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# Application of a Simple Enthalpy-Based Pyrolysis Model in Numerical Simulations of Pyrolysis of Charring Materials

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## Abstract

A new, simple pyrolysis model for charring materials is applied to several numerical and experimental test cases, with variable externally imposed heat fluxes. The model is based on enthalpy. A piecewise linear temperature field representation is adopted, in combination with an estimate for the pyrolysis front position. Chemical kinetics are not accounted for: the pyrolysis process takes place in an infinitely thin front, at the 'pyrolysis temperature'. The evolution in time of pyrolysis gases mass flow rates and surface temperatures are discussed. The presented model is able to reproduce numerical reference results, which were obtained with the more complex moving mesh model. It performs better than the integral model. We illustrate good agreement with numerical reference results for variable thickness and boundary conditions. This reveals that the model provides good results for the entire range of thermally thin and thermally thick materials. It also shows that possible interruption of the pyrolysis process, due to excessive heat losses, is automatically predicted with the present approach. Finally, an experimental test case is considered.

**Key words:** Pyrolysis, charring materials, enthalpy model

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## 1 Introduction

In the early stages of a fire, flame spread always plays an important role. In numerical simulations, this requires coupling of gas phase CFD (‘Computational Fluid Dynamics’) simulations, including combustion and radiation, to pyrolysis simulations in the solid material. To that purpose, it is advantageous to keep the pyrolysis model simple.

The real material behaviour is in general very complex. Phenomena like melting, surface oxidation, smouldering etc can occur. In the present paper we deliberately avoid discussion of these phenomena.

Depending on the residue left after pyrolysis, materials are called ‘charring’ (char is left after pyrolysis) or non-charring. A widely used charring material in the construction of buildings is wood. Although non-charring materials (e.g. PMMA) are also very important and experimentally and theoretically studied in great detail (e.g. [1, 2]), we focus here on dry charring materials for the basic application of our model. In [3, 4] we discuss the theoretical background in more detail and illustrate applications for charring materials with moisture content and for non-charring materials.

During the past two decades, several numerical models were developed for pyrolysis, of charring materials with different levels of complexity, such as: Arrhenius-type models [5]; ‘integral’ models [6-9]; an ‘extended’ integral model [10]; a moving mesh model [11]; a dual mesh model [12]. Reviews on pyrolysis modelling have been provided in e.g. [13, 14]. The motivation of the present paper, in which we describe a simplified pyrolysis model, based on enthalpy, is the relative ease to couple the model to gas phase CFD simulations for flame spread calculations.

The model, presented below, has compared to existing pyrolysis models as the most important advantages that:

- It is simple to implement;
- It is readily extended to more dimensions (in contrast to e.g. the integral model and moving grid models).

We apply the model to the series of basic numerical test cases, described in [11]. As such, the present paper can, to a certain extent, be regarded as a follow-up paper of [10]. In addition to the mentioned advantages, we illustrate that, with respect to variable heat fluxes in time, the present model performs very well. It performs better than integral type models as in [10]. The influence of the solid thickness and boundary conditions is shown. Finally, we discuss a comparison to experimental data and reveal the influence of material properties and model parameters on the results. First of all, we provide a brief model description. A more complete description and a sensitivity study with respect to numerical aspects (grid size and physical time step) are found in [3, 4].

## 2 Model description

### 2.1 Assumptions

An enthalpy based model approach is applied in the simulations below. Pyrolysis is modelled as an infinitely fast, irreversible, endothermic and isothermal process at the 'pyrolysis temperature' $T_{pyr}$, so that reaction kinetics are not considered and the pyrolysis zone in principle becomes infinitely thin ('pyrolysis front'). The endothermic transition process from virgin material to char material requires a constant amount of enthalpy per unit volume, equal to $\left(\rho_v - \rho_c\right)\Delta Q_{pyr}$ at temperature $T_{pyr}$. Note that $T_{pyr}$ and $\Delta Q_{pyr}$ are thus model parameters which are kept constant during the simulation. In [15], it is described, based on energy and mass balances, how to find $T_{pyr}$ such that the same amount of energy is consumed to produce the same amount of mass if a finite rate kinetics model is used for the entire charring process. Pyrolysis gases are assumed to leave the solid as soon as they are generated (no accumulation of gases). They are assumed in thermal equilibrium with the solid everywhere. Clearly, the mentioned simplifications imply limitations on the validity range of the models as described. In [3, 4], we extend the model for application to charring materials with moisture and non-charring materials. However, complex phenomena like melting, in depth radiation absorption, surface oxidation, smoldering, etc are not modelled. Effects of e.g. cracking could be incorporated by introduction of a transport model for pyrolysis gases in the solid, in the model framework as described in [3]. Introduction of multiple fronts can allow modelling of e.g. surface oxidation if the diffusion of oxygen is accounted for. All such aspects are considered beyond the scope of the present paper. Figure 1 shows the relation between enthalpy and temperature.

This makes the model appealing for coupling to gas phase combustion CFD simulations (e.g. for flame spread simulations). Once the (high-temperature) pyrolysis process start, the pyrolysis kinetics are indeed often not very important in this context. In CFD simulations, the detailed pyrolysis gas composition is typically not taken into account. Also, primarily the pyrolysis gases mass flow rate is an important input for the CFD and kinetics time scales are typically smaller than the time scale, related to variations in the pyrolysis gas mass flow rate.

For simplicity reasons, we only consider a one-dimensional configuration in the present study (Figure 2). The model concept is applicable in three dimensions, though, which is again interesting for general flame spread simulations.

### 2.2 Energy equation

As mentioned in the introduction, we use enthalpy per unit volume *'E'* as the basic variable[1]. The basic physical mechanisms that drive the changes in enthalpy in a fixed volume *'V'* are heat transfer by conduction in the solid material and by convective heat transfer due to movement of hot pyrolysis gases through the char layer:

$$\frac{\partial}{\partial t}\int_V E dV = -\int_S \left(\vec{\dot{q}}''_{\mathrm{cond}} + \vec{\dot{q}}''_{\mathrm{conv}}\right)\cdot\vec{n}\cdot dS \tag{1}$$

We adopt a finite volume formulation to represent eq. (1) in a discrete manner:

$$E_i^{n+1} = E_i^n + \frac{\Delta t}{\Delta x}\left[\left(\dot{q}''^{n+1}_{cond,i-\frac{1}{2}} - \dot{q}''^{n+1}_{cond,i+\frac{1}{2}}\right) + \left(\dot{q}''^{n+1}_{conv,i-\frac{1}{2}} - \dot{q}''^{n+1}_{conv,i+\frac{1}{2}}\right)\right] \tag{2}$$

In (2), $\Delta t = t^{n+1} - t^n$ is the physical time step size and $\Delta x$ is the grid spacing. Using Fourier's law for conduction and assuming the specific heat $c_{pyr}$ of the pyrolysis gases constant (for simplicity) the fluxes are discretized as:

$$\dot{q}''^{n+1}_{cond,i-\frac{1}{2}} = -k^{n+1}_{i-\frac{1}{2}}\left.\frac{\partial T}{\partial x}\right|^{n+1}_{i-\frac{1}{2}} \tag{3}$$

$$\dot{q}''^{n+1}_{conv,i-\frac{1}{2}} = -m''^{n+1}_{pyr,i-\frac{1}{2}} c_{pyr}\left(T^{n+1}_{i-\frac{1}{2}} - T_{pyr}\right) \tag{4}$$

---

[1] Note that, in (1), *E* is the energy density, rather than enthalpy density. In the solid material, these terms can both be used (no effect from static pressure) and we use 'enthalpy' from now on.

The discretisation of the temperature gradient in (3) is shown in fig. 3. A piecewise linear representation of the temperature field is necessary to provide acceptable results for the mass flow rate [4].

The pyrolysis gases mass flow rate equals the variation in mass, caused by the front motion. For each cell face, the expression depends on the relative position of the front ($x_f$) with respect to the position of the face ($x_{i-1/2}$):

$$\dot{m}''^{n+1}_{pyr,i-\frac{1}{2}} = \begin{cases} 0, if\ x_f^{n+1} < x_{i-\frac{1}{2}} \\ \dfrac{\left(x_f^{n+1} - x_f^n\right)\left(\rho_v - \rho_c\right)}{\Delta t}, if\ x_f^n \geq x_{i-\frac{1}{2}} \\ \dfrac{\left(x_f^{n+1} - x_{i-\frac{1}{2}}\right)\left(\rho_v - \rho_c\right)}{\Delta t}, if\ x_f^n < x_{i-\frac{1}{2}} \leq x_f^{n+1} \end{cases} \tag{5}$$

Eq. (2) can be integrated in time, provided that a closure is given for $x_f^{n+1}, T_{i-\frac{1}{2}}^{n+1}, \left.\dfrac{\partial T}{\partial x}\right|_{i-\frac{1}{2}}^{n+1}$ as a function of $E_i^{n+1}$. Also note that the value of $k_{i-\frac{1}{2}}^{n+1}$ depends on the position of the pyrolysis front $x_f^{n+1}$ at $t = t^{n+1}$.

### 2.3 Closure problem

Given the piecewise linear representation of the temperature field, a distinction is made between virgin, char and 'mushy' cells. We use storage of temperature at the centres (*i*). As such, given the temperatures at the cell centres and the pyrolysis front position, the cell-face temperature gradients can be constructed (as shown in fig. 3), and the function *T(x)* is known. The latter is used in the relationship between enthalpy and temperature:

$$E_i = \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} E(x)\cdot dx \quad \text{with} \quad E(x) = \begin{cases} \rho_v c_v \left(T(x) - T_{pyr}\right)\ if\ x > x_f \\ \left(\rho_v - \rho_c\right)\Delta Q_{pyr} + \rho_c c_c\left(T(x) - T_{pyr}\right)\ if\ x < x_f \end{cases} \tag{6}$$

At this level, yet another equation/constant is needed to close the system. This extra equation is derived by expressing a local mass and energy balance around the pyrolysis front. Indeed, the energy balance provides a relation between the conductive fluxes at both sides of the front and the possible motion of the front (thereby releasing pyrolysis gases at $T=T_{pyr}$) [3]:

$$\frac{\left(x_f^{n+1} - x_f^n\right)}{\Delta t}(\rho_v - \rho_c)\Delta Q_{pyr} = -k_c \left.\tfrac{\partial T}{\partial x}\right|_{f,l} + k_v \left.\tfrac{\partial T}{\partial x}\right|_{f,r} \qquad (7)$$

Combination of (2) - (7) provides a solvable set of equations. In practice, (2) is integrated using a pseudo-time stepping method, bearing in mind that, during the solution procedure, the pyrolysis front must not move backwards. For the details on the exact iterative solution procedure, we refer to [4].

## 3 Numerical reference results

### 3.1 Time dependent behaviour

Figure 2 is a schematic representation of the configuration under study. An external heat flux is imposed at one side. In flame spread simulations, the incoming heat flux onto the solid material stems from flames and their hot products (radiation and convection). We work with imposed heat fluxes here, in order to avoid uncertainty with respect to heat flux coming from flames. We consider the three most challenging cases of [11]. The intention is to illustrate that the simplified model, with a limited number of computational cells and relatively large time steps, reproduces the numerical reference results, obtained with the more complex moving grid model. Therefore, we apply identical settings for the boundary conditions, model parameters and material properties [16], as discussed next. The properties correspond to filter paper. Note that the numbers of cells used in all the simulations discussed in this work remain constant equal to 40 cells.

External heat loss from the exposed surface, by convection and re-radiation, is taken into account: $\dot{q}^{"}_{net} = \dot{q}^{"}_{ext} - h\left(T_{surf} - T_{amb}\right) - \varepsilon\ \sigma\ \left(T^4_{surf} - T^4_{amb}\right)$, while the back surface is perfectly insulated and impervious. The heat flux $\dot{\mathrm{q}}^{"}_{\mathrm{ext}}$ varies in time, as described below. The convection coefficient is set to $h = 15W/\left(m^2K\right)$, while the emissivity equals $\varepsilon = 1.0$. The pyrolysis temperature is set to $T_{pyr} = 573K$ and the heat of pyrolysis equals $\Delta Q_{pyr} = 7.54 \cdot 10^5\ J/kg$. Obviously, the choice of parameters is very important and results can be sensitive to this choice (see below). However, in the present section, focus is on the representation of the mentioned reference results. Therefore, we stick to the exact same settings as in [11]. As initial condition, there is only virgin material at temperature $T = T_{amb} = 300\mathrm{K}$. The solid has a thickness of 0.03m and the material properties are [16]:

$\rho_v$=650kg/m$^3$, $c_v = c_c$=1257J/$\left(\mathrm{kg\,K}\right)$, $k_v = k_c$=0.1257W/$\left(\mathrm{m\,K}\right)$, $\rho_c$=350kg/m$^3$, $c_{pyr}$=1040J/$\left(\mathrm{kg\,K}\right)$.
We use 40 cells and a physical time step equal to 0.5s.

**Case 1:** *Sudden increase of heat flux at start of pyrolysis*

The initially imposed external heat flux is 30kW/m$^2$. After 12.0s, reported as the onset of pyrolysis in [7], there is a sudden increase to 50kW/m$^2$. This sudden rise represents the additional heat flux due to combustion of the volatiles in the gas phase as they leave the solid. Figure 4 (top) reveals good agreement.

**Case 2:** *Sudden increase of heat flux at fixed time*

In this case, the initially imposed external heat flux of 30kW/m$^2$ is suddenly increased to 50kW/m$^2$ at t = 60s. This resembles e.g. additional heat flux due to a distant object catching fire or due to flashover. Figure 4 (middle) reveals that there is again good agreement of the present model with the moving grid results. In particular, the unphysical drop in the mass flow rate, as observed with the integral model of e.g. [17], is not seen here. Also, the second peak in the mass flow rate is predicted quite accurately. There is no overshoot as in the integral model.

**Case 3:** *Sudden increase and fall of external heat flux*

The initially imposed external heat flux is 30kW/m$^2$. At t = 12.0s, there is a sudden increase to 50kW/m$^2$. At t = 41s, the external heat flux is suddenly decreased again to 30kW/m$^2$. This models e.g. variable exposure to flames. Figure 4 (bottom) shows again good agreement of the present model with the moving grid reference results. The unphysical rise in mass flow rate with the integral model (at t = 41s) is again not encountered with the present enthalpy based model and the drop in the mass flow rate is well captured (no undershoot).

### 3.2. Influence of solid thickness

We now discuss the effect of the solid thickness, as in [10]. The thickness of the solid is varied from 2mm (thermally thin material) to 50mm (thermally thick). The boundary conditions are fixed: the front surface is exposed to a constant externally imposed heat flux of 50kW/m$^2$ and the back surface is perfectly insulated. The thermo-physical properties are now chosen exactly the same as in [10] (corresponding to particle board) again in order to illustrate representation of the numerical reference results:

$$\rho_v = 600\,\mathrm{kg/m^3}, \rho_c = 60\,\mathrm{kg/m^3}, c_v = c_c = 2500\,\mathrm{J/(kg.K)},\ k_v = 0.36\,\mathrm{W/(m.K)}, k_c = 0.23\,\mathrm{W/(m.K)},$$
$$c_{pyr} = 0\,\mathrm{J/(kg.K)}, \Delta Q_{pyr} = 8.7\ 10^5\ \mathrm{J/kg}, T_{pyr} = 648\,\mathrm{K},\ \varepsilon = 1.0,\ h = 15\,\mathrm{W/m^2K}.$$

Figure 5 confirms the good agreement with the moving grid results over the entire range of thicknesses. Clearly, onset of pyrolysis occurs earlier for the smaller thickness, due to more rapid heating of the material up to the pyrolysis temperature. For thickness larger than 10 mm, the start of pyrolysis remains practically unchanged. The heating process is then as if the solid were of infinite thickness.

For the thermally thin materials (L<10 mm), a single peak is observed in the mass flow rate. The peak is higher for the smaller thicknesses, due to the more rapid heating and thus faster pyrolysis front motion.

For the thermally thick materials, two peaks are observed. The second peak is due to the so called 'back effect' [8]. Note that the first peak is quasi-identical for all thermally thick materials, as they behave as infinitely thick materials during that stage. The duration of the pyrolysis obviously depends on the total mass of the solid and thus directly on the solid thickness.

### 3.3. Effect of boundary condition on the back side

As final numerical test, we vary the back side boundary condition, describing the convective heat loss as follows:

$$\dot{q}_{bs}^{"} = h_{bs}(T_{bs} - T_{amb}) \tag{8}$$

Unless mentioned otherwise, we use the same model parameters and material properties as in the previous section. We set the emissivity at the back surface equal to zero, as typically the temperature $T_{bs}$ is not high.

Before discussing the results, we perform a steady state analysis of the equilibrium situation. In that case, the net incoming heat flux at the front surface equals conduction through the solid material, as well as (convective) heat losses at the back surface. In the assumption that the steady state situation is complete charring of the material, this reads:

$$\dot{q}_{ext}^{"} - \varepsilon\sigma\left(T_{s,eq}^{4} - T_{amb}^{4}\right) - h_{s}\left(T_{s,eq} - T_{amb}\right) = k_{c}\frac{T_{s,eq} - T_{bs,eq}}{L} = h_{bs}\left(T_{bs,eq} - T_{amb}\right) \tag{9}$$

These are two equations for two unknown variables ($T_{s,eq}$ and $T_{bs,eq}$). The last identity shows that, in the relation between the two surface temperatures, the Biot number appears, based on the back surface convection coefficient:

$$T_{s,eq} = T_{bs,eq} + \frac{h_{bs} L}{k_c}\left(T_{bs,eq} - T_{amb}\right) \tag{10}$$

Elimination of $T_{s,eq}$ in (9) yields a single equation for $T_{bs,eq}$. The solution of this equation depends on $h_s$, $h_{bs}$ and $\varepsilon$. Figure 6 shows the result for $\varepsilon = 1$ and fixed $h_s$ (left) or fixed $h_{bs}$ (right). Obviously, if $T_{bs,eq} < T_{pyr}$, the assumption of complete charring of the material is incorrect.

Figure 6 confirms that, when $h_{bs} = 0\text{W/(m}^2\text{K)}$, i.e. perfect insulation at the back surface, the steady state situation yields $T_{s,eq} = T_{bs,eq}$. The higher the convection coefficient $h_s$, the lower the equilibrium temperature due to the lower net incoming heat flux. The left picture further reveals that the difference between the back surface temperature and the front surface temperature increases as the heat losses at the back surface increase (higher $h_{bs}$). The dashed line at $T = T_{pyr} = 648\text{K}$ reveals that the assumption of complete charring is no longer fulfilled for large values of $h_{bs}$ (e.g. $h_{bs} > 10.2\text{W/(m}^2\text{K)}$ for $h_s = 0\text{W/(m}^2\text{K)}$). The right picture of fig. 6 shows that complete charring is only possible for sufficiently low values of $h_{bs}$. For $h_{bs} = 10\text{W/(m}^2\text{K)}$, curve c, it is seen that complete charring only happens when $h_s < 1\text{W/(m}^2\text{K)}$.

We now discuss the results as obtained with the present pyrolysis model. Note that no case dependent adjustments are made to the model whatsoever. This is a particularly appealing model feature. First, the convective heat transfer coefficient $h_{bs}$ is varied from 0 (perfect insulation as in section 3.2) to $20\text{W/m}^2\text{K}$, while at the front surface $h_s = 0\text{W/m}^2\text{K}$

and $\varepsilon = 1$ [10]. The material properties are the same as in the previous section. The solid thickness equals 20mm. A constant heat flux of 50kW/m$^2$ is imposed.

Figure 7 (top left) confirms the agreement with the moving grid model results. When the pyrolysis front approaches the back boundary, the second peak (back effect) is only seen for sufficiently low values of the back boundary convective heat transfer coefficient. Indeed, there is no ‘piling up’ of heat when heat losses through the back surface are too high.

In [10], it is discussed that the integral model suffers the deficiency that mass flow rate curves cross each other when ‘$h_{bs}$’ is varied. This unphysical feature is not observed with the present model, as illustrated in the zoom (figure 7, top right).

The bottom picture (left) shows the effect of $h_{bs}$ on the front and back surface temperatures ($T_s$ and $T_{bs}$). Obviously, there is little effect on $T_s$. Note the onset of pyrolysis at t = 27s, in agreement with the top left picture of fig. 7. As $h_{bs}$ increases, $T_{bs}$ increases less and less rapidly, due to relatively higher heat losses through the back surface. Interestingly, differences become visible for t > 250s, which is also the period where differences become visible in the pyrolysis gases mass flow rates (top right figure). In other words, from t = 250s onwards, the back surface boundary condition affects the pyrolysis process.

Note here, that for $h_{bs}$<10.2 W/m$^2$K, where complete charring of the material should happen (see above), the steady state temperature of fig. 6 are indeed predicted. For higher values of $h_{bs}$, the steady state analysis is no longer applicable and indeed other steady-state temperatures are predicted as well as the ending of the pyrolysis process (see blow).

The bottom right picture of fig. 7 reveals the position of the pyrolysis front as function of time. Obviously, the higher $h_{bs}$, the lower the pyrolysis mass flow rate (see above) and, correspondingly, the slower $x_f$ increases in time. Interestingly, for $h_{bs}$ = 20W/m$^2$K, the pyrolysis process stops after a while: $x_f$ does not increase any more for t > 10000s. In other words, an equilibrium situation is met. The situation is then as follows: $T_{s,eq}$ = 946K, $x_{f,eq}$ = 0.0134m and $T_{bs,eq}$ = 555K. Thus, the net heat flux into the solid material equals: (50000 – 1 x 5.67 x 10$^{-8}$ (946$^4$ – 300$^4$)) ≈ 5100W/m$^2$). This indeed corresponds to the conduction through the char material (approx. equal to 0.23 x (946 - 648)/(0.0134 - 0)), the conduction through the virgin material (approx. equal to 0.36 x (648 - 555)/(0.02 – 0.0134)) and the convective heat losses at the back surface (20 x (555 - 300)). It is a very appealing model feature that the stopping of the pyrolysis process is automatically predicted when there is insufficient net incoming heat flux.

Figure 8 shows the results when the front boundary condition is varied, while keeping the back boundary condition fixed ($h_{bs}$ = 10W/m$^2$K). The bottom picture (left) shows the effect of $h_{bs}$ on the front and back surface temperatures ($T_s$ and $T_{bs}$). Obviously, the effect of the lower net incoming heat flux (due to relatively higher convective heat losses at the front surface for higher $h_s$ values), is that $T_s$ rises less rapidly. Consequently, the onset of pyrolysis occurs later for higher values of $h_s$. Also, the pyrolysis gases mass flow rate in general decreases, as the front moves less rapidly (see bottom right picture). This effect becomes negligible after a relatively long time. The bottom right picture, showing the position of the pyrolysis front as function of time, confirms that, with $h_{bs}$ = 10W/(m$^2$K), charring is only complete for the lowest $h_s$ values. When pyrolysis is incomplete, a similar energy balance is confirmed as described above for fig. 7.

## 4. Experimental test case

We now discuss the cone calorimeter experiments of [18]. The experiments were conducted on a 2.54cm thick plywood sample. The imposed external heat flux equals 50kW/m$^2$. The sample was placed in an inert nitrogen atmosphere, which prevents the ignition of the pyrolysis gases in the gas phase, so that there is no additional heat flux. We use 40 cells and a physical time step equal to 1.0s. The material properties are taken as in [19]:

$$\rho_v=462\,\mathrm{kg/m^3},\rho_c=60\,\mathrm{kg/m^3},c_v=4000\,\mathrm{J/(kg\,K)},c_c=2000\,\mathrm{J/(kg\,K)},\,k_v=0.60\,\mathrm{W/(m\,K)},$$
$$k_c=0.45\,\mathrm{W/(m\,K)},\,c_{pyr}=0\,\mathrm{J/(kg\,K)}.$$

Figure 9 below shows the result of the mass flow rate, compared to the experiments. As in [19] we use $\Delta Q_{pyr}=4.0\times10^5\,J/kg, T_{pyr}=623\,K, \varepsilon=1.0$ at the front surface and $\varepsilon=0.0$ at the back surface. We discuss the sensitivity of the results on these parameters below. As mentioned in [16], the back side boundary condition in the experiments was not fully described in [14]. For simplicity, we first assume perfect insulation. Afterwards, we illustrate the effect of a non-zero convection coefficient $h_{bs}$.

The model cannot capture the immediate onset of pyrolysis, as it needs to heat up to $T_{pyr}$ at the front surface. Yet, the peak around 100s is very well captured. The subsequent decrease is also very well reproduced as the pyrolysis front moves inside the solid and the char layer develops. Also the second peak seen around 1200s is well captured.

We now discuss the effect of the model choices $T_{pyr}$ and $\Delta Q_{pyr}$ (fig. 10). Obviously the higher the pyrolysis temperature, the longer it takes for pyrolysis to begin. Also, the peak becomes lower, due to slower pyrolysis front motion: more heat is conducted away from the front to the virgin material in (2), due to steeper temperature gradients (as the pyrolysis front temperature is higher). The influence of the heat of pyrolysis is less important. Obviously, the mass flow rate increases as $\Delta Q_{pyr}$ is lower, as less heat is required for the pyrolysis process. The onset of pyrolysis is independent of $\Delta Q_{pyr}$ as this only depends on the heating up stage up to $T_{pyr}$.

Finally, we discuss the effect of the front surface emissivity and the back surface convective heat transfer coefficient. As expected, figure 11 (top) reveals that the mass flow rate is lower for higher $\varepsilon$, as the net heat flux into the material decreases. Obviously, this also reduces the front and back surface temperatures (fig. 11, bottom).

## 6 Conclusions

A simplified enthalpy based pyrolysis model for charring materials, has been applied to a series of test cases. We first illustrated that numerical reference results, obtained with the more complex moving mesh method, are well reproduced: the transient behaviour of the present model is good (no unphysical drops or peaks in the mass flow rates) and the effect of variable solid thickness and back surface boundary condition is well captured. In particular, the model performs well for the entire range of thermally thin through thermally thick materials. Also, possible interruption of the pyrolysis process due to insufficient incoming net heat fluxes, is automatically predicted.

Finally, plywood cone calorimeter experiments, carried out in inert atmosphere, were discussed. Good agreement was again illustrated for the pyrolysis gases mass flow rate evolution in time. The effect of model parameters (pyrolysis temperature and heat of pyrolysis) and boundary conditions (emissivity and back surface convective heat transfer coefficient) on the mass flow rate, front and back surface temperatures and pyrolysis front position, was explained.

# 7 Nomenclature:

| | |
|---|---|
| $c$ | specific heat $\left(\mathrm{J/(kg.K)}\right)$ |
| $E$ | enthalpy density $\left(\mathrm{J/m^3}\right)$ |
| $h$ | convective heat transfer coefficient $\left(\mathrm{W/(m^2.K)}\right)$ |
| $h_{pyr}$ | enthalpy of pyrolysis gases $\left(\mathrm{J/kg}\right)$ |
| $k$ | thermal Conductivity $\left(\mathrm{W/(m.K)}\right)$ |
| $\dot{m}''$ | mass flux $\left(\mathrm{kg/(m^2.s)}\right)$ |
| $\Delta Q_{pyr}$ | pyrolysis heat $\left(\mathrm{J/kg}\right)$ |
| $\dot{q}''$ | heat flux $\left(\mathrm{W/m^2}\right)$ |
| $S$ | surface area $\left(\mathrm{m^2}\right)$ |
| $t$ | time $\left(\mathrm{s}\right)$ |
| $T$ | temperature $\left(\mathrm{K}\right)$ |
| $V$ | volume $\left(\mathrm{m^3}\right)$ |
| $\Delta x$ | cell size $\left(\mathrm{m}\right)$ |

| Subscripts | |
|---|---|
| $i$ | cell number |
| $i + \frac{1}{2}$ | face between cell $i$ and cell $i + 1$ |
| $pyr$ | pyrolysis |
| $c$ | char |
| $v$ | virgin |
| $amb$ | ambient |
| $cond$ | conduction |
| $conv$ | convection |
| $surf$ | surface |
| $ext$ | external |
| $bs$ | back surface |
| $r$ | right |
| $l$ | left |
| $f$ | front |
| $eq$ | equilibrium |

| Superscripts | |
|---|---|
| $n$ | physical time level |
| $n + 1$ | physical time level |

Greek symbols

| | |
|---|---|
| $\rho$ | density $\left(\mathrm{kg/m^3}\right)$ |
| $\varepsilon$ | emissivity |
| $\sigma$ | Stefan-Boltzmann constant $\left(\mathrm{W/\left(m^2K^4\right)}\right)$ |

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