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# Modelling charring of timber exposed to natural fire



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## Abstract

Charring of timber structural elements in fire is one of the most fundamental phenomena that affect the fire resistance of these elements. For an accurate and safe design of structural fire resistance, it is important to consider charring of timber in natural fire exposures, since determining charring for standard fire exposure, which is a common practice, is outdated and in some cases unsafe, due to the fact that some natural fires can be much more severe. Currently, the prescriptive approach and simplified design methods fail to give information about charring of timber elements exposed to natural fire and thus, a performance-based design is needed. Therefore, this paper presents an upgrade and extension of a recently developed heat-mass-pyrolysis model named PYCIF. Originally, PYCIF model was developed only for standard fire conditions. In the present paper, several studies and analyses are performed to extend model application to natural fire conditions. Firstly, the sensitivity study is performed, where the impact of model parameters on the charring development is investigated. It is discovered, that the kinetic parameters for the reaction rate of the active cellulose production, namely activation energy  $E_1$  and pre-exponential factor  $A_1$ , are the most influential. In the next analyses the model calibration for small-scale cone calorimeter tests and large-scale natural fire tests of cross-laminated timber (CLT) floor system is performed. A robust nature of the model is identified since minor parameter calibration is required for an accurate prediction of the charring depth and temperatures in timber elements exposed to various fire conditions. Furthermore, a strong connection between the heating rate of fire and kinetic parameters is discovered. In cases of faster heating rate, the kinetic parameters govern slower reaction rate of active cellulose.

Keywords Heat-mass-pyrolysis model—PYCIF, Pyrolysis, Charring, Natural fire, Sensitivity analysis

## Introduction

In the last decade, the use of timber for construction purposes has increased significantly. Besides traditional prefabricated lower timber buildings, the trend nowadays is also in construction of taller timber buildings and skyscrapers up to 25 stories so far (Ascent, Mjøstårnet tower, Hoho Wien), with the plans of constructing 80 story buildings and more in the future (River Beech Tower,

Jamova 2, Ljubljana, Slovenia

W350 Project, etc.). One of the main reasons of timber construction over other typical materials is sustainability and a need for an environmentally friendly environment. Although the transition to clean and  $CO_2$  neutral environment is undoubtedly needed, the main question arises whether this can prevail over the safety of the structure. Especially in terms of fire safety, since the current design practice can hardly keep up with the sudden urge for sustainability.

The most common way to determine fire resistance of timber structures follows standards and regulations, where different simple design rules and methods are given. These are usually developed based on the knowledge acquired from the ISO standard fire exposure [1-4], which is a fire curve proposed by the international



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organization for standardization (ISO) [1]. However, the use of ISO standard fire curve, to prove fire safety of the structure is outdated, since the presence of modern highly combustible materials such as foams, plastics and other, often found in buildings nowadays, can lead to much more severe natural fires. Therefore, a use of natural fire curve is necessary for a safe design of fire resistance of timber buildings.

Fire resistance of timber structures exposed to natural fire strongly depends on the development of charring, since it governs how much of sound wood remains to provide load-bearing capacity during fire. Therefore, a precise prediction of charring of timber in natural fire is important and needed. However, current simple design rules and methods do not provide any information about charring development in natural fire. For instance, the European standard for the structural fire design of timber structures EN 1995-1-2 [5] gives charring rates only for standard and parametric fire exposures. The latter is a very simple model of natural fire and, due to its limitations, cannot be widely and generally used. What is more, recent advanced studies show that simplified methods to determine fire resistance of timber structures exposed to parametric fire are not accurate and also on the unsafe side [6]. Thus, precise determination of charring during natural fire exposure still remains a challenge nowadays. One of the ways towards this is developing advanced calculation models that are formed on a precise physical description of the phenomena. At elevated temperatures, timber is subjected to thermo-chemical decomposition. As a result, different products are formed, the most visible one is charcoal. Physically, this process can be described by the coupled heat and mass transfer and the pyrolysis reaction in timber. In the past, a few coupled heat-mass-pyrolysis models have already been developed. Some of them were designed for specific conditions to simulate the drying of wood [7-9] or the conditions with the temperatures up to 600 °C [10], while some of them were developed explicitly for fire conditions [11, 12]. The latter were very simple in the description of pyrolysis reaction and transfer of mass, and thus, not fully general and applicable for natural fire conditions. Lately, a very precise model to simulate charring of timber in fire conditions was proposed by the authors [13]. However, the model was still not applicable for natural fire conditions.

Therefore, the main objective of this paper is to extend and upgrade a coupled heat-mass-pyrolysis model, previously presented by the authors [13], to simulate charring of timber in natural fire conditions. Since this is a very complex process, several studies are needed. Firstly, a model sensitivity study is conducted to discover the parameters that have the most influence on charring. Once these parameters are discovered, a set of calibration studies is performed. Model calibration studies are based on the small-scale tests in cone calorimeter, where the sample is exposed to different external heat fluxes, and three large-scale natural fire tests of the cross-laminated timber (CLT) floor system. All experimental data were found in the literature [14, 15].

#### Theory

#### Coupled heat-mass-pyrolysis model—PYCIF

Coupled heat-mass-pyrolysis model named PYCIF couples heat and mass transfer in timber with the process of timber pyrolysis and is designed for the analysis in fire condition. The primary objective of the model is to accurately determine the charring of timber. The model accounts for the transfer of bound water, water vapour and residual gas mixture (air and gases formed during pyrolysis) coupled with the heat transfer as well as timber decomposition due to the pyrolysis reaction. Mathematically, this is described by a system of three mass conservation equations for bound water, water vapour and residual gas mixture, an energy conservation equation and five equations describing the pyrolysis reaction. The mass continuity equations are:

$$\frac{\partial c_{\rm b}}{\partial t} = \nabla \cdot \left( \boldsymbol{D}_0 \exp\left(-\frac{E_{\rm b}}{RT}\right) \nabla c_{\rm b} + \boldsymbol{D}_0 \exp\left(-\frac{E_{\rm b}}{RT}\right) \frac{c_{\rm b} E_{\rm b}}{RT^2} \nabla T \right) + \dot{c},$$
(1)

$$\frac{\partial \left(\varepsilon_{g}\widetilde{\rho}_{v}\right)}{\partial t} = \nabla \cdot \left(-\varepsilon_{g}\widetilde{\rho}_{v}\frac{KK_{g}}{\mu_{g}}\nabla P_{g} + \varepsilon_{g}\widetilde{\rho}_{g}\boldsymbol{D}_{vg}\nabla\left(-\frac{\widetilde{\rho}_{v}}{\widetilde{\rho}_{g}}\right)\right) - \dot{c},$$
(2)

$$\frac{\partial \left(\varepsilon_{g}\widetilde{\rho}_{g}^{*}\right)}{\partial t} = \nabla \cdot \left(-\varepsilon_{g}\widetilde{\rho}_{g}^{*}\frac{KK_{g}}{\mu_{g}}\nabla P_{g} + \varepsilon_{g}\widetilde{\rho}_{g}\boldsymbol{D}_{gv}\nabla\left(-\frac{\widetilde{\rho}_{g}^{*}}{\widetilde{\rho}_{g}}\right)\right).$$
(3)

In the left-hand side of Eqs. (1)–(3),  $c_b$ ,  $\tilde{\rho}_v$  and  $\tilde{\rho}_g^*$  represent the concentration of bound water, water vapour and residual gas mixture, respectively. The latter consists of the concentration of pyrolytic gases  $\tilde{\rho}_{g,p}$  and air  $\tilde{\rho}_a$ . Symbol *t* denotes time and  $\varepsilon_g$  is the porosity of timber. In the right-hand side of Eqs. (1)–(3),  $D_0$ , K and  $D_{vg}$  (= $D_{vg}$ ) are diagonal matrices that, for different material directions (longitudinal and transverse) contain bound water diffusion coefficients, coefficients of residual gases into vapour, respectively.  $E_b$  is the activation energy, R is universal gas constant, T is temperature and  $\dot{c}$  is the sorption rate, which represents the phase change from bound

water to water vapour or vice versa.  $K_{\rm g}$  is relative permeability of gas,  $\mu_{\rm g}$  is dynamic viscosity of gas,  $P_{\rm g}$  is pressure of the gas mixture and  $\tilde{\rho}_{\rm g}$  is the concentration of gas mixture determined as:  $\tilde{\rho}_{\rm g} = \tilde{\rho}_{\rm v} + \tilde{\rho}_{\rm g}^*$ . The energy conservation equation is:

$$\rho C \frac{\partial T}{\partial t} = \nabla \cdot (\mathbf{k} \nabla T) - \left(\rho C \frac{KK_{g}}{\mu_{g}} \nabla P_{g}\right) \nabla T - \Delta H_{s} \dot{c} - Q,$$
(4)

where  $\rho C$  is the heat capacity of timber, **k** is the matrix that contains thermal conductivities for different material directions,  $H_s$  is latent heat of sorption and Q is energy sink or release due to the pyrolysis reaction.

At the contact between the timber volume and surroundings, the boundary conditions are prescribed in form of bound water flux  $J_b$ , water vapour flux  $J_v$ , pressure  $P_g$  and heat flux  $h_{cr}$ , which consist of the convective  $h_c$  and radiative part  $h_r$ :

$$\frac{d\rho_{\rm c}}{dt} = -k_1\rho_{\rm c}, \frac{d\rho_{\rm ac}}{dt} = k_1\rho_{\rm c} - (k_2 + k_3)\rho_{\rm ac},$$

$$\frac{d\rho_{\rm ch}}{dt} = 0.35k_2\rho_{\rm ac}, \frac{d\tilde{\rho}_{\rm g,p}}{dt} = 0.65k_2\rho_{\rm ac}, \frac{d\rho_t}{dt} = k_3\rho_{\rm ac}.$$
(6)

Notations  $\rho_c$ ,  $\rho_{ac}$ ,  $\rho_t$ ,  $\rho_{ch}$  represent the densities of the cellulose, active cellulose, tar and char, respectively. The kinetic parameters  $k_1$ ,  $k_2$  and  $k_3$  are the reaction rates for the formation of active cellulose, char with gasses and volatiles, respectively. They follow the Arrhenius law:  $k_i = A_i \exp\left(\frac{-E_i}{RT}\right)$ , where reference values of pre-exponential factors  $A_i$  and activation energies  $E_i$  (i=1, 2, 3) are taken from Bradbury et al. [17] and shown in Table 1.

The energy generated or consumed due to the pyrolysis reaction, *Q*, is determined as:

$$Q = k_1 \Delta h_1 \rho_{\rm c} + (k_2 \Delta h_2 + k_3 \Delta h_3) \rho_{\rm ac},\tag{7}$$

$$\mathbf{n} \cdot \mathbf{J}_{\mathrm{b}} = 0, \quad \mathbf{n} \cdot \mathbf{J}_{\mathrm{v}} = \beta_{\mathrm{v}} (\widetilde{\rho}_{\mathrm{v},\infty} - \widetilde{\rho}_{\mathrm{v}}), \quad h_{\mathrm{cr}} = k \frac{\partial T}{\partial n}, \quad P_{\mathrm{g}} = P_{\mathrm{g},\infty}.$$

Here **n** represents the unit vector normal to the outer surface of timber volume,  $\beta_v$  is mass transfer coefficient determined according to Cengel [16],  $\tilde{\rho}_{v,\infty}$  is the ambient vapour concentration and  $P_{g,\infty}$  is the ambient pressure.

The model to describe the pyrolysis of timber at elevated temperatures is adopted from the Broido-Shafizadeh reaction scheme [17], the pyrolysis of timber is considered based on the pyrolysis of cellulose, since it is one of the main constituents of the timber. In general, however, the pyrolysis reaction is a complex phenomenon of thermo-chemical decomposition of all three main wood constituents, i.e. cellulose, hemicellulose and lignin [18-20]. Especially lignin gives higher char yields and also the products produced during the lignin reaction are completely different compared to the cellulose pyrolysis. In addition, significant interaction occurs in cellulose-lignin pyrolysis [21-24]. However, as discovered by Richter et al. [25], the Broido–Shafizadeh (BS) scheme gives the best balance between model accuracy and complexity, since its reaction scheme is the most appropriate for macroscale fire models and the complexity beyond the BS scheme is not required if the main purpose is to estimate the fire resistance of timber elements exposed to fire. Based on the BS model, the cellulose pyrolysis is firstly initiated by the decomposition on the active cellulose, subsequently followed by two competing reactions yielding the volatiles or char and gasses. The mathematical description of this phenomena is given by a set of ordinary differential equations:

where the enthalpies of the individual pyrolysis reactions are labelled as  $\Delta h_i$  and are, according to Park et al. [26]  $\Delta h_1 = 0 \text{ kJ/kg}, \Delta h_2 = 110 \text{ kJ/kg} \text{ and } \Delta h_3 = -210 \text{ kJ/kg}.$ 

#### The solution

For the solution of Eqs. (1)–(6), the entire time domain  $[0 t_{end}]$  is divided into time steps  $dt = t^i - t^{i-1}$ . The solution is than numerically obtained within each time step, since the problem is transient and non-linear. Own developed software is used, that is based on the Galerkin finite element method built in Matlab<sup>®</sup> environment [27] where implicit time integration scheme is used. Within the software, a system of Eqs. (6) is considered as a submodel, solved with Matlab embedded solver ode23s. Since the PYCIF model has already been developed for standard fire conditions, the reader is referred to Pečenko and Hozjan [13] for more detailed description of the model derivation and solution.

#### **Materials and methods**

#### Sensitivity analysis

The influence of model parameters on the charring development is performed by means of sensitivity analysis. The

Table 1 Reference values of kinetic	parameters $E_i$ and $A_i$
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i	1	2	3
E; (kJ/mol)	242.6	153.1	197.9
$A_i$ (s <sup>-1</sup> )	$1.7 \times 10^{21}$	$7.9 \times 10^{11}$	$1.9 \times 10^{16}$

(5)

influence of model parameters associated with the coupled heat and mass transfer was previously investigated in Pečenko et al. [28], where it was discovered that convective heat transfer in timber does not have significant effect on the development of charring, and the model was simplified accordingly. Since PYCIF model is an upgrade of the previous coupled heat and mass transfer model it is the aim to continue the sensitivity study and to analyse the parameters associated with the pyrolysis model, which represents a new addition to the coupled heat and mass transfer model. Therefore, the emphasis is on discovering the most influential parameters of the pyrolysis reaction, represented by  $A_i$  and  $E_i$  (i = 1, 2, 3), which govern the reaction rate of the individual pyrolysis reaction path. For this purpose, the reference values of parameters  $A_i$  and  $E_i$ , given in Table 1, are varied by the following rule:

$$E_{i,\Delta} = \{0.85\ 0.9\ 0.95\ 1.05\ 1.1\ 1.15\ 1.2\} \cdot E_i,\tag{8}$$

$$A_{i,\Delta} = \{0.2\ 0.4\ 0.6\ 0.8\ 1.2\ 1.4\ 1.6\ 1.8\} \cdot A_i. \tag{9}$$

Local sensitivity study is employed, since the influence of each varied parameter is examined individually. In total, 45 analyses are conducted, for  $E_i$  (i=1, 2, 3),  $7 \times 3 = 21$  analyses and for  $A_i$  (i=1, 2, 3),  $8 \times 3 = 24$  analyses. To quantify the influence of each parameter  $E_{i,\Delta}$  and  $A_{i,\Delta}$ , sensitivity index  $S_{\text{char},x_i}$  is introduced:

$$S_{\text{char},x_i} = \frac{d_{\text{char},x_i} - d_{\text{char},\text{ref}}}{d_{\text{char},\text{ref}}},$$
(10)

where  $x_i$  represents the input variable  $(E_{i,\Delta} \text{ or } A_{i,\Delta})$ ,  $d_{\text{char},x_i}$  is the final charring depth determined based on the input parameter  $x_i$ , while  $d_{\text{char},\text{ref}}$  represents the reference final charring depth, calculated considering the reference value of the parameters  $E_i$  and  $A_i$  (see Table 1).

All model parameters, except for varied parameters  $E_{i,\Delta}$  or  $A_{i,\Delta}$ , are in accordance with the test conducted by Konig [29] (test C3), where a spruce specimen exposed to parametric fire from one side was analysed. This case is selected since it was a basis for the model validation presented in Pečenko and Hozjan [13] and is therefore a firm basis for the sensitivity study. A timber member with the height of 95 mm, width of 45 mm, density of 430 kg/m<sup>3</sup> and initial moisture content of 12% was investigated. For more details of model input parameters, the mesh discretization and other, the reader is referred to Konig [29] and Pečenko and Hozjan [13].

#### Model calibration studies

To extend the PYCIF model application and use in random natural fire exposures, several calibration analyses are performed, where, based on the findings of the sensitivity study, model parameters are fitted to different fire conditions. The calibration is performed for small-scale cone calorimeter tests and large-scale natural fire test of CLT floor system.

#### Model calibration based on the cone calorimeter tests

First series of model calibration studies are based on the cone calorimeter tests performed by Terrei et al. [14]. The tests were conducted on a spruce specimens exposed to different external heat fluxes, i.e. 38.5 kW/m<sup>2</sup>, 60 kW/m<sup>2</sup> and 93.5 kW/m<sup>2</sup>. The average density and initial moisture content of the samples were 490 kg/m<sup>3</sup> and 9.5%, respectively, while the specimen dimension were 50 mm  $\times$  100 mm.

For numerical analyses, the computational domain is discretized to 50 finite elements and treated as a 1D problem, since the specimen is exposed to external heat flux from only one side. For the boundary conditions on the exposed side, the radiative and convective heat transfers are accounted for. The surface emissivity of 0.8 is considered according to EN 1995-1-2 [5]. The convective heat transfer coefficient  $\alpha_c$  is calculated based on the Newton law of cooling, where the Nusselt number is considered for a horizontal hot plate in initially quiescent air:

$$Nu = 0.54 Ra^{\frac{1}{4}}; 10^4 \le Ra \le 10^7,$$
(11)

where Ra represents the Reynolds number (see Bergman et al. [30], p. 579). The values of convective heat transfer coefficients, for 38.5, 60 and 93.5 kW/m<sup>2</sup> heat flux exposures are 10, 12 and 16 W/m<sup>2</sup>K, respectively. The specific heat and thermal conductivity of timber and char layer are considered in accordance with EN 1995-1-2 [5]. Other model input data for the numerical analysis can be found in Pečenko et al. [31] and Pečenko and Hozjan [13], which are the porosity of timber  $\varepsilon_{g}$ , relative permeability of gas  $K_{\rm g}$  and dynamic viscosity of gas, activation energy  $E_{\rm b}$ , universal gas constant *R*, matrices  $D_0$ , *K* and  $D_{vg}$  (= $D_{vg}$ ), heat of sorption  $\Delta H_s$ , initial bound water concentration  $c_{b,0}$ , initial water vapour concentration  $\tilde{\rho}_{v,0}$ , initial gas pressure  $P_{g,0}$ , initial temperature  $T_0$ , specific heat of active cellulose, specific heat of tar, specific heat of pyrolytic gases. The model is calibrated to the development of temperatures in different locations of the specimens and the development of charring depth, since these quantities are measured during the experiment. For the calibration, several numerical analyses are performed where following rules are applied for varying the kinetic parameters, i.e.  $E_i$  by the following rule:  $E_{i,\Delta} = \{0.8 : 0.1 : 1.2\} \cdot E_i$ and  $A_{i,\Delta} = \{0.3 : 0.05 : 1.5\} \cdot A_i$ . The reference values for  $E_i$  and  $A_i$  are given in Table 1. The calibrated parameters  $E_i$  and  $A_i$  are obtained based on the minimum value of the least square cost function, determined from the normalized squared difference between the numerically and

experimentally determined charring depth and temperatures in different locations of the specimens.

# Model calibration based on the large-scale natural fire tests on CLT floor system

To calibrate the model in cases of big-scale tests and natural fire exposures, the results from the natural fire test of the CLT floor system found in literature [15] are used. The behaviour of CLT floor systems in fire conditions was tested by Mindeguia et al. [15]. Three natural fire test of CLT slabs with the thickness of 165 mm were performed. The natural fire tests were conducted in the outdoor experimental facility, with the compartment dimensions of  $6 \times 4 \times 2.52$  m<sup>3</sup>. The walls of the compartment were composed of aerated concrete with the thickness of 300 mm, while the floor was covered with calcium silicate boards (thickness 25 mm) on top of mineral wool insulation (thickness 25 mm). For each natural fire test different ventilation conditions were introduced. The opening factors, as defined in EN 1991-1-2 [32] were  $0.144 \text{ m}^{1/2}$ , 0.050 m<sup>1/2</sup> and 0.032 m<sup>1/2</sup> for fire scenarios 1,



Fig. 1 The development of temperatures for different natural fire tests [15]

2 and 3, respectively. The wood crib fuel loads were used in the test to simulate a representative fire load density for dwellings. The total fire load in the compartment was 891 MJ/m<sup>2</sup>. The development of room temperatures with time is presented in Fig. 1. For all three natural fire tests, the temperature increase in the heating phase was faster compared to the ISO fire curve. The fastest temperature increase was monitored in case of the scenario 1, the slowest in case of the scenario 3. During the tests, temperature developments in pre-installed thermocouples were measured. The charring depth was evaluated from the measurements of temperatures in this thermocouples and also by physical measurements at the end of the tests.

The total number of finite elements for the numerical analyses is 110, giving the element size of 1.5 mm  $\times$  1.5 mm. Due to the exposure of CLT floor system to fire from one side, the computational procedure is treated as 1D problem.

On the exposed edge, the parameters for the boundary conditions for natural fire exposure are considered according to EN 1991-1-2 [5], i.e. the surface emissivity  $\varepsilon_m = 0.8$  and convective heat transfer coefficients  $\alpha_c = 35 \text{ W/m}^2\text{K}$ . The values of initial moisture content considered in the analyses are 12.6, 11.05 and 10.60% for the scenario 1, 2 and 3, respectively. The density of timber is 450 kg/m<sup>3</sup>. Other input data can be found in Pečenko et al. [31] and Pečenko and Hozjan [13].

The best fit between numerical and experimental results is obtained similarly as for the calibration study of cone calorimeter tests, by varying parameters  $E_i$  and  $A_i$ .

## **Results and discussion**

#### Results of the sensitivity analysis

The influence of each varied parameter  $E_{i,\Delta}$  or  $A_{i,\Delta}$  is shown by two different but correlated results, i.e. the development of charring depth with time of fire exposures (Figs. 2a, 3, 4, 5, 6 and 7a) and the value of



**Fig. 2** a The development of charring depth for varied parameter  $E_{1,\Delta}$ . **b** Sensitivity index  $S_{char,E_1}$  showing the influence of parameter  $E_1$  on the final charring depth

sensitivity index  $S_{\text{char},x_i}$  (Figs. 2b, 3, 4, 5, 6 and 7b), which is a normalized measure for the final charring depth (see Eq. 10). The influence of the varied parameter  $E_{1,\Delta}$  is presented in Fig. 2a and b. Varying the activation energy  $E_i$ has a major influence on the development of charring depth and on the sensitivity index  $S_{char,E_1}$ . The lower the value of  $E_{1,\Delta}$ , the faster is the reaction rate (see Eq. 6) for the production of the active cellulose. In turn, this leads to the faster development of the charring depth and also bigger final charring depth. The final charring depth



**Fig. 3** a The development of charring depth for varied parameter  $A_{1,\Delta}$ . **b** Sensitivity index  $S_{char,A_1}$  showing the influence of parameter  $A_1$  on the final charring depth



**Fig. 4** a The development of charring depth for varied parameter  $E_{2,\Delta}$ . **b** Sensitivity index  $S_{char,E_2}$  showing the influence of parameter  $E_2$  on the final charring depth



**Fig. 5** a The development of charring depth for varied parameter  $A_{2,\Delta}$ . **b** Sensitivity index  $S_{charA_2}$  showing the influence of parameter  $A_2$  on the final charring depth

increases from 34 to 49 mm if the reference value  $E_1$  is reduced by a factor of 0.85. This means that reducing the parameter  $E_1$  by only 15% induce 44% increase of the final charring depth, seen in the index  $S_{\text{char},E_1}$  in Fig. 2b. Similarly, but vice versa, increasing  $E_1$  by 20% results in 23.4% decrease of the final charring depth. Varying the preexponential factor  $A_1$ , does not have such a significant influence on the final charring depth. When the parameter  $A_1$  is varied from 0.2 to 1.8 regarding the reference value, the final charring depth increases or decreases by a maximum of 3% (Fig. 3b). The development of charring depth with time (Fig. 3a) is very similar for all cases.

Varying the parameters  $E_2$  and  $A_2$ , that govern the reaction rate for the char production and gases, does not have a significant influence on the development and final charring depth, as observed from Figs. 4 and 5. The final charring depth increases by a maximum of 3% when varying parameter  $E_2$  (see Fig. 4b) and around 3% when varying the parameter  $A_2$  (see Fig. 5b).

Similar conclusions apply when changing the parameters that govern the reaction rate for the tar production,  $E_3$  and  $A_3$ . For both varied parameters, the charring depth increases by a maximum of 3% (Figs. 6b and 7b).

The sensitivity study demonstrates, that the most influential parameter for the development of charring depth is the activation energy  $E_1$ . Other parameters have minor influence. Therefore, to calibrate the model for different fire conditions and natural fire exposures, the parameter  $E_1$  is calibrated in the following. In addition, the parameter  $A_1$  is calibrated as well, since  $E_1$  and  $A_1$  jointly govern the reaction rate of active cellulose productions and must be considered together in the calibration.

# Results of model calibration analysis—cone calorimeter tests

The comparison between calculated and measured development of temperatures and charring depth, for a  $38.5 \text{ kW/m}^2$  heat flux exposure, is given in Fig. 8a and b, respectively. The development of temperatures in points



**Fig. 6** a The development of charring depth for varied parameter  $E_{3,\Delta}$ . b Sensitivity index  $S_{char,E_3}$  showing the influence of parameter  $E_3$  on the final charring depth



**Fig. 7** a The development of charring depth for varied parameter  $A_{3,\Delta}$ . b Sensitivity index  $S_{char,A_3}$  showing the influence of parameter  $A_3$  on the final charring depth

of the specimen that are 10 and 14 mm away from the exposed edge agree well. Some more discrepancies are observed in points closer to the exposed edge (2 mm and 6 mm), where the measured temperatures are higher than calculated values. For instance, the measured temperature plateau in the point 2 mm from the exposed edge is 685 °C, compared to the calculated temperature plateau of 645 °C, giving the total difference of 5.8%, which is, however, within the reasonable boundaries. Although minor discrepancies occur regarding temperature development, there is, on the other hand, a very accurate agreement between measured and calculated charring depth as seen from Fig. 8b. The calibrated value of activation energy  $E_1$  for 38.5 kW/m<sup>2</sup> heat flux exposure, given in Table 2, is 3% less than the reference value (see Table 1), while the calibrated parameter  $A_1$  is the same as the reference value (Table 1).

**Table 2** Kinetic parameters  $E_1$  and  $A_1$  for different heat flux exposures in cone calorimeter tests

	38.5 kW/m <sup>2</sup>	60 kW/m <sup>2</sup>	90 kW/m <sup>2</sup>
E <sub>1</sub> (kJ/mol)	235.3	242.6	254.7
$A_1(s^{-1})$	$1.7 \times 10^{21}$	$1.7 \times 10^{21}$	$8.5 \times 10^{20}$

The results for the 60 kW/m<sup>2</sup> heat flux exposure are given in Fig. 9a and b. The measured and calculated development of temperatures and charring depth correspond very accurately, since the deviations are less than 2% for all the observed quantities. The analysis showed that the best fit between experimental and numerical results was obtained by considering the reference values of  $E_1$  and  $A_1$  (see Tables 1 and 2).

Comparison of temperature development for 93.5 kW/  $m^2$  heat flux exposure (Fig. 10a) shows good agreement



Fig. 8 Comparison of experimental and numerical results for 38.5 kW/m<sup>2</sup> cone calorimeter test. **a** The development of temperatures in different points of the specimen. **b** The development of charring depth



Fig. 9 Comparison of experimental and numerical results for 60 kW/m<sup>2</sup> cone calorimeter test. **a** The development of temperatures in different points of the specimen. **b** The development of charring depth



Fig. 10 Comparison of experimental and numerical results for 90 kW/m<sup>2</sup> cone calorimeter test. **a** The development of temperatures in different points of the specimen. **b** The development of charring depth

between experimental and numerical results. The development of charring depth demonstrates some discrepancies between measured and calculated values, especially after 10 min of the exposure, when the measured charring depth starts increasing faster than the calculated charring depth. The final value of charring depth is 26.6 mm (at t=25 min), which is 4.6 mm more than the final calculated value (22 mm), resulting in 17% difference. This, nevertheless, is a moderate deviation regarding all the uncertainties when analysing the behaviour of timber in fire conditions. As known, timber is associated with large scatter of material parameters. In Terrei et al. [14], no specific values of thermal conductivity, specific heat and other parameters were given. Therefore, some of these data in the numerical model were assumed. For instance, thermal conductivity and specific heat of timber were assumed to follow EN 1995-1-2 [5] proposal. However, this sometimes is not consistent with the real parameters of the timber used in the experiment. For this reasons, some discrepancies between the experimental and numerical results and numerical are expected. The best fit for the 93.5 kW/m<sup>2</sup> exposure was obtained considering the activation energy  $E_1$  of 254.7 kJ/mol (5% more regarding the reference value of  $E_1$ ) and the preexponential factor  $A_1$  of  $8.5 \cdot 10^{20}$  s<sup>-1</sup> (50% more regarding the reference value of  $A_1$ ).

The model calibration studies based on the cone calorimeter tests show a robust behaviour of the model, since a small calibration of the pyrolysis reaction parameters is needed for an accurate prediction of the temperature and charring developments at different heat flux exposures. An important observation is also that for lower heat flux exposures lower values of  $E_1$  and bigger values of  $A_1$  are obtained, which means that faster reaction rates of the active cellulose production at lower heat flux exposures occur.

# Results of model calibration analysis—large-scale natural fire tests on CLT floor system

In the following part of the paper, the model calibration for the large-scale natural fire tests of CLT floor system is presented. All together three fire scenarios were considered. Temperature-time curves for all scenarios are presented in Fig. 1. Experientially determined charring depths are determined from temperature positions at 4 points along the slab in reference marked as points A to D. Based on the experimental setup the CLT slabs are heated only from one side, thus the problem is one dimensional, which is also considered in the numerical model. Experimentally determined charring depths are based on the 300 °C isotherm, meaning that marks in Figs. 11b, 12, 13b represent the time when temperature 300 °C is reached. For the comparison with the experiment, average (linear) numerical charring rates of first or second lamella are obtained (Table 3). Although as seen from Figs. 11b, 12, 13b, charring developments and consequently charring rates are non-linear.

#### Scenario 1

The developments of measured and calculated temperatures and charring depths for fire scenario 1 (see Fig. 1) are given in Fig. 11a and b. According to test reports [15], the plan was to measure the temperatures in 4 points (A to D), but for this scenario temperature developments in points C and D are given. In addition, only the charring of first lamella occurred in the experiment. Good agreement for the development of temperatures and charring depth is discovered (Fig. 11). The mean value of experimentally determined charring rates in the first lamella



Fig. 11 Fire scenario 1. a The development of temperatures at the interlayer between first and second lamella. b The development of charring depth



Fig. 12 Fire scenario 2. a The development of temperatures at the interlayer between first and second lamella. b The development of charring depth



Fig. 13 Fire scenario 3. a The development of temperatures at the interlayer between first and second lamella. b The development of charring depth

	Charring rates (mm/min)			
	1st lamella		2nd lamella	
	Experiment	Numerical	Experiment	Numerical
Scenario 1	1.43 (min 1.29–max 1.65)	1.58	No charring	No charring
Scenario 2	1.19 (min 1.13–max 1.4)	1.39	0.8 (min 0.72–max 0.86)	0.72
Scenario 3	0.85 (min 0.76–max 0.9)	0.98	0.92 (min 0.73–max 1.17)	1.09

Table 3 Charring rates for different fire scenarios

was 1.43 mm/min, while numerically determined value is 1.58 mm/min (see Table 3), yielding the difference of 9.5%.

#### Scenario 2

The temperature developments fit well in the heating phase (Fig. 12a) and a bit less at the beginning of the cooling phase. When the cooling phase starts a fall off of the first lamella occurs, seen as a sudden temperature jump at positions A, C and D. The model fails to predict this phenomenon, since delamination of layers is not modelled. However, later on in the cooling phase, the temperatures agree well. In case of fire scenario 2, charring of first and second lamella occurred. The model slightly overestimates the charring of the first lamella and underestimates the charring of second lamella (Fig. 12b). The mean value of the measured charring rates of the first lamella is 1.19 mm/min. Compared to the computed value of 1.39 mm/min (Table 3), this gives a difference of 14%. The charring rate (mean experimental value) of the second lamella is 0.8 mm/min. A bit slower value of 0.72 mm/min is predicted numerically, which is 10% less compared to the experiment.

#### Scenario 3

For fire scenario 3, a good agreement of temperatures in the heating phase is found as well (Fig. 13a), however, same observation as for the scenario 2 is detected, i.e. the delamination at positions A and B causes sudden jump in temperature development, which the model cannot predict. Similarly, as for scenario 2, also in case of scenario 3, the charring of both first and second lamella happened. The model somewhat overestimates the charring of first and second lamella, compared to the experiment (Fig. 13b). The experimentally measured charring rates (mean values) for the first and second lamella are 0.85 and 0.9 mm/min, respectively. The model predicts slightly higher charring rates of 0.98 and 1.09 mm/min, which is 14% and 17% more than experimentally determined values, for first and second lamella, respectively.

Although for all three fire scenarios some discrepancies are observed between numerically predicted charring rates and mean values of experimentally measured charring rates, the numerical determined charring rates are, except for the 1st lamella in scenario 3, within the boundaries of minimum and maximum experimentally measured charring rates (see minimum and maximum charring rates that supplement the mean values in Table 3). Note that a large scatter of experimental results is observed, meaning that a lot of variability is present in the experiment, which is quite common for timber elements exposed to fire, since charring is by its nature a stochastic phenomenon [33]. This is one of the drawbacks of current PYCIF model, since modelling of charring is not fully probabilistic. By varying the parameters of the pyrolysis reaction, it is possible only to some extent describe the stochastic nature of charring. For a fully general stochastic model a variability of room temperatures, boundary conditions, thermal characteristic of timber and other should be implemented, which is planned in the next step of the PYCIF model development. However, already in this stage of development the PYCIF model gives satisfactory results and enables to predict the chairing of timber elements in various fire conditions.

In addition, the charring rates determined by Mindeguia et al. [15] were obtained under load, while in the simulation, the unloaded specimen was considered. This could also be a potential reason for the differences between the numerical and experimental result, especially for fire scenarios 2 and 3, where considerable deflection occurred. This means that the deformation of the slab can have some influence on the thermal response of the slab and can potentially lead to delamination of the slab or occurrence of cracks, which probably happened in fire scenarios 2 and 3.

#### Fitting of the model parameters

The best fit with the experimental results is found based on the kinetic parameters of pyrolysis reaction given in

**Table 4** Kinetic parameters  $E_1$  and  $A_1$  for different fire scenarios

	Scenario 1	Scenario 2	Scenario 3
E <sub>1</sub> (kJ/mol)	246.8	247.3	253.9
$A_1(s^{-1})$	$1.7 \times 10^{21}$	$1.7 \times 10^{21}$	$8.5 \times 10^{20}$

Table 4. As observed, the parameter  $E_1$  is for all three scenarios higher than the reference value. The parameter  $A_1$  is lower compared to the reference value only for scenario 3. This means that in all cases, the reaction rate for the active cellulose production  $(k_1)$  is slower compared to the reaction rate with the reference value of kinetic parameters, which are calibrated for standard ISO fire exposure. This study therefore shows, that in case of natural fire with faster heating rate than the ISO standard fire, the kinetic parameters take lower values and govern slower reaction rate for the active cellulose production. This is in accordance with basic laws of thermochemical decomposition of timber, since in case of faster temperature increase less charcoal is produced, which is a consequence of slower reaction for the active cellulose production [17, 34].

#### Relationship between the model parameters $E_1$ and $A_1$ and characteristics of fire (heat) exposure

In the following, the influence of parameters that define fire or heat exposure on the kinetic parameters  $E_1$  and  $A_1$  is examined. In Fig. 14a, the parameters  $E_1$  and  $A_1$ are plotted against the external heat flux exposure in the cone calorimeter tests. Interestingly, Fig. 14a demonstrates a linear dependence of the parameter  $E_1$  on the external heat flux exposure. A bilinear relationship is observed between the parameter  $A_1$  and the external heat flux exposure, since at 38.5 and 60 kW/m<sup>2</sup> heat flux exposures, the parameter  $A_1$  does not change, while at 93.5 kW/m<sup>2</sup> this parameter drops by 50%. However, more research is needed to identify the threshold of heat flux exposure, at which parameter  $A_1$  starts decreasing. In Fig. 14b the parameters  $E_1$  and  $A_1$  are shown depending on the parameter  $t_{g,max}$ , which is the time when maximum temperature is reached in case of large-scale natural fire tests of CLT floor system. The parameter  $t_{g,max}$  is chosen since it gives the information about the duration of the heating phase and as shown in the recent research [6], the development of charring depth strongly depends on the parameter  $t_{g,max}$ . For scenarios 1, 2 and 3, times  $t_{g,max}$  are 21.1 min, 42.4 min and 50.6 min, respectively. In general, the parameter  $E_1$  increases with time  $t_{g,max}$  and exponential relationship can be assumed. The relationship between parameter  $A_1$  and  $t_{g,max}$  is bilinear. The plateau of 253.9·10<sup>21</sup> s<sup>-1</sup> between  $t_{g,max} = 21.1$  min and  $t_{g,max} = 42.4$  min is observed, which than drops by 50% at  $t_{g,max} = 50.6$  min.

# Discussion on the suitability of Broido–Shafizadeh pyrolysis model

As calibration analyses show ("Model calibration studies" section), with the implemented BS pyrolysis submodel in the PYCIF model, an accurate determination of the charring of wood for the various fire conditions can be achieved. It is, however, necessary to identify why implementing rather simple pyrolysis model (such as BS model) for determination of charring depths is appropriate when fire resistance of timber elements is assessed. As defined by EN 1995-1-2 [5], from a fire resistance point of view, charring of wood occurs when wood fibre cannot carry load anymore, i.e. when completely loses its strength characteristics. As well known, cellulose is responsible for strength in the wood fibre [35]. Therefore, when cellulose completely decomposes at elevated temperatures, wood fibre is no longer able to carry load. For this reason, the BS model, that considers only the cellulose pyrolysis, represent a good approximation of how wood fibre decomposes and loses strength at elevated temperatures. This is also shown in sections "Results of model calibration analysis-cone calorimeter tests" and "Results of model calibration analysis-large-scale natural fire tests on CLT floor system" by comparing



**Fig. 14** A relationships between the parameters  $E_1$  and  $A_1$  and **a** the external heat flux exposure in cone calorimeter tests, and **b** time  $t_{g,max}$  for fire scenarios 1, 2 and 3 in case of natural fire tests of CLT floor system

experimental and numerical results, where good agreement is obtained. However, charring criterion that is based on the decomposition of cellulose is appropriate only for determining fire resistance of timber structures. In terms of other aspects of fire safety, complex multiconstituent models that describe the pyrolysis of cellulose, lignin and hemicellulose are needed in order to accurately determine which products are formed during fire exposure and also their quantity. This can be especially of great importance in case of modelling the evacuation from the building, where accurate prediction of smoke, toxic gases, etc., is crucial to evaluate the critical evacuation time.

## Conclusions

The paper presents an improvement and upgrade of a recently developed heat-mass-pyrolysis model named PYCIF, to predict charring in case of natural fire exposure, which, to the authors knowledge, has not been presented till date. For this purpose, firstly a sensitivity study was performed with a goal to discover which kinetic parameters of pyrolysis reaction are the most influential. Once these parameters were identified, model calibration analyses for cone calorimeter tests and large-scale natural fire tests on CLT floor system were performed. The following was discovered:

- The kinetic parameters *E*<sub>1</sub> and *A*<sub>1</sub>, which describe the reaction rate for the production of active cellulose, have the most influence on the development of charring depth.
- First set of calibration analyses were based on a small-scale cone calorimeter tests, with different exposures to the external heat flux. With calibration of kinetic parameters, the model predicted accurately the development of charring depth and temperatures compared to the experiment. Additionally, it was discovered that for lower heat flux exposures, the calibrated parameters  $E_1$  and  $A_1$  govern faster reaction rate of active cellulose.
- The second set of calibration analyses were based on the large-scale natural fire tests of CLT floor system. The model yielded accurate charring depth and temperature developments after the model calibration was performed. The study also revealed, that for natural fires with faster heating rates than the standard ISO fire, the kinetic parameters were modified, so that the reaction rate of active cellulose was slower compared to the reaction rate for ISO curve.
- A significant connection between the heating rate in cone calorimeter tests and kinetic parameters that govern the reaction rate of active cellulose was discovered. The faster the heating rate, the slower

the reaction rate of active cellulose. This is consistent with the basic laws of pyrolysis reaction, since, at faster temperature increase, less charcoal is produced (as a consequence of less active cellulose production). This observation is very important for the next step of modelling, i.e. implementing the stochastic approach to model charring, since model parameters can now be correlated with different natural fire curves.

- Similar finding was also discovered in the analysis with different natural fire scenarios, where the reaction rate of active cellulose slows down with longer and more intense fires (more heat is generated in case of fire scenario 3 compared to the scenario 1). In order to find more accurate relationships between the parameters of natural fire curve and kinetic parameters of the model, further investigation is needed. This will also give a better understanding of the charring phenomena in general.
- In order to reduce some minor discrepancies that appear between numerical and experimentally determined development of charring, the following improvements are important in the future: (1) considering a fully stochastic nature of charring in order to implement uncertainties and probabilistic approach to model charring. This is especially important in cases of natural fire conditions, since more uncertainties are present. (2) Modelling a possible thermo-mechanical interaction in cases of loaded timber elements, especially when large deflections appear.

#### Abbreviations

3S	Broido–Shafizadeh
CLT	Cross-laminated timber
SO	International Organization for Standardization
PYCIF	Heat-mass-pyrolysis model

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#### Author contributions

RP, TH and SH conceived and designed the numerical studies. RP, TH and SH performed the numerical studies and analysed the data. RP wrote the draft of this manuscript. RP, TH and SH reviewed and edited the manuscript. All authors read and approved the final manuscript.

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#### Availability of data and materials

All data generated or analysed during this study are included in this published article.

#### Declarations

#### **Competing interests**

The authors declare that they have no competing interests.

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