Original article

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A novel approach to determine charring of wood in natural fire implemented in a coupled heat-masspyrolysis model

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Abstract: The paper presents a novel approach to determine charring of wood exposed to standard and natural fire that is based on a new numerical model named PyCiF. The new model couples an advanced 2D heat-mass model with a pyrolysis model. A new charring criterion based on a physical phenomenon is implemented in the PyCiF model to determine charring of wood. This presents the main advantage of the new PyCiF model in comparison to common modelling approaches, which require an empirical value of the charring temperature that is often called the char front temperature. The fact that the char front temperature is not an explicit value as assumed by the isotherm 300 °C is advantageously considered in the presented approach where an assumed empirical value of the char front temperature is not directly required to determine the thickness of char layer. The validation of the PyCiF model against experimental results showed great model accuracy, meaning that the model is appropriate for the evaluation of charring depths of timber elements exposed to the standard fire as well as the natural fires. Additionally, as shown in the case study, the presented approach also enables to determine the char front temperature for various natural fire exposures. This will be especially important for the upgrade of the new design methods for fire safety of timber elements exposed to natural fire given in the various design codes such as Eurocode 5.

Keywords: charring; charring criterion; coupled numerical model; fire; pyrolysis; wood.

1 Introduction

The behaviour of timber structures in fire largely depends on charring, which causes the reduction of the strength and increases the deformability of the structure (Moraes et al. 2004; Sinha et al. 2011). In the past, numerous studies have been carried out to investigate the charring of timber and the related fire resistance of timber structures as well as the phenomenon of wood pyrolysis. To start with, a large number of experiments have been carried out to provide the empirical expressions to calculate charring depth of timber under standard fire exposure (Lawson et al. 1952; Schaffer 1967; White and Nordheim 1992), while the experiments to determine charring depths for non-standard fire exposures (Lau et al. 1999; Mikkola 1990) were less numerous. The observations from these experimental investigations were adopted in standards such as EN 1995-1-2 (2005) and AS 1720 (1990), where empirical expressions to determine charring depths can be found. Due to the experimental background, these empirical expressions are only valid for standardized fires. The standard EN 1995-1-2 (2005) also provides expressions to calculate charring depth for parametric fire curves, which represent the simplest way of describing natural fire, but their use is limited and cannot be generalized.

Despite numerous empirical expressions to determine charring depth, their range of application for assessing the fire resistance of timber elements is usually limited to cases with simple geometry, standard fire exposure or precisely defined non-standard fires and to only a particular wood species under investigation. The researchers tried to improve the mentioned deficiency by using heat (Fragiacomo et al. 2012; Frangi et al. 2008; Tsai et al. 2013) and heat-mass transfer numerical models (Pečenko et al. 2015). In these models, the charring depth is determined based on the calculated temperature isotherm, often referred to as the char front temperature, in a timber cross-section. According to the standard EN 1995-1-2 (2005), the suggested char front temperature is 300 °C and is validated for the standard fire exposure. However, recent research studies (Lange et al. 2015) suggested that the char front

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temperature in case of non-standard fire exposure varies and is dependent on the fire curve. Thus, the use of heat and heat-mass transfer models for the calculation of charring depth is limited to the standard fire or to fires with a similar temperature development since isotherm 300 °C criterion is not appropriate to determine charring depth in cases of natural fire.

It is evident that a new, more general approach to determine charring of wood is required. This can be accomplished with the help of advanced mathematical models based on the appropriate physical description of the governing phenomena. Thus, the knowledge of the associated process of pyrolysis and the heat and mass transfer in wood exposed to elevated temperatures is essential. Pyrolysis describes the thermo-chemical decomposition of wood to various products (Araújo et al. 2017). At the same time, the pyrolysis reaction is a time-dependent process, meaning that the rate of temperature development in wood has an impact on the rate of thermo-chemical decomposition of wood and consequently on the rate of char formation, which is crucial for a more general description of charring. The thermochemical processes that take place at elevated temperatures are primarily controlled by the cellulose, which is the main wood constituent (Di Blasi 1994). In literature, various pyrolysis models can be found, which differ in complexity of the pyrolysis reaction, i.e. in the number of reaction processes (components). In the simplest models, cellulose pyrolysis is described by a single reaction (Antal et al. 1998). More advanced models describe thermo-chemical degradation of cellulose with two, three or four consecutive-parallel reactions (Kilzer and Broido 1965; Broido and Nelson 1975; Bradbury et al. 1979a; Ranzi et al. 2008), while the most complex pyrolysis models take into account up to nine reactions (Grieco and Baldi 2011). Nonetheless, knowing the pyrolysis reaction of cellulose is not enough to determine the charring of timber elements. It is also necessary to know the precise temperature development within timber elements, which can be determined on the basis of heat-mass transfer models. Therefore, for the general description of charring of timber elements in natural fire, it is necessary to couple the products of the pyrolysis reaction and the released/ consumed energy during the reaction with the process of heat and mass transfer. At the moment, a few specific coupled heat-mass-pyrolysis models can be found in the literature, which were developed for particular problems, thus making their use limited. Some of these models were devoted to the analysis of drying and thermal treatment of wood (Melaaen 1996; Turner et al. 2010). Flash pyrolysis analysis model, characterized by a rapid warming rate and a moderate maximum temperature (400 - 600 °C) was developed by Di Blasi (1997). Park et al. (2010) investigated and

developed a model for the analysis of dry wood spheres, where the influence of mass transfer on pyrolysis development was not taken into account. Yuen et al. (2013) introduced a 3D model for wet wood pyrolysis neglecting the influence of the bound water diffusion and the diffusion of gas mixture components. However, as shown in Pečenko et al. (2016), where multiphase mass transfer is considered, the process of bound water diffusion in the cell wall significantly affects the charring depth and should not be disregarded. In addition, the multi-phase models are in comparison to single-phase models, such as (Younsi et al. 2006, 2007) more accurate since the actual physical state in wood during the moisture and temperature variation is taken into account (Frandsen et al. 2007a, b; Hozjan and Svensson 2011).

Although the complexity and accuracy of the above described models are not arguable, these models are not suitable for an application in fire conditions. For the fire condition, some generalized pyrolysis model for combustible solids can be found (Stoliarov and Lyon 2008; Lautenberger and Fernandez-Pello 2009a), which, however do not consider some specific phenomena related to moisture transfer in wood. Furthermore, for fire conditions, also some simple models can be found in literature. Fredlund (1993) presented a model where simple charring criterion based on the density threshold was proposed. In the model only single-phase transfer of mass was considered, where the moisture content was the only variable and a simple model of sorption defined as an isotherm was taken into account. In addition, pyrolysis was modelled by only one reaction describing the decomposition of wood. Even more simplified model was introduced by Janssen (2004), where mass transfer was completely neglected. Similar model was presented in Thi et al. (2016). In both models (Janssen 2004: Thi et al. 2016) the isotherm 300 °C was used as a charring criterion. To summarize, some of the heat-mass-pyrolysis models currently in use are not directly applicable for fire conditions, some of them take into account coupled problems in a simplified way, while the rest of them still use isotherm 300 °C as a charring criterion. Therefore, the main goals of the present paper are i) the development of a new numerical model for charring of timber elements in fire conditions based on the precise physical description of the associated heat and mass transfer phenomena and pyrolysis of wood and ii) to provide a new more general charring criterion.

The basis for the development of the new numerical model presents the coupled heat transfer and multiphase mass transfer model given in Pečenko et al. (2015). The model is based on the bound water diffusion in wood cell walls, the diffusion and convection of water vapor and air in lumens, and precise formulation of the interaction between the bound water and the water vapour, known as sorption. Compared to other coupled heat-mass models (Younsi et al. 2006, 2007), this model presented a very accurate description of the heat-mass transfer in wood. However, as already described, the main disadvantage of the model (Pečenko et al. 2015) was simple estimation of charring, determined from the temperature isotherm (300 ° C), which is suitable only for standard or similar fire exposure. Therefore, to make a transition to natural fire, the model (Pečenko et al. 2015) is upgraded in the presented paper, to couple the process of heat-mass transfer with the process of pyrolysis. The coupling arises from the combination of pyrolysis reaction products (gases) with the mass transfer in timber elements. Furthermore, the equation of heat conservation includes also endo/exothermic pyrolysis reaction, which has an influence on the development of temperatures in timber elements exposed to fire. Due to its more general formulation, the newly developed numerical model is suitable for determining the charring depth and char front temperature of timber elements exposed to various design fires, including natural fires, and is applicable for the performance based design of timber structures in fire.

2 Materials and methods

A new 2D model for coupled heat-mass and pyrolysis process, named PyCiF, is divided in two sub-models, which are presented in detail in the following sections. In section 2.1, background and main governing equations of here used pyrolysis model are presented. In section 2.2, the implementation and coupling of pyrolysis model with the heat-mass transfer model presented in Pečenko et al. (2015) is shown. At the end, coupled computational solution procedures are explained in section 2.3.

2.1 Pyrolysis model

The pyrolysis of wood can be in a good approximation substituted by the cellulose pyrolysis, because cellulose is the main wood constituent and governs chemical and physical processes during thermal degradation of wood (Di Blasi 1994). For an application to fire conditions, Richter and Rein (2017) showed that the Broido-Shafizadeh (hereinafter BS) pyrolysis model (Bradbury et al. 1979b) is accurate enough and any complexity beyond this model is unnecessary. The BS model describes cellulose pyrolysis with three reactions. Firstly, initiation reaction leading to active cellulose, which is the intermediate substance with relatively simple composition and lower degree of polymerization (Liu et al. 2008), is followed by two competing reactions, the first one resulting in volatile production, and the second one in char and gas formation. The Broido-Shafizadeh reaction scheme is given in Figure 1.



Figure 1: Broido-Shafizadeh pyrolysis kinetics.

The cellulose pyrolysis is mathematically written by a system of ordinary differential equations:

$$\frac{d\rho_c}{dt} = -k_1 \rho_c,\tag{1}$$

$$\frac{d\rho_{ac}}{dt} = k_1 \rho_c - (k_2 + k_3)\rho_{ac},\tag{2}$$

$$\frac{d\rho_{\rm t}}{dt} = k_2 \rho_{ac},\tag{3}$$

$$\frac{d\rho_{ch}}{dt} = 0.35k_3\rho_{ac},\tag{4}$$

$$\frac{\rho_{g,p}}{dt} = 0.65k_3\rho_{ac},\tag{5}$$

where ρ_c , ρ_{ac} , ρ_t and ρ_{ch} represent the density of the individual component, i.e. cellulose (*c*), active cellulose (*ac*), tar (*t*) and char (*ch*), $\tilde{\rho}_{g,p}$ is the concentration of gases produced during the pyrolysis and *t* is time. Kinetic parameters k_i govern the rate of *i*th pyrolysis reaction and follow the Arrhenius law:

$$k_i = A_i \exp\left(\frac{-E_i}{RT}\right), i = 1, 2, 3$$
(6)

where *R* is universal gas constant and *T* is temperature. Preexponential factors A_i and activation energies E_i are considered according to Bradbury et al. (1979b) and are given in Table 1.

2.2 Coupling heat-mass transfer model with the pyrolysis model

In Pečenko et al. (2015, 2016), a model for multiphase transfers of different mediums coupled by the heat transfer was introduced. There, the heat-mass transfer in wood is described by an energy conservation equation and multiple mass conservation equations for air, water vapour and bound water taking into account the sorption process between bound water and water vapour as well. The model (Pečenko et al. 2015, 2016) is upgraded in this paper, where, in addition, the phenomena occurring during wood pyrolysis are coupled with heat and moisture transfer processes.

Air transfer equation is replaced by the equation describing the transfer of residual gas mixture, i.e. pyrolytic gases and air combined. The energy conservation equation is modified to include the endo-thermic or exothermic reaction during the production of different pyrolysis products. In addition, some of the constitutive relations are modified.

Table 1: Kinetic parameters for ith reaction.

Reaction #1	Reaction #2	Reaction #3
$E_1 = 242.6 \text{ kJ mol}^{-1}$	$E_2 = 153.1 \text{ kJ mol}^{-1}$	$E_3 = 197.9 \text{ kJ mol}^{-1}$
$A_1 = 1.7 \cdot 10^{21} \text{ s}^{-1}$	$A_2 = 7.9 \cdot 10^{11} \text{ s}^{-1}$	$A_3 = 1.9 \cdot 10^{16} \text{ s}^{-1}$

Mass conservation equations for bound water and water vapour are given as:

$$\frac{\partial c_b}{\partial t} = \nabla \cdot \left(\mathbf{D}_0 \exp\left(\frac{-E_b}{RT}\right) \nabla c_b + \mathbf{D}_0 \exp\left(\frac{-E_b}{RT}\right) \frac{c_b E_b}{RT^2} \nabla T \right) + \dot{c}, \quad (7)$$

$$\frac{\partial (\varepsilon_g \tilde{\rho}_v)}{\partial t} = \nabla \cdot \left(-\varepsilon_g \tilde{\rho}_v \frac{\mathbf{K} K_g}{\mu_g} \nabla P_g + \varepsilon_g \tilde{\rho}_g \mathbf{D}_{vg} \nabla \left(\frac{\tilde{\rho}_v}{\tilde{\rho}_g} \right) \right) - \dot{c}, \qquad (8)$$

where ∇ is the nabla operator, *t* is time, c_b , $\tilde{\rho}_v$ and $\tilde{\rho}_g$ denote the concentrations of bound water, water vapour and gas mixture in the lumen (water vapour, pyrolytic gases and air), respectively, ε_g is porosity of timber, E_b is the activation energy (Siau 1995), *R* is universal gas constant, \dot{c} is sorption rate (see Pečenko et al. 2015; Frandsen et al. 2007b), K_g , μ_g and P_g are relative permeability, dynamic viscosity and pressure of gas mixture, respectively. Matrices **D**₀, **K** and **D**_{vg} in the diagonals contain base values for bound water diffusion coefficients, specific permeabilities of dry wood and diffusion coefficients of residual gases into vapour for different material directions, i.e. longitudinal (*L*) and transverse (*T*). The values of **D**₀, **K** and **D**_{vg} can be found in Pečenko et al. (2015).

The last equation describing the mass conservation includes the transport of the residual mixture of gases:

$$\frac{\partial \left(\varepsilon_{g}\tilde{\rho}_{g}^{*}\right)}{\partial t} = \nabla \left(-\varepsilon_{g}\tilde{\rho}_{g}^{*}\frac{\mathbf{K}K_{g}}{\mu_{g}}\nabla P_{g} + \varepsilon_{g}\tilde{\rho}_{g}\mathbf{D}_{gv}\nabla\left(\frac{\tilde{\rho}_{g}^{*}}{\tilde{\rho}_{g}}\right)\right),\tag{9}$$

where $\tilde{\rho}_g^*$ represents the concentration of the residual gas mixture, defined as:

$$\tilde{\rho}_g^{\star} = \tilde{\rho}_{g,p} + \frac{M_{g,p}}{M_a} \tilde{\rho}_a. \tag{10}$$

Above, $M_{g,p}$ is the molar mass of pyrolytic gases, M_a is the molar mass of air and $\tilde{\rho}_a$ is the concentrations of air in lumen. The molar mass of pyrolytic gases is calculated as an average value ($M_{g,p}$ = 24.8 g/ mol) from the main gases formed during fast heating regime (Dufour et al. 2009). The molar mass of air is M_a = 28.96 g/mol.

The equation describing the energy conservation has the following form:

$$\left(\rho C\right)\frac{\partial T}{\partial t} = \nabla \cdot \left(\mathbf{k} \nabla T\right) - \left(\rho C \mathbf{v}\right) \nabla T - \Delta H_s \dot{c} - Q, \tag{11}$$

where *T* is temperature, matrix **k** in the diagonal contains thermal conductivities for different material directions and ΔH_s is latent heat of sorption (see Pečenko et al. 2015). ρC represents the heat capacity of the entire volume of the body, determined as:

$$\rho C = \varepsilon_g \left(\tilde{\rho}_a C_a + \tilde{\rho}_{g,p} C_{g,p} + \tilde{\rho}_v C_v \right) + c_b C_w + \rho_c C_c + \rho_{ac} C_{ac} + \rho_t C_t + \rho_{ch} C_{ch}.$$
(12)

In (12), C_i (*i*=*a*, (*g*, *p*), *v*, *w*, *c*, *ac*, *t*, *ch*) denotes the specific heat of individual component. The contribution due to the convective heat transfer of gases, $\rho C \mathbf{v}$ is given as:

$$\rho C \mathbf{v} = \left(\tilde{\rho}_{g}^{*} C_{g,p} + \tilde{\rho}_{v} C_{v} \right) \varepsilon_{g} \mathbf{v}_{g}. \tag{13}$$

The source term *Q* in Eq. (11) represents energy sink or release due to the endo- or exo-thermic pyrolysis reaction. The source term has the following form:

$$Q = k_1 \Delta h_1 \rho_c + (k_2 \Delta h_2 + k_3 \Delta h_3) \rho_{ac}$$
(14)

where Δh_i is the enthalpy of the individual pyrolysis reaction. According to Park et al. (2010), the values are: $\Delta h_1 = 0 \text{ kJ/kg}$, $\Delta h_2 = 110 \text{ kJ/kg}$, $\Delta h_3 = -210 \text{ kJ/kg}$.

2.2.1 Boundary and initial conditions: At the contact between timber volume and the surrounding, the boundary conditions for pressure, heat flux, vapour flux and bound water flux need to be given. These are:

$$P_{g} = P_{g,\infty}, h_{cr} = k \frac{\partial T}{\partial n}, \mathbf{n} \cdot \mathbf{J}_{v} = \beta \left(\tilde{\rho}_{v,\infty} - \tilde{\rho}_{v} \right), \mathbf{n} \cdot \mathbf{J}_{b} = 0,$$
(15)

where $P_{g,\infty}$ and $\tilde{\rho}_{\nu,\infty}$ are gas pressure and vapour concentration in the ambient, respectively, h_{cr} is the heat flux composed of convective and radiative part, **n** is the unit vector normal to the outer surface of timber or char layer and β is mass transfer coefficient given in Cengel (1998).

The initial conditions are:

$$\mathbf{u}(t=0) = \left[T_0 P_{g,0} \tilde{\rho}_{\nu,0} c_{b,0} \right]$$
(16)

2.3 Solution procedure

The problem of coupled heat-mass and pyrolysis model is non-linear and transient. For this reason, the solution can only be obtained numerically. Solution is found for each time step $dt = t^{i}-t^{i-1}$, which divides the entire time domain [0 t_{end}]. Coupling between heat-mass and pyrolysis model is performed within local loop, where firstly the basic unknowns of the pyrolysis model are computed and then imported into the heat-mass model (Figure 2). Subsequently, the basic unknowns of the heat-mass model are calculated. The accuracy of the results (convergence criterion) is examined at the end of the local loop. If the desired accuracy is met, then the computation at the new time step begins, otherwise the local loop is repeated.

The basic system of ordinary differential Eqs. (1)-(5) of the pyrolysis model is solved with Matlab built-in solver "ode15s", which uses implicit time integration scheme and is suitable for solving "stiff" problems, such as this one. Because the solution of Eqs. (1)-(5) is



Figure 2: Computational procedures of PyCiF model.

obtained within each time step $dt=t^{t}-t^{t-1}$, for the solution at time t^{i} , the results from previous time step t^{i-1} are implemented as initial conditions: $\rho_{c,in}(t=t^{i})=\rho_{c}(t=t^{i-1}), \rho_{ac,in}(t=t^{i})=\rho_{ac}(t=t^{i-1}), \rho_{t,in}(t=t^{i})=\rho_{t}(t=t^{i-1}), \rho_{c,in}(t=t^{i})=\rho_{ch}(t=t^{i-1}), \rho_{a,p,in}(t=t^{i})=\rho_{a,p}(t=t^{i-1}).$

Modified governing Eqs. (7)–(9) and (11) of the heat-mass model together with the corresponding boundary and initial conditions are discretized and solved by finite element method, applying the Galer-kin method and implicit finite difference scheme. The derivation of non-linear partial differential equations expressed with basic unknowns (T, c_b , $\tilde{\rho}_v$, P_g) and subsequent finite element formulation is analogous to the procedures presented in Pečenko et al. (2015). Thus, for an extensive and thorough description, the reader is referred to Pečenko et al. (2015).

2.4 Model validation

The aim of model validation is to compare the calculated and the measured charring depths during fire. Note that validation of temperatures distribution over timber section was already presented in Pečenko et al. (2015) and is thus not given here. The measured charring depths are extracted from the series of fire tests conducted by König and Walleij (1999) and König (2006), where spruce members exposed to standard and parametric fire curves from one side were investigated, respectively. Timber members with the height of 95 mm were composed of five lamellas of width 45 mm glued together, giving the total width of 225 mm, as presented in Figure 3. The density of timber varied between 420 and 430 kg/m³, while the initial moisture content was around 12% for all the analysed members.

In the numerical model, due to 1D problem, the cross-section is discretized with only 95 finite elements, giving the element size of 1×1 mm². The specific heat and the thermal conductivity of the timber and char layer for the analysis with standard fire exposure is considered according to EN 1995-1-2 (2005). In case of the parametric fire exposure, the thermal conductivity of timber and char is used as given in König (2006). For the heat exchange at the interface between timber volume and the surroundings, the considered coefficient of heat transfer by convection is $\alpha_c = 25 \text{ W/m}^2\text{K}$, while surface emissivity ε is 0.56, as proposed by König (2006). All the data for boundary conditions are depicted in Figure 3. Basic model input data and parameters used in the analyses are summarized in Table 2. The parameters not listed here can be found in Pečenko et al. (2015). Since timber volume is represented in the model by cellulose, the initial cellulose density $\rho_{c,0}$ is assumed equal to initial dry density of timber.

Table 2: Basic input data of PyCiF model.

Material parameter	Value	Unit	
Inital density of cellulose	425	kg m⁻³	
Inital bound water concentration	50.42	kg m⁻³	
Inital water vapour concentration	9	g m⁻³	
Specific heat of act. cellulose	1200	J (kg K)-1	
Specific heat of tar	1470	J (kg K)-1	
Specific heat of pyrolytic gases	1148	J (kg K)-1	

2.5 Case study

In the case study, the capabilities of a newly developed model PyCiF are demonstrated and additionally char front temperatures are given as well. A wood specimen is exposed to two natural fire curves, i.e. "slow" and "fast" fire curve. The natural fire curves are generated in the commercial software Ozone (Cadorin and Franssen 2003). The considered size of the fire compartment is $b \times l \times h = 10 \times 12 \times 4$ m³. Other basic input parameters to generate natural fire curves are given in Table 3. Data for boundary conditions, thermal properties of wood as well as specimen geometry are the same as under section 3.2.

3 Results and discussion

3.1 Model validation – standard fire exposure

The decomposition of cellulose, degradation/formation of active cellulose and the formation of char, in point P1 located 20 mm away from the exposed edge 1 (see Figure 3),

 Table 3: Basic input data in software Ozone for fast and slow fire curve.

	Fast fire	Slow fire	
Openings	$2 \times 5 \text{ m}^2$, $2 \times 3 \text{ m}^2$	$2 \times (2 \times 10) \text{ m}^2$	
Fire growth rate	Ultra fast, 75 s	Medium, 300 s	
Fire load density	300 MJ m ⁻²	1000 MJ m ⁻²	
RHRf	250 kW m ⁻²	250 kW m ⁻²	



Figure 3: Experimental and numerical setup and data for boundary conditions.

are depicted in Figure 4a. The values of each constituent are normalized against initial cellulose density $\rho_{c,0}$. In addition, the decomposition of solid is given, which is determined as sum of fractions of each constituent at a given time. The cellulose decomposition starts after 21 min of fire exposure, when the temperature in this point reaches around 190 °C. Simultaneously, the formation of active cellulose begins, which achieves peak value at t = 26.5 min. Afterwards, the normalized density of solid starts decreasing, given the fact that active cellulose is only a transitional phase. The formation of char starts at t = 25 min. The process of pyrolysis in point P1 ends after 28.1 min of fire exposure, when the cellulose and active cellulose are fully decomposed and the char reaches its final vield which represents 12.6% of the solid. Thus, the density of solid decreases from the initial 425 kg/m³ to the final 53.7 kg/m³.

The charring depth is determined using the proposed charring criterion. This way charring is connected with process of pyrolysis and it is determined when final char yield is reached as presented on Figure 4a. Note that the temperature when this occurs is the corresponding char front temperature T_{char} . From Figure 4a it is seen that the charring depth of 20 mm is reached after 28.1 min of fire exposure. Based on the proposed charring criterion, the charring depths and the corresponding charring times over the entire cross-section are determined and presented in Figure 4b. The calculated charring depths are compared against the measured values given in König and Walleij (1999), and, as observed, the results agree very well, with the absolute difference being less than 1.5 mm throughout the entire fire exposure. This indicates that the model with the proposed charring criterion accurately predicts charring depth in case of standard fire exposure.

The development of moisture content and gas pressure with time in points 5, 20 and 50 mm away from the exposed edge is depicted in Figure 5a, b, respectively. In addition, the development of temperature with time in the same points is plotted as well. The process of drying. i.e. the decrease of the moisture content, starts at the temperature about 100 °C. Before that, for points 20 and 50 mm away from the exposed edge, the moisture content increases as a consequence of the moving moisture front in the interior of the specimen. The drying ends at the temperatures around 300–350 °C, which corresponds well to the temperature when the final char yield forms. The gas pressure increases with time as expected, reaching the peak values of 0.12, 0.135 and 0.15 MPa, for points 5, 20 and 50 mm away from the exposed edge, respectively. Since porosity of wood is quite high, the increase of air pressure in the lumen is small.

3.2 Model validation – parametric fire exposure

In this study, the results of two different natural fire tests (C3 and C6) carried out by König (2006) were used to validate the capability of the model to predict charring depth in conditions different from standard fire. Natural fires were designed by parametric fire curves with different opening factors used in the experiments (Figure 6).

Parametric fire curve C3 had similar temperature development as standard fire curve in the heating phase, while fire curve C6 had faster temperature increase and consequently reached higher maximum temperature.

The time development of the calculated and the measured charring depths for tests C3 and C6 are depicted in Figure 7a, b, respectively. The charring depth was calculated based on a charring criterion, as described in section 3.1. For test C3 the model slightly underestimates the final charring depth compared to the experiment, although absolute difference is small (<2 mm). Almost perfect agreement is observed for test C6. This implies that the presented model with the corresponding charring criterion is capable of accurate prediction of charring depth in cases of natural fire.



Figure 4: a) Decomposition/formation of solid constituent (cellulose, active cellulose and char) in point P1, b) calculated and measured charring depth for the standard fire exposure.

1000

800

600 🖸

400 E

200

0.1

20

 $\begin{array}{cc} 40 & 60 \\ t & [min] \end{array}$

50 mm

80



80

1200 Standard fire curve 1000 Test C6 (König 2006) 800 $O = 0.06 \text{ m}^{\circ}$ $= 120 \text{ MJ/m}^{2}$ [] 00600 Test C3 (König 2006 $O = 0.04 \text{ m}^{0.5}$ $= 120 \text{ MJ/m}^{2}$ a 400 200 Ω 0 20 40 60 80 100 120 t [min]

60

a)

t [min]

20 mm

14

8

ä

mm

20

Figure 6: Parametric fire curves C3 and C6 from the test (König 2006) and comparison with standard fire curve.

3.3 Case study

The calculated hot zone temperatures for analysed natural fires are depicted in Figure 8. For the fast fire, maximum temperature of 1200 °C is reached after 20 min, afterwards the cooling phase initiates. For the slow fire, quasi plateau with the temperatures between 570 and 610 °C is reached and lasts for around 45 min (between 25 and 70 min of fire exposure), before the cooling of compartment starts.

The development of temperatures with time (T-t curves) in the chosen points of the cross-section (from 5 to 50 mm away from the exposed edge) are presented in Figure 9a (fast fire) and Figure 9b (slow fire). As anticipated, much faster temperature development is found in

Figure 5: The development of different quantities (a) moisture content m (b) pressure P_g with time in points 5, 20 and 50 mm away from the exposed edge.



Figure 8: The development of temperatures within the fire compartment for the fast and slow fire determine with Ozone software.

the case of fast fire. Similarly, the cooling phase is significantly faster in case of fast fire as well.

Figure 10b, d represent the development of moisture content and gas pressure, respectively, for points 5, 15 and 25 mm away from the exposed edge in case of slow fire. For points 5 and 15 mm away from the exposed edge, very similar conclusions can be drawn compared to Figure 5a, b, i.e. the extensive drying process starts at the temperature around 100 °C and ends at around 300 °C. For point 25 mm away from the exposed edge, the drying process is not completed on the account of the mild temperature increase. In case of fast fire (Figure 10a), the drying in points 10 and 30 mm away from the exposed edge slightly differs. The highest (maximum) moisture content is observed at a temperature around 200 °C, caused by the bound water



Figure 7: Measured and calculated time development of charring depths for a) test C3 and b) test C6



diffusion in the direction towards the exposed edge. After that, extensive drying takes place.

Based on the charring criterion presented in section 3.1 and Figure 4, the char front temperatures for different distances from the exposed edge are presented in Figure 11. The representation of char front temperature for fast and slow fire is only up to 45 and 25 mm from the exposed edge, respectively, since, beyond that charring did not occur. In general, the char front temperature decreases with the distance from the exposed edge, since for charring to take place, it is important for how long wood is exposed to a certain temperature. As observed from Figure 9, the T-tcurves differ from point to point of the cross section, which result in different char front temperature. Thus, slower temperature increase and longer exposure to temperatures above 250 °C, that are required for charring to occur, result in lower char front temperature. For this reason, the char front temperatures in case of slow fire are around 50 °C lower compared to the fast fire. The average char front temperatures for fast and slow fire are 331 and 284 °C,



respectively. Some studies have already discussed whether the char front temperature remains 300 °C for fire exposures different from the standard one (Lange et al. 2015; Tiso et al. 2019). However, this problem has not been particularly investigated in the literature so far. From the results of the analysis it is evident that the newly developed model is able to adress this issue and as shown, the char front temperatures are not constant in case of natural fires and highly dependent on the type of fire.

3.4 Future work

Although the presented model is applicable also for natural fires, there are some specific conditions where its use is limited. For instance, in fires with forced convection where the phenomena of oxidative pyrolysis of wood (Lautenberger and Fernandez-Pello 2009a, b) may have an important effect on charring, the presented model cannot be directly applied. The second phenomenon not explicitly addressed in the presented model is smouldering of wood



Figure 10: Numerically determined development of moisture content (a, b) and pressure (c, d) with time in different points of the cross section for fast fire (a, c) and slow fire (b, d).



Figure 11: Numerically determined development of char front temperature with a distance from the exposed edge for the fast and slow fire.

(Anca-Couce et al. 2012), which may have a dominant effect on charring in fires with a slow heating regime. In the future, these two processes are planned to be included, thus making the presented model even more general.

4 Conclusions

The paper presents a new numerical model PyCiF that is suitable to determine charring of timber exposed to fire by a completely novel approach. The model is based on a thorough description of the multiphase mass transfer and the sorption phenomena, coupled by the heat transfer and pyrolysis processes in timber structural elements exposed to fire. With the presented model, beside the temperature, water vapour, bound water and pressure distributions, also the distribution of wood density and densities of individual pyrolysis products are possible to predict. This way, charring depths can be determined. Accordingly, the time development of charring depths of timber structural elements during fire is based on a detailed physical background, i.e. pyrolysis reaction.

The model validation performed by comparing experimentally (König and Walleij 1999; König 2006) and numerically obtained charring depths shows that the model is accurate and appropriate for predicting the charring depths for the standard fire as well as natural fires. The main advantage of the presented model is that the char front temperature is no longer necessary input data. For instance, the determination of char front temperature in case of nonstandard fire is not trivial (Alastair et al. 2015). PyCiF overcomes this shortcoming, because the charring depth is determined from the char yield (charring criterion) that is calculated based on the differential equation with the reaction rate coefficient following the Arrhenius law. Thus, more general description of charring is provided, which allows a wider range of model applications, especially for the use in natural fire conditions. This is one of the main goals of the wider research community in this field (Lennon et al. 2010; Östman et al. 2017) and represents an important step towards performance based design. The model also enables to determine the exact value of char front temperature for various natural fire exposures, which will be especially important for the upgrade of new design methods for fire safety of timber elements exposed to natural fire given in the future versions of various codes such as Eurocode 5.

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