathbf{k}\right) - C_g\frac{\partial T}{\partial x}\int_l^x \frac{\partial \rho}{\partial t}dx + \frac{\partial \rho}{\partial t}(Q + h - h_g) = 0 \quad (5)$$

with $\mathbf{i}, \mathbf{j}, \mathbf{k}$ being the unit vectors in the x, y, z-directions respectively.

With respect to the fire-structure coupled simulations, first a fire is simulated by the program Fire Dynamics Simulator FDS), which has been verified to correctly predict smoke and heat phenomena [13]. The thermal data from FDS is transferred to the HT analysis via ASTs [7], from which in the HT analysis the heat flux q_{total} on the structure can be calculated by:

$$q_{total} = \varepsilon\sigma\left(AST^4 - T_{surf}^4\right) + h_{cv}(AST - T_{surf}) \quad (6)$$

where ε and h_{cv} are the emissivity and heat transfer coefficient of the surface, σ is the Stefan Boltzmann constant 5.6703×10^{-8}[W/(m^{2}K^4)], and T_{surf} is the surface temperature in the HT analysis [K]. The implementation of the pyrolysis model in the fire-structure simulations (the latter based on Feenstra et al. [8]) is shown in Figure 1, which presents the software and scripts used. In the outer loop, blue boxes refer to public or commercial software (FDS and Abaqus), and orange boxes to in-house developed C++ or Fortran programs and Python scripts. In the middle, **FDS-2-Abaqus** is the name of the management program, which (re)starts and stops the programs and scripts, and controls overall variables like the load step size.

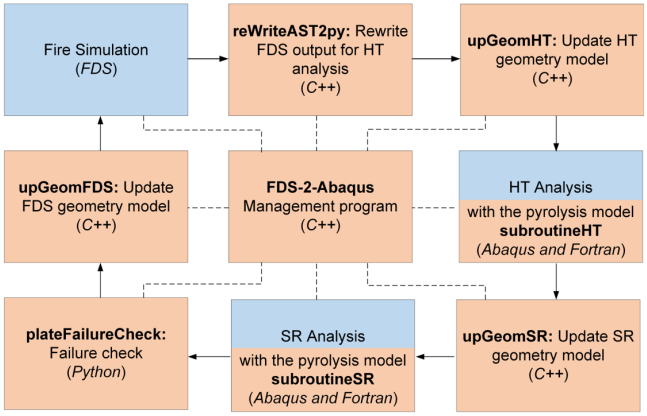

Figure 1 Implementation of the pyrolysis model in fire-structure simulations, one clockwise cycle equals one load step.

A fire-structure simulation starts with an FDS fire dynamics simulation, whereafter the AST data are rewritten by the **reWriteAST2py** program to a format that can be read by the HT model (itself updated by **upGeomHT**). During the HT analysis, the pyrolysis model, implemented by the user subroutines UMATHT and USDFLD in Abaqus [12], is involved in giving a more accurate prediction for the temperature distribution within the structure. Subsequently, the resulting temperature data is transferred to the SR model (as updated by **upGeomSR**) for the SR analysis, in which material properties depend on their pyrolysis level). After the SR analysis, structural failure is checked by the script **plateFailureCheck**, and failed parts are removed

before the next load step, both in the HT and SR models.

3 Pyrolysis model verification

Both the pyrolysis model and the coupled fire-structure simulations should be verified before application. The fire-structure simulations were verified by Feenstra and De Boer [8,9], so here only the pyrolysis model is verified, by a case by Zhang [11], shown in Figure 2 bottom right. Using a 2D scheme, a sample is loaded by a heat flux equal to 25 kW/m^2 on the left, and initial temperatures are set to 27 °C for all surfaces. Material properties are listed in Table 1.

Table 1 Material properties for case Zhang [11].

Material properties	Values
Virgin density ρ_v [kg/m³]	1700
Pyrolyzed density ρ_c [kg/m³]	1255
Solid specific heat C_s [J/(kgK)]	1100
Solid thermal conductivity k_s [W/(mK)]	0.3
Gas specific heat C_g [J/(kgK)]	3000
Heat of decomposition Q [J/kg]	-2.0×10^5
Pre-exponential factor A [s^{-1}]	5.0×10^{28}
Activation energy E [J/mol]	3.62×10^5
Order of reaction n	4.6

The simulation is carried out by a transient HT analysis, using 2D DS4 shell elements with a size of 1.0×0.625 mm (20 elements in total). A fixed increment size of 50 seconds is used. Figure 2 shows temperatures versus time for the results from Zhang (green line) [11], and the pyrolysis model in this paper (orange circles).

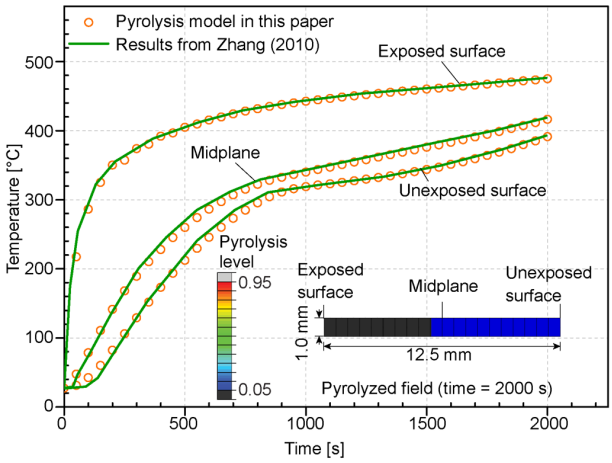

Figure 2 Verification of the pyrolysis model.

Despite slightly different implementations, the two models predict the same behaviour for all three surfaces (exposed surface, midplane, and unexposed surface). Using user-subroutine USDFLD in Abaqus, the contour in Figure 2 shows the pyrolysis level (by a so-called field variable) at the end of the simulation (t=2000 s), from 0 to 1, with 0 for fully pyrolyzed. It can be concluded that the pyrolysis model functions correctly and can be used for fire-structure simulations.

4 Case study

In this section, the pyrolysis model is used in concert with fire-structure simulations, modelling an academic/practical case, consisting of an office room with a façade of sandwich panels. The setup is explained in Section 4.1, and for illustration purposes a typical simulation is demonstrated in Section 4.2. Section 4.3 then presents simulations that show the effects of pyrolysis, as well as the effects of using either OWC or TWC type of simulations.

4.1 Model setup

The simulations start with a fire simulation by FDS, which models an office compartment, sized 5.4×3.6×2.7 m^3, see Figure 3 on the left, and using cubic CFD elements sized 0.15×0.15×0.15 m^3. On the sides of the office room, two additional spaces are modelled (not shown in Figure 3), for a corridor and outside space respectively, to allow for airflow into the office. A door with a width of 1.2 m and a height of 2.1 m is modelled between the corridor and the office. A 1h fire is simulated, with cellulose selected as a fuel, having a specified heat release rate of 4.0 kW, as suggested by Eurocode 1991-1–2 for a standard compartment fire [14]. The walls, floors (except the façade) and ceiling of the office room are assumed to be concrete, in FDS being "obstructions" with a thickness of 0.3 m, density of 1800 [kg/m^3], specific heat of 1.00 [kJ/(kgK)], conductivity of 1.15 [W/(mK)], and an emissivity of 0.8. The façade consists of 12 sandwich panels (4×3) with adiabatic properties, each having 4 measuring points to record the AST values, as mentioned in Section 2.

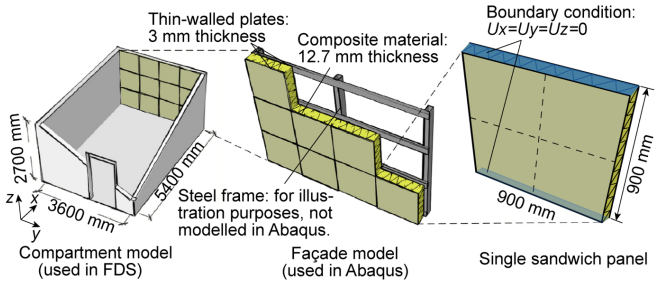

Figure 3 Compartment with a façade that consists of sandwich panels with an insulation core.

Only the façade needs to be modelled for the HT and SR analyses. Therefore, in the corresponding finite element models, 12 panels are modelled as shown in Figure 3 in the middle. For the HT analyses, each panel is divided into four partitions (indicated by dotted lines on the right), where each partition is related to a single AST point in the fire simulation. Each sandwich panel, sized 0.9×0.9 m^2, consists of two thin-walled steel faces and an insulation core. Conductivity between the faces and core is defined by so-called interaction properties. The sandwich panels are assumed to be thermally (and structurally) independent. For the panel faces, shell elements DS4 (size 150×150 mm^2) are used, which are tied to volume elements DC3D8 (150×150 mm × 5 layers along the thickness) for the insulation core. Although as such the volume elements are distorted, they show to relay the temperatures from the shell elements correctly. The faces of steel grade S355 have temperature-dependent thermal properties, as given by Eurocode EN 1993-1-2 [15]. Regarding the insulation core, thermal material properties from Table 1 are used for

demonstration purposes. For e.g. sandwich panels with PIR insulation, properties can be used as given in [12]. The following boundary conditions are used: The thin-walled steel faces have a convection coefficient equal to 25 [W/(m^{2}K)] and an emissivity coefficient of 0.8. For the fire-exposed side, the ambient temperature is set to the AST (different for each AST point and so partition), whereas on the outside, the uniform ambient temperature is 0 °C. The problem is solved using an Abaqus transient heat transfer step, with automatic (increment) time stepping, with a maximum step size of 10 seconds.

For the SR simulations, the geometry is similar to the HT simulations: again for 12 panels, two thin-walled steel faces are tied to an insulation core. Shell elements S8 are used for the steel faces, and volume elements C3D20R are applied for the core. Mesh sizes are the same for the SR and HT models, see above. The temperature-dependent thermal expansion coefficient of the S355 steel faces follows EN 1993-1-2 [15], and the density is set to be a constant 7850 kg/m^3. The constitutive stress-strain relation of the steel is taken from the conceptual prEN 1993-1-14 [16], and the temperature-dependent properties are from EN 1993-1-2 [15], all visualised in Figure 4. Note that for Abaqus, the Eurocode engineering stress-strain (σ_{eng}-ε_{eng}) curves should be converted to true stress-strain (σ_{true}-ε_{true}) curves by:

$$\sigma_{true} = \sigma_{eng}(1 + \varepsilon_{eng}) \quad (7)$$

$$\varepsilon_{true} = \ln(1 + \varepsilon_{eng}) \quad (8)$$

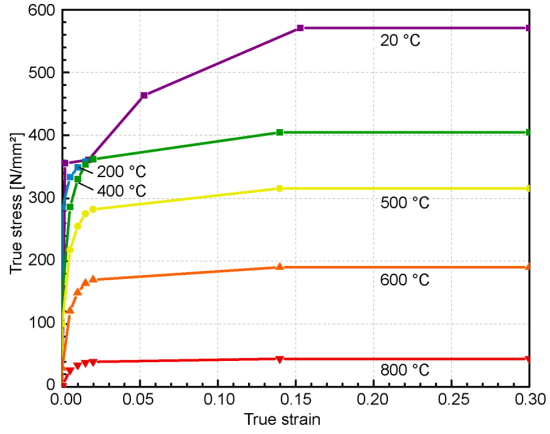

Figure 4 Temperature-dependent properties of S355 steel.

The Young's modulus of the insulation core at ambient temperature is 6.75×10^{10} [N/m^2] [10], which in this paper is assumed to be dependent on the pyrolysis level: the Young's Modulus decreases linearly from the above value for virgin material (density of 1700 [kg/m^3]) to half this value (3.375×10^{10} [N/m^2]) for fully pyrolyzed material (density of 1255 [kg/m^3]). Thermal expansion is not considered for the insulation core. Since the frame as shown in Figure 3 is not modelled, each panel is supported at the top and bottom edge (indicated by blue in the figure) by restraining all related finite element nodes in all three directions. Loading is applied via the results of the HT analysis, i.e. temperatures in time. An implicit dynamic solver is used, including geometric and material non-linearities. Automatic (increment) time stepping is applied, with a maximal increment size of 10 seconds.

4.2 Demonstration

To illustrate the fire-structure simulations, including the effects of pyrolysis, a typical TWC simulation is shown in Figure 5, using the software and scripts as explained in Figure 1, and the setup as presented in the previous section.

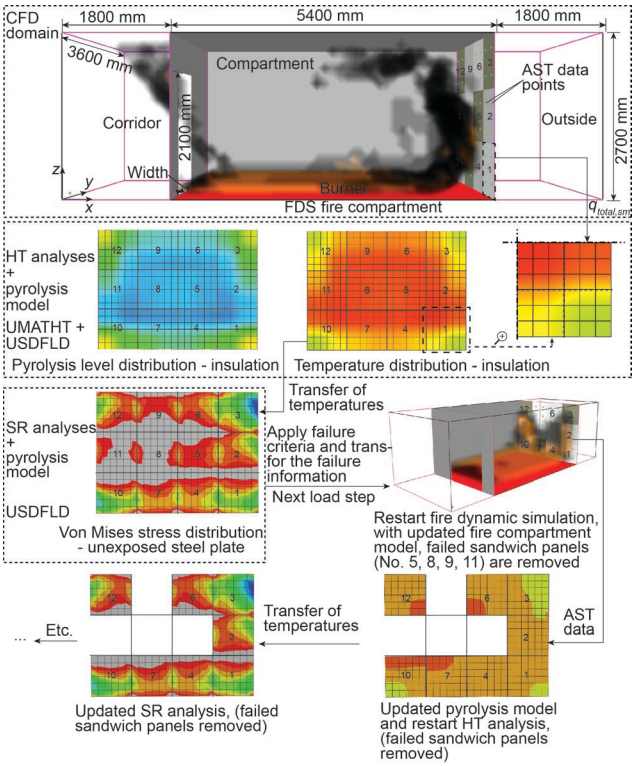

Figure 5 Demonstration of a typical TWC fire-structure simulation, including pyrolysis.

The top part of Figure 5 shows the fire simulation, including the corridor, compartment, burner, outside region, and the façade with AST data points. Following the procedure in Figure 1, a 1h fire is divided into 18 load steps of 200 seconds each. For each load step, the fire simulation is carried out, whereafter the AST data is transferred to the HT analysis. For the same load step, the HT analysis predicts (by the UMATHT and USDFLD subroutines) the pyrolysis levels (next row, on the left) in combination with the temperature distribution (in the middle). Then, the nodal temperatures vs. time as found in the HT analysis are transferred to the SR analysis, where the pyrolysis level of each integration point is recalculated by the user subroutine USDFLD. After the SR analysis, failure criteria are applied, and if a panel has failed, it is removed for the next load step. Since in the next section models with and without pyrolysis will be studied, the failure criterion is selected to be a panel having an overall temperature of 420 °C (or higher), since 95% of the material will be pyrolyzed at this temperature. In the figure, panels 5, 8, 9, and 11 fail, which is of influence on the fire behaviour and the subsequent HT and SR analyses.

4.3 Effects of pyrolysis in coupled fire-structure simulations

In this section, the pyrolysis model is used in fire-structure simulations such that the effects can be studied of (a) pyrolysis on structural failure and (b) structural failure on the fire.

For an arbitrary panel, here panel 5, Figure 6(a) compares the TWC simulation of Section 4.2 with pyrolysis to a similar simulation but without pyrolysis. In both simulations, after some time panel 5 becomes so hot that it is regarded as failed. However, for the simulation with pyrolysis, this clearly takes more time, due to the endothermic character of the pyrolysis. Panels show a complex mechanical response (e.g. deformations), further elaborated in [12]. Figure 6(b) shows the number of failed panels vs. simulation time for the complete TWC simulation. The model with pyrolysis shows a later start of failures, for which the total duration is also longer, which indicates that fire risks may be overestimated in a model without pyrolysis. Of course, this overestimation depends on the amount of pyrolysis material, the ability of decomposition gasses to escape, etc.

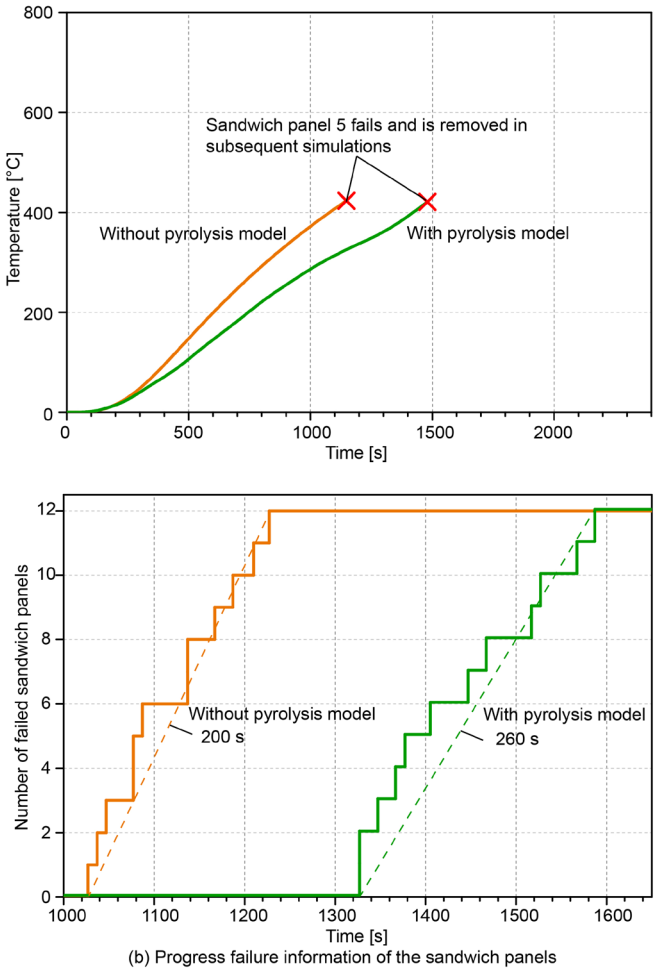

Figure 6 TWC fire-structure coupled simulations with and without pyrolysis.

To put the above effects in perspective, the differences between OWC and TWC simulations are investigated in the following, with all simulations including the pyrolysis model. Three door widths (0.9, 1.05, and 1.2 m) are tried in the FDS model, to obtain different fire scenarios, i.e. fuel or ventilation controlled. All other aspects of the simulations are the same as those already demonstrated. Results are shown in Figure 7.

Figure 7(a) shows the Heat Release Rate (HRR) in time. If the HRR matches the specified value in the FDS simulations (the horizontal black line), the fire scenario is considered fuel controlled. This is the case for a door width equal to 1.2 m, as its green line (on average) always equals the specification. For a door width equal to 1.05 m, the beginning of the simulation sees a ventilation-controlled fire, as not enough oxygen can be supplied. However, as soon as panels fail, also this simulation leads to a fuel-controlled fire. For the smallest door width (0.9 m), the fire is less severe as oxygen supply is limited. Consequently, no panels fail, and so the fire stays ventilation-controlled.

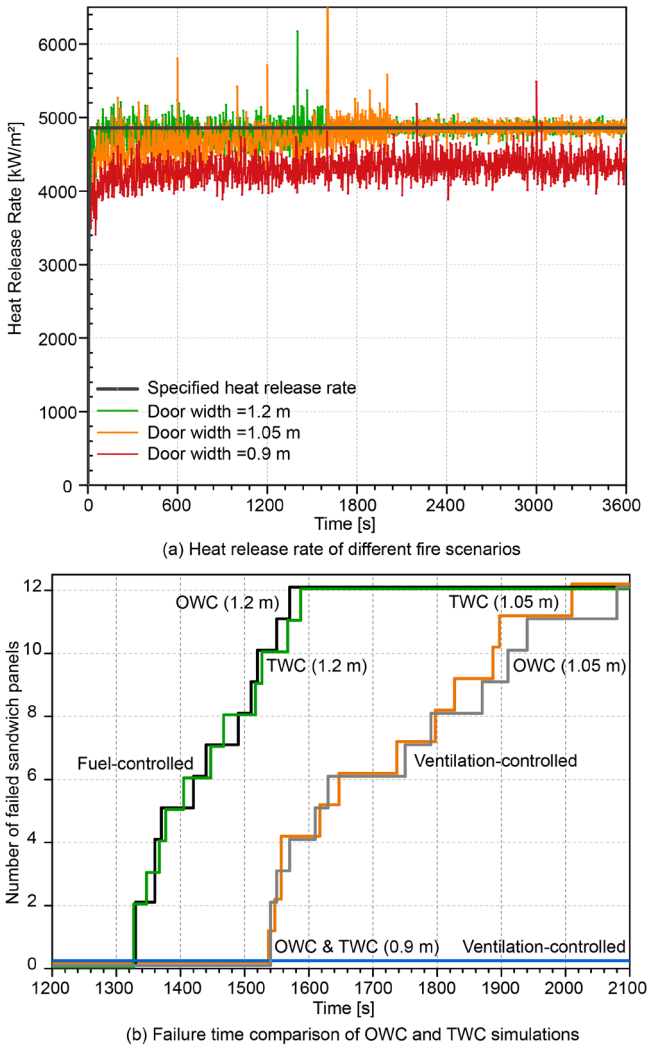

Figure 7 (a) Failed panels vs. time and (b) heat release rate vs. time for different door widths.

The number of failed sandwich panels vs. time is shown in Figure 7(b), for the three door widths and OWC and TWC simulations. OWC and TWC simulations are equal within a time envelope of 5% of the total time, which indicates that the structural behaviour does not significantly influence the fire behaviour. Nevertheless, for the ventilation-controlled situation, structural failure is somewhat accelerated by the TWC simulation, as the openings make the fire fuel-controlled and so more severe. For the case in this paper, the difference between simulations with and without pyrolysis (Figure 6(b)) is more than 15% of the total time, somewhat equal to the effect of the difference between a fuel-controlled and ventilation-controlled fire. Therefore, here the modelling of pyrolysis (and the fire scenario) are more important than the selected coupling method (OWC or TWC). However, naturally, this conclusion depends on

the type of problem studied.

5 Conclusions and future work

An existing theory for 1D pyrolysis has been implemented, verified by an existing model, and incorporated in 3D coupled fire-structure simulations.

A case study has been used to demonstrate 3D TWC fire-structure simulations, including pyrolysis. For this an office room was modelled, including a sandwich panel façade, which showed to progressively fail under fire, influencing the fire behaviour and subsequent HT and SR analyses.

To quantify the effects of pyrolysis, TWC simulations with and without pyrolysis were compared. This showed that a panel fails later if pyrolysis is considered, due to the endothermic character of the pyrolysis. Finally, including pyrolysis, OWC and TWC simulations have been compared, for different door openings, which results in different fire scenarios. For the case studied, the effects of pyrolysis and the developed fire scenario were about equally strong, and much more important than the small differences between OWC and TWC simulations. Naturally, TWC simulations only made a difference for ventilation-controlled fires, since panel failures result in openings, which improve oxygen supply.

In this paper, the mechanical properties of the insulation core were assumed as dependent on the density. More realistic properties, related to and including thermochemical expansion, pore formation, viscoelasticity, and delamination behaviour, should be studied.

Future research will study the inclusion of both a pyrolysis model and a two-scale method (providing detailed simulations of bolt and screw connections) in TWC fire-structure simulations.

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