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RESEARCH ARTICLE

A multiscale model for wood combustion

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Abstract

Understanding wood combustion has become increasingly critical as fire safety engineering moves toward a performance-based approach to building design. Although different kinetic models have been developed for wood burning, chemical kinetics remains a significant challenge for accurate prediction. This work has developed a novel multiscale model by implementing kinetic parameters calculated from molecular dynamics simulations using reactive forcefield into a kinetic model of wood burning. The calculated kinetic parameters of the main components in wood, namely, cellulose, hemicellulose, and lignin, are first utilized to model microscale thermogravimetric experiments for validation. Subsequently, the mesoscale and full-scale fire tests have been simulated by the multiscale model. Furthermore, the fire properties of various wood species at different heat fluxes have been predicted and compared with results from the cone calorimeter test. Our multiscale model outperforms existing kinetic models in predicting wood combustion and can effectively discern the influence of chemical components on fire properties.

1 | INTRODUCTION

Timber-based materials are undergoing a renaissance recently driven by an unprecedented push for sustainable development with lower energy demands and less pollution (Östman et al., 2017). Better insulation capabilities relative to traditional building materials such as concrete or steel, minimal energy usage during the life cycle from processing to final disposal, and convenient recyclability provide the basis for using wood as an innovative renewable construction material (Cai & Chow, 2018; Rathnayake et al., 2020). However, the combustibility of timber limits its wide application (H. Cheng & Hadjisophocleous, 2012; Qin et al., 2021). The load-bearing capacity of wood structures is degraded and controlled by the process of

thermal decomposition, namely charring (Kim et al., 2006; Richter et al., 2019). Understanding the fire behavior of wood is critical to figure out the strength decay in fire and to estimate the safety of timber buildings, offering a determinable role in their fire safety management.

Numerical simulations have become essential in the fire safety design of buildings, where the outputs can be used for detailed analyses of passive and active fire protection for building structures, protection of persons during evacuation, and fire intervention during its liquidation (Arias, 2007). As the strength decay of wood is highly dependent on the charring, various kinetic models have been developed to model wood pyrolysis (Anca-Couce, 2016; C. H. Cheng et al., 2021; Miao & Chow, 2018; Richter & Rein, 2019; Rinta-Paavola & Hostikka, 2021). However, the most

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commonly used kinetic model with a single-step reaction scheme cannot identify the difference among various wood species, ignoring the influence of chemical components, namely, cellulose, hemicellulose, and lignin (Hostikka & Matala, 2017). While the parallel reaction scheme controlling the degradation of cellulose, hemicellulose, and lignin independently outperforms the single-step reaction scheme in reproducing bench-scale fire test, the deviation of fire properties between prediction and experiment can be as high as 50% (Ding et al., 2020). As fire modeling has become a fundamental part of fire engineering, it is crucial for a robust and reliable kinetic model that can be confidently used to predict the wood burning. More importantly, charring, a critical parameter to estimate the fire resistance of wood and the fundamental reason for the strength decay, is required to be accurately estimated. The accuracy of the fire modeling approach lies in the chemical kinetics that can describe the pyrolysis and oxidation of wood burning. The kinetic parameters of the reaction scheme in existing kinetic models are deduced from different integral and differential kinetic models based on microscale experiments, such as thermogravimetry, differential scanning calorimetry, and microscale combustion calorimetry (D'Acierno et al., 2020). To achieve a more comprehensive understanding of the burning behavior of wood elements, including wood materials, wood structures, and timber buildings, it is crucial to develop models that can accurately simulate the chemical kinetics of wood.

Recently, reactive forcefield (ReaxFF) has been developed to model bond breaking and formation in molecular dynamics (MD) simulations (Hao et al., 2020a; Qiu et al., 2020; Yu et al., 2021). MD simulations using ReaxFF enable the simulation of chemically reactive systems. The parameters of ReaxFF are trained for optimization against data from experiments and quantum mechanics (QM) calculations (Chenoweth et al., 2008; Hao et al., 2020a). MD simulations using ReaxFF can efficiently simulate the molecular behaviors in chemical reactions in large-scale systems with a high accuracy close to QM at a much lower computational cost (Qiu et al., 2020). The chemical reaction pathway can be decided by this approach so that the kinetics parameters, such as activation energy, reaction rate, and heat of reaction for different systems, can be deduced. MD simulations using ReaxFF have been successfully utilized to predict hydrocarbon oxidation, polymer decomposition, and coal combustion (Aryanpour et al., 2010; Weismiller et al., 2010). The chemical kinetics, including the reaction mechanism and kinetic parameters of polymers, can be accurately calculated by MD simulations using the ReaxFF approach in an economical and time-saving way.

The objective of this work is to develop a multiscale model that can predict the burning behavior of various wood structures. The chemical kinetics, including reac-

tion schemes and kinetic parameters calculated from the nanoscale modeling, are implemented into a mesoscale kinetic model to simulate the fire behavior of various wood species; the full-scale fire performance of corresponding structures can be predicted by the developed multiscale model as shown in Figure 1. At the nanoscale, the reaction schemes of wood's main components, namely, cellulose, hemicellulose, and lignin, are determined from MD simulations using ReaxFF, and the corresponding kinetic parameters are deduced. The calculated chemical kinetic is first applied to model the thermal decomposition test at microscale, and the predicted results are compared with the thermogravimetric experiment for validation. Subsequently, the validated chemical kinetics of cellulose, hemicellulose, and lignin are implemented into the kinetic model with a parallel reaction mechanism to model the mesoscale fire test, namely, cone calorimeter, by using Fire Dynamics Simulator (FDS). Fire properties of different wood species, such as oak, larch, and red cedar at various external heat fluxes, are predicted and compared with experiments to evaluate the accuracy of the multiscale model. Furthermore, the multiscale model is utilized to predict the fire behavior of full-scale wood structures, such as wood furniture.

The developed multiscale modeling can predict the fire properties of structures related to wood elements, such as wood furniture, and timber buildings. The ability to distinguish the effect of chemical components on fire properties makes it possible to predict the burning behavior of different wood species, significantly reducing the costs and effort for experimental testing. Additionally, the fundamental understanding of how wood performs in fire leads to much more reliable and sustainable wood building designs and the appropriate choice of wood species in consideration of fire safety concerns. The multiscale developed in this work can be extended to model the fire behavior of plant materials, such as bamboo, as they are also mainly composed of cellulose, hemicellulose, and lignin with different contents. It should be noted that as the burning behavior is complex, the multiscale model is simplified, including the molecular structure of components and the oxidation mechanism of char. Therefore, the disparities between the results obtained from the developed multiscale modeling and experimental outcomes are inevitable.

2 | METHODOLOGY

2.1 | MD simulations using ReaxFF

In contrast to the traditional non-ReaxFF, ReaxFF is a bond-order dependent interatomic potential. The connectivity between every pair of atoms in ReaxFF is determined

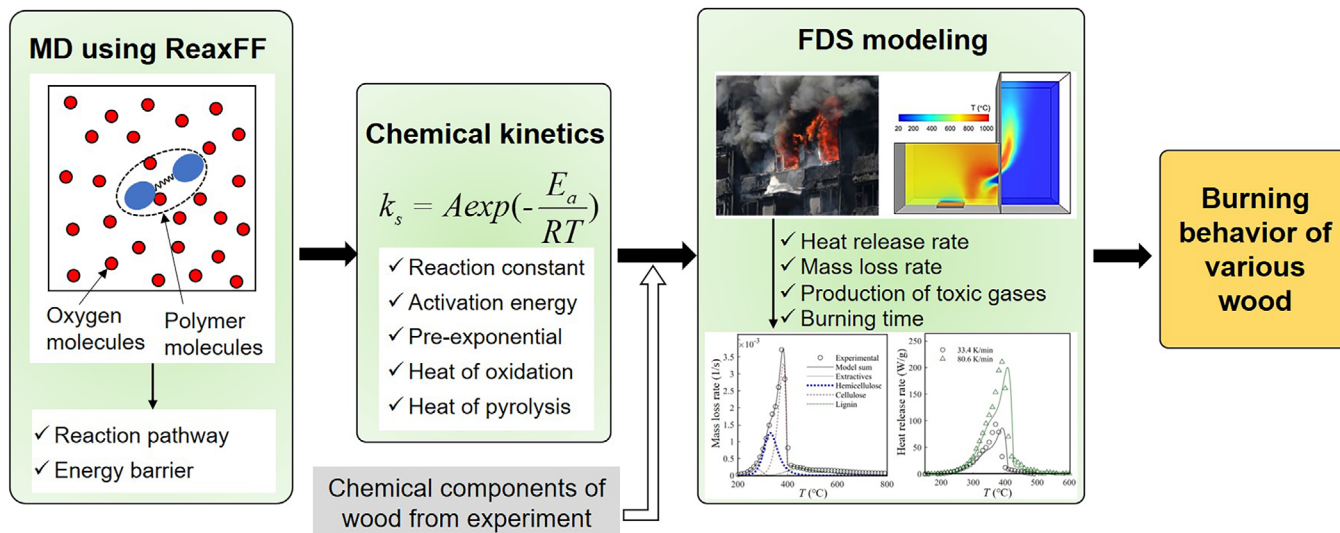


FIGURE 1 The schematic diagram of the developed multiscale model for fire modeling of wood. The combustion kinetic parameters of cellulose, hemicellulose, and lignin can be deduced from molecular dynamics (MD) simulations using reactive forcefield (ReaxFF). These parameters are then employed as input parameters to control the pyrolysis and oxidation of timber structures within Fire Dynamics Simulator (FDS) simulation. When combined with the chemical compositions specific to each wood species, this approach enables the prediction of burning properties of structures made up of various wood species.

at each time step, enabling to simulate the smooth formation and dissociation of bonds. The following equation is used to find the energy and force of each atom (van Duin et al., 2001):

$$E = E_{\text{bond}} + E_{\text{val}} + E_{\text{tor}} + E_{\text{over}} + E_{\text{under}} + E_{\text{conj}} + E_{\text{vd}} + E_{\text{Coul}} \quad (1)$$

where E_{bond} , E_{val} , and E_{tor} are the energy related to bond, angle, and torsion angles, respectively; E_{over} and E_{under} are over-coordinated and under-coordinated energy penalties; E_{conj} is the contribution of conjugation effects to the molecular energy; E_{vd} , and E_{Coul} are the energy of the van der Waals force and Coulomb force. All covalent interactions, such as E_{bond} , E_{val} , and E_{tor} are expressed in terms of bond orders; their contribution diminishes upon bond breaking (Goddard et al., 2006; Trnka et al., 2018). The nonbonded interactions in ReaxFF like Coulomb and van der Waals are calculated between every pair of atoms irrespective of their connectivity, and any excessive short-range nonbonded interactions are avoided by including a shielding term. ReaxFF allows for dynamic adjustments of bond orders during simulations based on the local atomic environment. This distinctive feature empowers ReaxFF to accurately model the changes in chemical bonding that are correlated with char formation and oxidation during polymer decomposition. Furthermore, ReaxFF can effectively represent non-covalent interactions between molecules, influencing the formation and structure of char. As a result, MD

simulations using ReaxFF can reveal the chemical reaction pathway, providing an accurate estimation of the activation energy related to char formation. The reaction pathway of pyrolysis and oxidation for cellulose has been successfully predicted by MD simulations using ReaxFF (Hao et al., 2020a). The essential reactions occurring during pyrolysis and oxidation of cellulose, such as the cleavage of linkages between monomers, the production of intermediates, and the oxidation of small molecules can be captured by MD simulations using ReaxFF, similar to the experimental findings. The reasonability and reliability of utilizing MD simulations with the ReaxFF approach predict covalent properties of polymers containing glucose and benzene rings, such as hemicellulose, and lignin, have been demonstrated. The kinetics of cellulose, hemicellulose, and lignin are studied by MD simulations with ReaxFF.

In wood, cellulose is made up of glucose monomers linked by the β (1-4) glycosidic linkage (Gibson, 2012); hemicellulose is composed of many sugars, such as xylose, arabinose, mannose, and galactose, and the xylose is the main composition (Delbecq et al., 2018); lignin is mainly composed of three monolignols, namely, p-coumarylalcohol, coniferyl alcohol, and sinapyl alcohol, and these monomers are connected by various types of linkages, such as β -O-4, α -O-4, β - β , β -5, 5-5, 4-O-5, β -1 (Wen et al., 2013). The most common sinapyl alcohol monomers connected with β -O-4 linkages are used to represent lignin structure (Habibi et al., 2016). As the model consisting of two building blocks can effectively

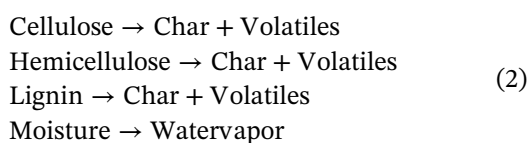


capture the essential reactions occurring during pyrolysis and oxidation, the structures of cellulose, hemicellulose, and lignin are simplified considering the accuracy and efficiency. The linked glucose, xylose units, and sinapyl alcohol monomers are selected as representatives of cellulose, hemicellulose, and lignin. MD simulations are used to derive chemical kinetic parameters of pyrolysis for cellulose, hemicellulose, and lignin, such that various wood species can be accommodated in FDS modeling, considering the variation in composition.

The MD simulations of reactions are performed in the large-scale atomic/molecular massively parallel simulator (LAMMPS) (Plimpton, 1999). The atom number for reaction systems is significantly lower than the number of atoms found in solid materials, spanning several orders of magnitude. A much higher temperature is used in MD simulations for the possibility of a reaction occurring. The extent of oxidation determines the total simulation time of the systems, and the simulations are terminated when all hydrogen and carbon atoms in polymer molecules are transferred to water molecules and carbon dioxide. The reaction mechanism and energy barriers at different temperatures are directly obtained based on MD simulations. The kinetic parameters, such as the pre-exponential factor and activation energy, are inferred according to the Arrhenius equation.

2.2 | FDS modeling

The burning behavior of different wood species is studied using FDS Version 6.7.5 developed by the National Institute of Standards and Technology (McGrattan et al., 2013). The pyrolysis and oxidation reactions occur when wood is heated in air. More specifically, wood undergoes pyrolysis when exposed to a heat flux, with the generation of fuel gases and char; fuel gases and char layer then react with oxygen, causing the increment in surface temperature until fire decays and dies down. A kinetic model that includes the pyrolysis and char oxidation is proposed to model wood burning. The pyrolysis of wood is governed by a parallel reaction mechanism, where cellulose, hemicellulose, and lignin degrade independently. The reaction scheme for pyrolysis is described by the following equations:



The oxidation is controlled by a single-step reaction scheme. The kinetics parameters, such as pre-exponential

factor, activation energy, heat of reaction, and heat of combustion, for cellulose, hemicellulose, and lignin obtained from MD simulations are applied to control the pyrolysis model.

As described above, the kinetics parameters of cellulose, hemicellulose, and lignin are the most important to determine the accuracy of pyrolysis in wood combustion model. The thermal decomposition for cellulose, hemicellulose, and lignin at a heating rate of 10 K/min has been carried out by FDS with the kinetic parameters from MD simulations. During the decomposition process, it is assumed that cellulose, hemicellulose, and lignin decompose with the production of volatile gases, leaving a char residue. The decomposition process is predominantly governed by a first-order reaction mechanism. The solid residual contents of cellulose, hemicellulose, and lignin in FDS modeling are set to 8.6%, 27.3%, and 46.2%, respectively, based on thermogravimetric analysis (TGA) experimental results (H. Zhou et al., 2015). To assess the reliability of the kinetic parameters obtained from MD simulations for predicting the pyrolysis of cellulose, hemicellulose, and lignin, the predicted results are compared with those obtained from traditional numerical modeling where the kinetic parameters are inferred from experimental data. Additionally, the predicted properties are also compared directly with TGA results for validation.

The multiscale model for wood combustion is developed by combining the validated kinetic parameters from the nanoscale into the kinetic model for the fire model at the mesoscale. The most common mesoscale fire test, cone calorimeter, is simulated by the developed multiscale model. The predicted results have been compared with the cone calorimeter test to estimate the reliability and accuracy of the developed multiscale model. The computational domain of FDS modeling is defined based on our previous cone calorimeter test (Hao et al., 2020b). The FDS model of the cone calorimeter test at mesoscale is constructed to resemble the experimental setup as shown in Figure 2. The simulated computational domain of FDS cone calorimeter modeling is $300 \times 300 \times 700$ mm, so all flames can be captured. The four sides of the domain have been specified as closed glasses (Dutta et al., 2019; Moinuddin et al., 2020). The size of the modeled sample is $100 \times 100 \times 50$ mm, identical to the experimental test; the sample is placed horizontally and centrally near the bottom of the domain. The wood combustion behavior at different cone radiative heat fluxes (20, 35, and 50 kW/m²) has been predicted by our multiscale model. As the fire properties of oak, larch, and red cedar have ever been tested, they have been selected as representatives. The chemical compositions and thermal properties of oak, larch, and red cedar are shown in Table 1. The heat release rate (HRR), one critical parameter to understand the



TABLE 1 Chemical composition and thermal properties of different wood species.

Wood type	Composition (wt.%)				Specific heat (kJ/kg·K)	Thermal conductivity (W/m·K)
	Cellulose	Hemicellulose	Lignin	Water		
Oak	41.6	26.8	25.7	5.9	1.2	0.1
Larch	37.8	28.4	29.0	4.8	1.2	0.1
Red cedar	40.0	20.0	34.0	6.0	1.3	0.1

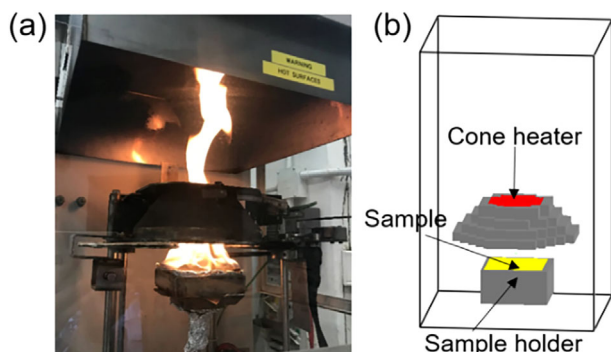


FIGURE 2 (a) Experimental set-up of cone calorimeter; (b) FDS model set-up of cone calorimeter. The modeled sample size is the same as that in the cone calorimeter.

combustion process, characteristics, and propagation rate of fire (Zou et al., 2018), has been predicted and compared with results tested by cone calorimeter.

The grid size is an essential factor for FDS modeling. The balance between simulation accuracy and computational time needs attention in deciding the grid size. According to the geometric features of modeling, the grid is made of a structured mesh with dimensions of $2 \times 2 \times 2$ mm. Grid dependence analysis is performed prior to the main simulations to guarantee that the predicted results are acceptable. Although there are some temperature variations in the system with a coarser grid, consistent temperature profiles across different elevations are observed in FDS simulations regardless of grid size variations. A grid dimension of 2 mm can provide accurate predictions where the effect of grid size on the time history of temperatures simulated by FDS can be negligible. As a result, it can be inferred that the grid size is appropriate for studying fire behavior of wood.

3 | RESULTS AND DISCUSSION

3.1 | Chemical kinetics of cellulose, hemicellulose, and lignin

In MD simulations using ReaxFF, a high temperature is used to ensure the reaction occurrence. The elevated temperature can provide the necessary energy to overcome

barriers to reactions. The chosen temperature range for pyrolysis ensures the initial cleavage of bonds connecting the monomers of cellulose, hemicellulose, and lignin, aligning with experimental observations. Beyond the specified temperature values, bonds within the monomer are initially broken, leading to a diversified reaction mechanism. It has been observed that, in the MD simulations, the bonds linking the glucose, xylose, and sinapyl alcohol monomers are the first to be broken during the reaction. When all carbon atoms in linked molecules are in the form of CO and CO₂, CO starts to be oxidized. The snapshots of different modeled systems with the highest number of CO are shown in Figure 3.

The kinetics of reactions is calculated based on the trajectories of the simulations. The rate constant is calculated by the following equation (Dontgen et al., 2015):

$$\Delta G(T) = -RT \ln \left(\frac{h \cdot k(T)}{k_B T} \right) \quad (3)$$

where R is the gas constant, T is temperature, h is Planck's constant, k_B is Boltzmann's constant, and ΔG is ReaxFF free-energy barriers for the reactions. According to the Arrhenius equation, the rate constant is dependent on the temperature, calculated by (Liu et al., 2020; Smith et al., 2011):

$$k_s = A \exp \left(\frac{-E_a}{RT} \right) \quad (4)$$

$$\ln k_s = \frac{-E_a}{RT} + \ln A \quad (5)$$

where k_s is the rate constant, E_a is the activation energy, and A the pre-exponential factor.

Figure 4 shows the curves of the rate constant as a function of temperatures. The deduced E_a and A of cellulose, hemicellulose, and lignin are listed in Table 2. Compared with the experimental data, where the E_a for cellulose and lignin can be as high as 200 kJ/mol and that of hemicellulose up to 160 kJ/mol (Liang et al., 2023; Mamleev et al., 2007; Paajanen & Vaari, 2017; Anca-Couce et al., 2020), the E_a deduced from MD simulation using ReaxFF is underestimated, directly correlated to the intrinsic limitations of MD simulations in adequately modeling phenomena associated with evaporation. For instance, processes such as the pyrolysis and oxidation of polymers

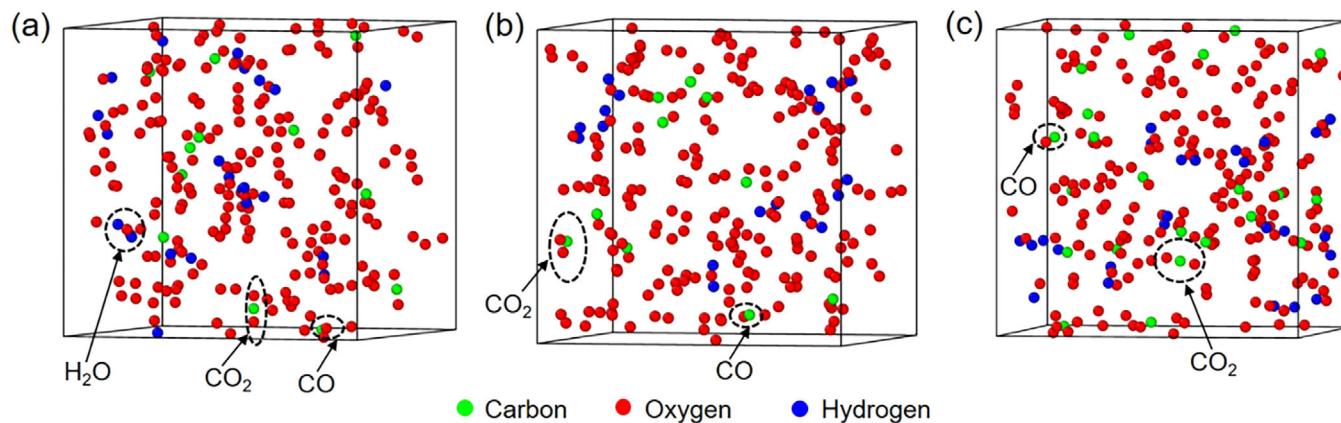


FIGURE 3 The snapshot for different systems at 2000 K when CO has the highest content: (a) Linked glucose and oxygen molecules. The number of CO and CO₂ is 4 and 8, respectively. (b) Linked xylose and oxygen molecules. The number of CO and CO₂ is 8 and 2, respectively. (c) Linked syringyl units and oxygen molecules. The number of CO and CO₂ is 14 and 8, respectively. The hydrogen atoms in linked molecules are in the form of water molecules.

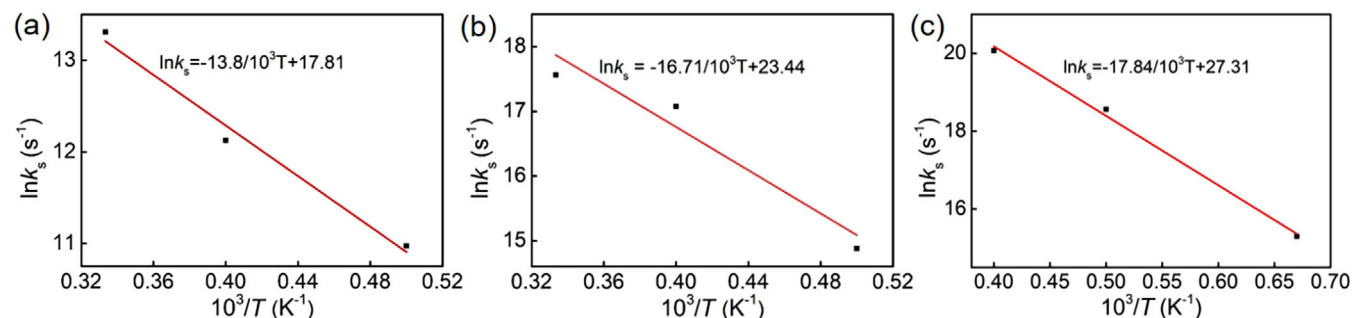


FIGURE 4 Arrhenius plot for pyrolysis of cellulose, hemicellulose, and lignin. The Arrhenius equation is obtained through the fitted curves. (a) System for linked glucose with oxygen molecules, (b) system for linked xylan with oxygen molecules, and (c) system for linked sinapyl alcohol monomers with oxygen molecules.

TABLE 2 Physical and thermal properties of cellulose, hemicellulose, and lignin obtained from molecular dynamics simulation.

Primary component	Density (kg/m ³)	Heat of reaction (kJ/kg)	Heat of combustion (kJ/kg)	A (1/s)	E _a (kJ/mol)
Cellulose	1559	1791	19,075	5.43 × 10 ⁷	114.73
Hemicellulose	1520	2430	16,233	1.76 × 10 ¹⁰	140.42
Lignin	1350	1230	16,268	7.25 × 10 ¹¹	148.32

involve the transfer of volatile fragments from the condensed phase to the gas phase. This phase transfer process encompasses both the breaking and forming of chemical bonds, as well as evaporation. While MD simulations using ReaxFF can effectively capture the bond-breaking and forming aspects, explicit modeling of evaporation is lacking. During evaporation, molecules must overcome diverse intermolecular interactions, including van der Waals forces, Coulombic forces, and hydrogen bonding, to transition from the condensed phase to the vapor phase. While ReaxFF accounts for nonbonded interactions and

covalent bonding changes, its resolution may not be sufficient to represent the intricate sequence of individual molecules transitioning during evaporation in fine detail. Consequently, MD simulations using ReaxFF tend to underestimate the overall E_a due to the absence of explicit modeling of molecule-by-molecule evaporation.

The activation energy deduced from MD simulations using ReaxFF, despite potential underestimation, is suitable for integration into FDS simulations, which also emphasize char formation and oxidation. In FDS simulations, the decomposition of polymers involves both the

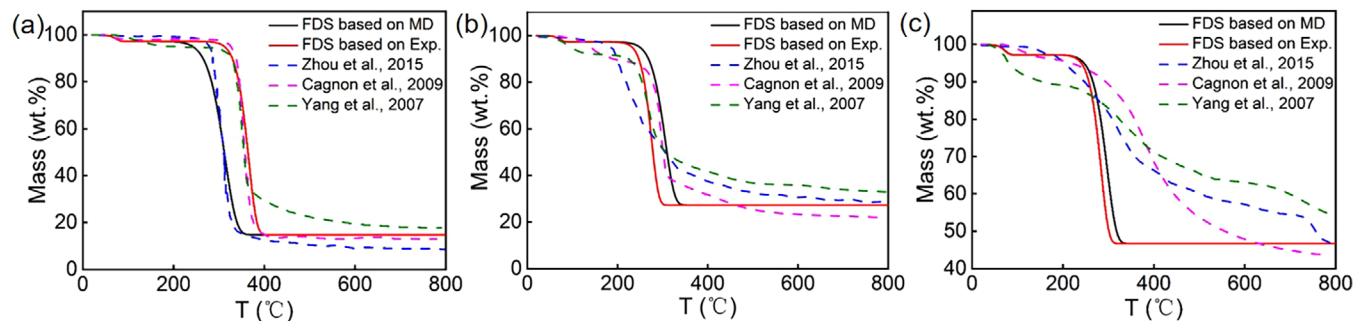


FIGURE 5 Thermogravimetric analysis of pyrolysis at a heating rate of 10 K/min for (a) cellulose, (b) hemicellulose, and (c) lignin. The mass loss curves predicted by FDS modeling based on kinetics parameters from MD simulations have a good agreement with those predicted by FDS based on parameters from experiments.

formation and subsequent oxidation of char. It is essential to note that FDS does not explicitly model the production of reaction-correlated volatiles during polymer decomposition. Kinetic parameters derived from MD simulations, especially details regarding char formation and oxidation kinetics, can be integrated into FDS to simulate how this char reacts and influences overall combustion and temperature profiles during polymer decomposition.

3.2 | Kinetic parameters validation

Figure 5 shows the thermal decomposition characteristics of cellulose, hemicellulose, and lignin predicted by FDS modeling based on kinetics parameters from MD simulations and experiments. The FDS results are compared with experimental results from the TGA test (Cagnon et al., 2009; Yang et al., 2007; H. Zhou et al., 2015). It is found that from predicted mass loss curves, cellulose starts pyrolysis at 248°C, lower than the experimental results of 300°C (D'Acerno et al., 2020). This can be attributed to the low activation energy resulting in a low pyrolysis temperature (Shen & Gu, 2009). The predicted decomposition of hemicellulose mainly occurs between 230 and 345°C, falling in the experimental range of 220–315°C (Yang et al., 2007). The pyrolysis of lignin predicted by FDS happens at a narrow range from 235 to 350°C, whereas the pyrolysis of lignin occurs over a wide temperature range from 10 to 900°C tested by experiment (Waters et al., 2017).

The difference in the pyrolysis behavior of lignin between FDS modeling and the experimental test is correlated to its complex structure. Lignin is full of aromatic rings with different monolignol monomers connected through various linkages. The different linkages and functional groups in lignin cause the reactivity of lignin covering an extremely wide range so that lignin can pyrolyze in a wide temperature range (Kawamoto, 2017; Nawawi et al., 2017). For example, the monomers connected by β -O-4

linkage in lignin can be decomposed within a temperature range of 200–450°C with less than 10% residual produced, whereas the monomers connected by β - β linkage start decomposition at a higher temperature above 300°C with more than 30% residual solid (Ando et al., 2019). In the modeling, the structure of lignin is simplified, where the sinapyl monomers are connected through β -O-4 linkage.

Consequently, the pyrolysis of lignin predicted by FDS modeling occurs within a narrow temperature range, deviating from the experimental test. As the thermal stability of β -O-4 linkage is the lowest in lignin and the char produced during wood combustion is mainly from lignin (Dorez et al., 2014), the simplified structure of lignin is reasonable with the production of a high content of solid residual. The narrow temperature range predicted for lignin pyrolysis in the simulation approach is inevitable. This limitation arises from the utilization of a one-step reaction model incorporating specific kinetic parameters to govern the lignin pyrolysis process. Additionally, even when FDS simulations are coupled with kinetic parameters acquired from the experimental approach, they fail to exhibit strong consistency with experimental outcomes (Cagnon et al., 2009; Yang et al., 2007; H. Zhou et al., 2015). The difference can be attributed to the variation in the material source, the methodologies employed, and the underlying assumptions of the kinetic models used to derive the kinetic parameters in the TGA test.

3.3 | Mesoscale fire modeling

The comparison of HRR for oak, larch, and red cedar predicted by our multiscale model against the results from experimental measurements is shown in Figure 6. Compared with the HRR curve exposed to a heat flux of 20 kW/m², our multiscale model can relatively well predict the overall variation trend at a heat flux of 35 and 50 kW/m². The two peaks in the HRR curve under the

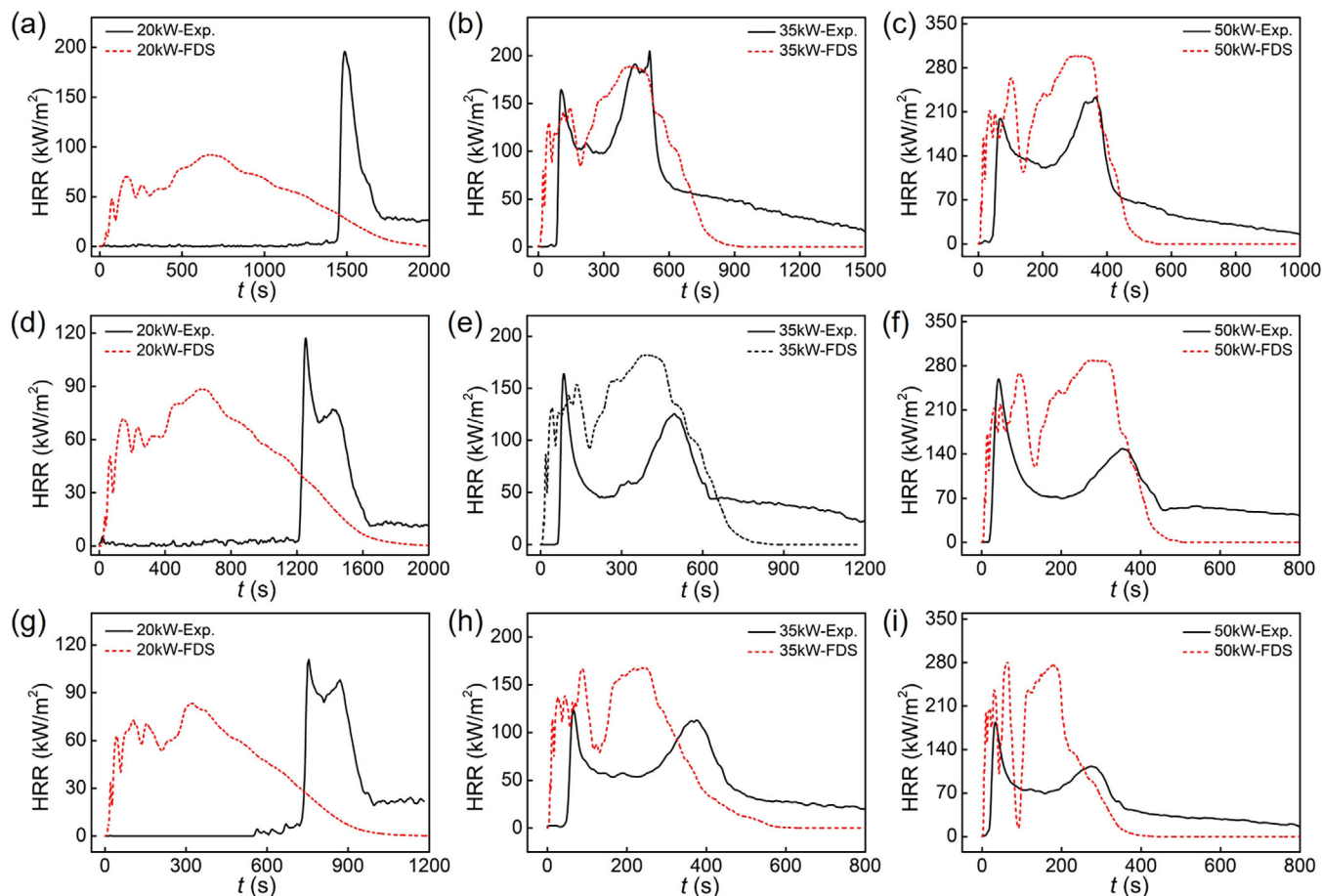


FIGURE 6 Comparison of heat release rate (HRR) exposed to different external heat fluxes between experimental test and FDS prediction (a)–(c): oak; (d)–(f): larch; and (g)–(i): red cedar. The critical characteristic of wood burning, namely, pyrolysis, has been predicted. And the effect of chemical components on the pyrolysis has been distinguished.

heat flux of 35 and 50 kW/m², correlated to the formation and reaction of char, are one of the most important characteristics of wood burning. Our multiscale model can successfully reproduce this fundamental feature of wood burning. The apparent difference in the HRR curve at 20 kW/m² between predictions and experiments is correlated to the homogeneous burning at 20 kW/m² in the experiment. The pyrolysis of wood causes warping of the wood so that a homogeneous burning from the sides, bottom, and up occurs (Hao et al., 2020b). The lower surface temperature and longer pyrolysis time at the low heat flux of 20 kW/m² enable wood distributing the heat throughout its structure, resulting in a homogeneous pyrolysis. Moreover, the charring rate at higher heat fluxes is higher than that at the heat flux of 20 kW/m² (Hao et al., 2020b). The char layer acts as insulation, preventing it from burning homogeneously. However, the burning of wood specimens in FDS modeling is simulated starting from the surface, and such homogeneous burning cannot be modeled. Despite the difference between the predicted HRR curve at 20 kW/m² and the experimental results,

the predicted trend with the presence of a distinct peak is similar to the experiment results. Different from the cone calorimeter test where the wood specimens have been ignited after a long time, the developed multiscale modeling predicts that wood specimens ignite within a short time. The difference of peak value between experimental test and simulations is correlated to the assumption in modeling that wood specimens undergo one-dimensional conductive heat transfer. Such an assumption indicates that wood specimens burn layer by layer. However, in the cone calorimeter test, wood specimens are burnt homogeneously at the heat flux of 20 kW/m².

It is clear that as the heat flux increases, the onset of heat release decreases, which is consistent with the experimental test. According to the cone calorimeter test performed in the previous work, the oak is ignited at 1440 s, 90 s, and 45 s at the heat flux of 20, 35, and 50 kW/m², respectively (Hao et al., 2020b). However, the ignition time predicted by the model is found to be lower than the experimental results obtained from the cone calorimeter test. This underestimation primarily arises



from the simplified kinetic models employed in the FDS simulation of the cone calorimeter. For instance, in the experiment, moisture evaporation takes a longer duration, resulting in a slower temperature rise on the sample surface under lower heat flux conditions. Nevertheless, in FDS simulations, the precise influence of moisture evaporation on the temperature rise of the wood surface remains inadequately captured. The impact of moisture evaporation on heat transfer diminishes with an increase in heat flux. Hence, the observed discrepancy in ignition time between FDS-predicted outcomes and experimental results becomes insignificant at a heat flux of 50 kW/m², compared to that observed at 20 and 35 kW/m².

The deviation of value between prediction and experiment (θ) can be calculated by:

$$\theta = \frac{|V_{\text{FDS}} - V_{\text{Exp}}|}{V_{\text{Exp}}} \quad (6)$$

where V_{FDS} represents the value predicted by FDS modeling, and V_{Exp} is the value tested by the experiment. The θ value of the first HRR peak at 35 kW/m² for oak, larch, and red cedar is 14.5 %, 14.1%, and 31.2%, respectively; the θ value of the corresponding time for the first HRR peak at 35 is 8.6 %, 20.4 %, and 33.6 %. Except for oak, both larch and red cedar show a much larger θ for the second HRR peak. The deviation of HRR between prediction and experiment at 50 kW/m² is slightly higher. Specifically, the first peak of HRR at the heat flux of 35 and 50 kW/m² is governed by pyrolysis of the kinetic model; its reduction is due to the formation of char with low thermal conductivity providing thermal insulation for fire. The deviation of HRR between prediction and experiment is much smaller, compared to existing works (Ding et al., 2020). The pyrolysis mechanism employing the three parallel reactions with the parameters from MD simulations in our developed multiscale model outperforms current models in the prediction of pyrolysis.

Although the first peak of HRR is predicted with reasonable accuracy, the second peak of HRR predicted is overestimated, compared with the experimental results. The second peak of HRR is correlated to the char oxidation in the kinetic model. The main discrepancy between the prediction and experiment for the second peak of HRR is correlated to the reaction mechanism of char combustion. First, in the multiscale modeling, an ideal reaction mechanism of char combustion is considered, namely, char \rightarrow ash + gas. However, the actual reaction mechanism of char combustion is more complex, where the char can be consumed not only by oxygen but also by carbon dioxide (Turns, 2012). Second, the char reactivity between chars from cellulose, hemicellulose, and lignin is different (Richter & Rein, 2019). Third, the kinetics parameters

obtained based on the simplified structure of lignin from MD simulations underestimate the pyrolysis temperature range. All these contribute to the undervalued second peak value of HRR as well as the corresponding time.

Furthermore, the effect of chemical components on the HRR can be revealed by our multiscale model. Lower content of lignin in wood can lead to a smaller deviation of HRR between prediction and experiment. This is correlated to the narrow temperature range of pyrolysis caused by the simplified lignin structure. Lower lignin content in wood can significantly weaken the simplification influence on fire properties. Additionally, it is found that wood with a higher content of lignin releases less heat at the second HRR peak. The predicted effect of lignin is consistent with the experimental data, where lignin can effectively reduce flammability (Hao et al., 2020b). Although the multiscale model cannot predict the oxidation mechanism of wood with high lignin content, the discrepancy is acceptable as the trend of fire properties for different wood species can be forecasted and compared.

The snapshots of oak burning exposed to the heat flux of 50 kW/m² are shown in Figure 7. The flame temperature distribution at different stages is represented. As shown in Figure 7a, wood has been instantly ignited in the modeling, and the temperature rises quickly, leading to pyrolysis. The heat released during wood pyrolysis results in a significant increment in flame temperature as shown in Figure 7b. The formed char on the surface of the specimen hinders fire spread resulting in a reduction in flame temperature in Figure 7c. The oxidation of char damages its protection of wood, causing the pyrolysis front proceed to wood in the depth direction. More heat is released at this stage in Figure 7d. Finally, the fire starts to die with the flame temperature decrease in Figure 7e.

Multiscale model for wood combustion has been proposed, integrating the reaction kinetics and reaction energetics from MD simulations into the kinetic model that includes the pyrolysis and oxidation of wood. The pyrolysis reaction scheme depends on the independent degradation of cellulose, hemicellulose, and lignin. The developed multiscale model can offer a significant advantage in reproducing cone calorimeter experiments, especially at high heat flux where the instant ignition occurs. Pyrolysis as well as the corresponding HRR can be estimated. The developed multiscale model can effectively identify the fire properties of different wood species, which is often overlooked by the traditional FDS model implemented with a single-step reaction scheme. Compared with the existing kinetic models with a parallel reaction mechanism, the developed multiscale model demonstrates higher precision in predicting fire properties for wood. It can accurately capture the essential characteristics of wood pyrolysis, such as the presence of two peaks commonly observed in

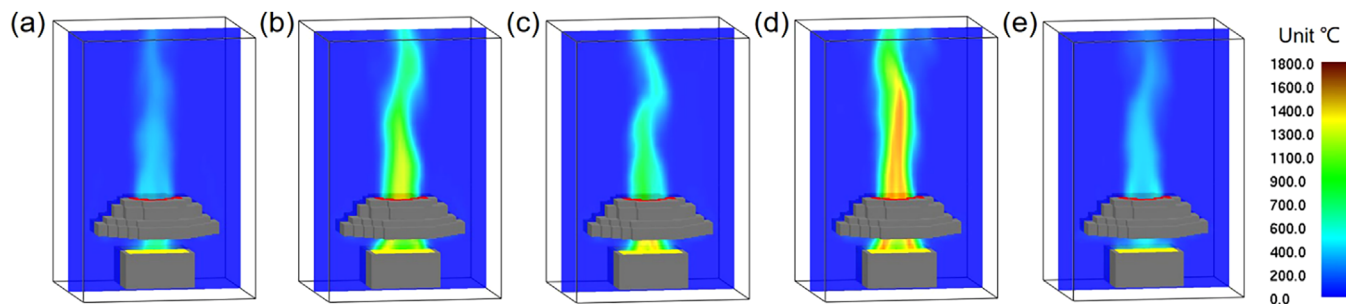


FIGURE 7 The flame temperature distribution at the center plane parallel to z -axis of oak burning at 50 W/m^2 : (a) 10 s where the specimen has been ignited from the surface. (b) 100 s where the HRR reaches the first peak. (c) 140 s where the HRR decreases to the local minima. The formed char starts combustion. (d) 350 s where the HRR reaches the second peak. The combustion of char releases more heat resulting in a higher temperature in the whole domain. (e) 450 s where the fire has already started to die with decreased temperature.

wood pyrolysis. A typical HRR curve of wood usually has two peaks, where the first peak in HRR is a response to the surface ignition and the second peak is a result of material burn-through and char cracking (Sanned et al., 2023; ScharTEL et al., 2007).

Furthermore, the HRR curves predicted by the multiscale model are compared with those from other researchers, and our results exhibit better agreement with experimental data. For example, Moinuddin et al. (2020) used FDS to model the cone calorimeter test of pine, and it has been found that, compared with the experimental data, the value of the first peak in the HRR curves is higher than 70% at 30 and 50 kW/m^2 . Similarly, X. Wang et al. (2016) employed the FDS to model the cone calorimeter test of wood, and the deviations between prediction and experimental results are more than 30% at the heat flux of 35 kW/m^2 and more than 50% at the heat flux of 50 kW/m^2 . Zhang et al. (2015) also modeled the cone calorimeter of wood by FDS simulation, and their results exhibit good agreement with experimental data. However, they relied on inputted data from the cone calorimeter test, such as HRR and ignition temperature of wood material, into the FDS program for simulations. In contrast, the developed multiscale model predicts the trend and peak values of the HRR curves at heat fluxes of 30 and 50 kW/m^2 without relying on any prior experimental data input from the cone calorimeter. Our model demonstrates lower deviations when compared to other FDS simulations reported in the literature (Moinuddin et al., 2020; X. Wang et al., 2016; Zhang et al., 2015).

All the kinetic parameters in our multiscale model are obtained from the simulation approach, which is economical, time-saving, and eco-friendly. The reliability of predicted wood combustion properties using our developed multiscale model is highly contingent on the quantity of ReaxFF parameters and the kinetic model employed for FDS modeling. The parameterization of ReaxFF may not fully capture the intricacies of every elemental reaction.

Moreover, the reaction pathways associated with elemental reactions and their intermediates are complex, and ReaxFF simplifies these complexities. The simplifications in representing chemical reactions and the limited scope of force field parameters can introduce potential deviations from the true energy landscape of a system, impacting the accuracy of activation energy estimates. In FDS simulations, which primarily emphasize capturing overall combustion and temperature effects, explicitly modeling reaction-correlated volatiles remains challenging due to the complexity of the involved chemical reactions.

Despite the inherent limitations and potential underestimation, incorporating the kinetic parameters from ReaxFF MD simulations into FDS simulations in the developed multiscale model is a practical approach. This enhances the overall representation of combustion processes, especially char formation and oxidation. While the results predicted by the developed multiscale model may not precisely represent absolute values, the relative trends and patterns obtained from the simulations offer valuable insights for understanding the behavior of a system. Considering the burning behavior of various wood species under general conditions, with the primary heat source recognized as the predominant factor in wood combustion scenarios, the developed model has been specifically tailored for wood combustion scenarios without the inclusion of any catalyst.

The developed multiscale model can improve the understanding of burning behavior of wood materials, allowing for a comprehensive assessment of the fire spread dynamics among wood elements. Figure 8 shows an application of the developed multiscale model to simulate fire behavior of large-scale structures. The FDS setup for a scenario involving the burning of wooden furniture and fire spread in a two-floor building is shown in Figure 8a. The bedroom contains a wooden table and an oak floor, while the walls, stairs, and second floor are protected using gypsum wallboard. The fire scenario initiates on the surface of the

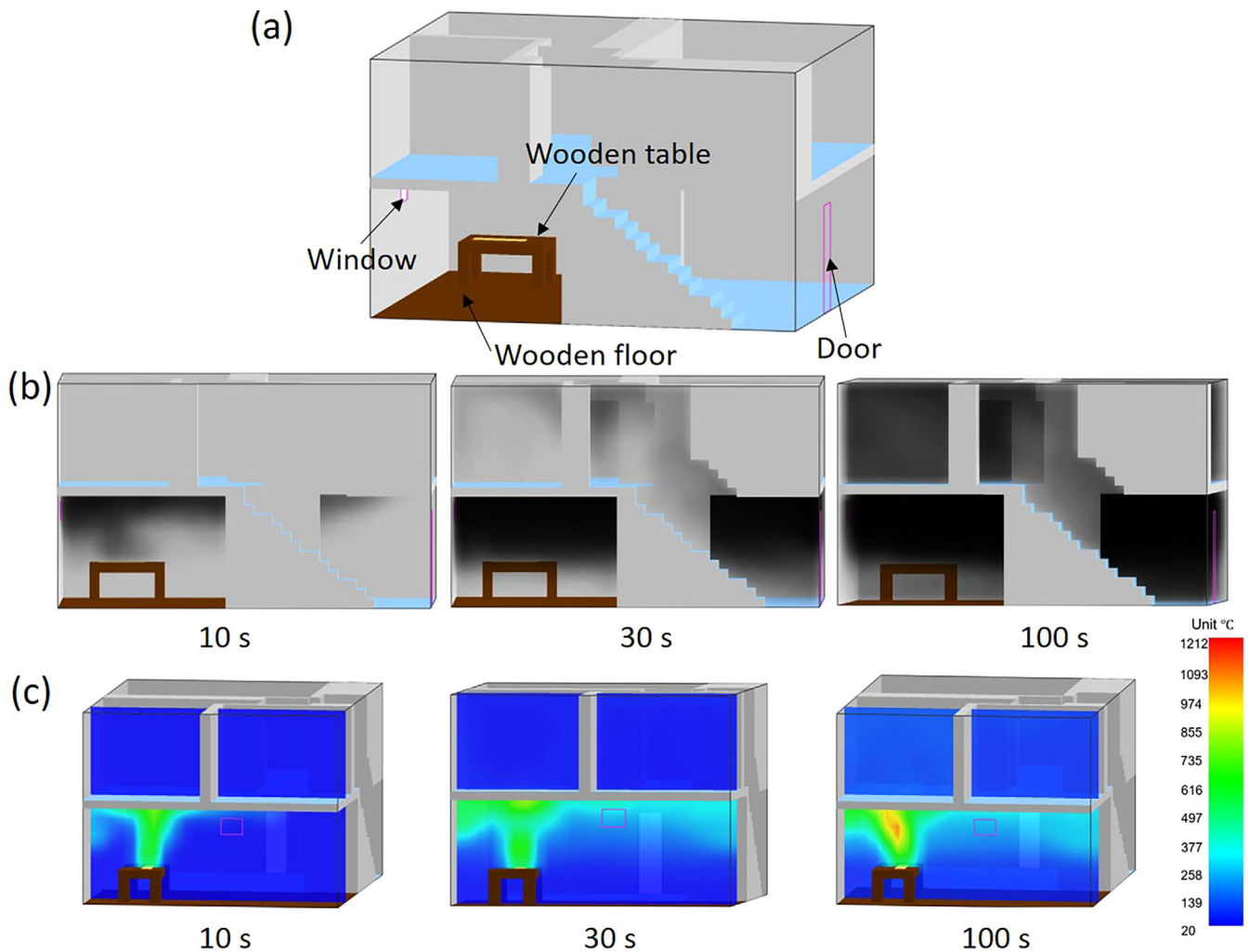


FIGURE 8 (a) The setup of fire spread in a two-story building. The fire originates from the surface of a wooden table composed of oak. (b) The smoke density distribution as a function of time during fire spread. (c) The temperature distribution on the centered plane of the wooden table as a function of time during fire spread.

wooden table in the bedroom, and the spread of the fire throughout the entire building is predicted by the multi-scale model. As the fire grows, smoke and heat gradually accumulate, making it increasingly challenging for occupants to survive. Smoke development within the building is consistent with the trend of fire propagation as shown in Figure 8b. The temperature rises as the heated smoke moves. Figure 8c shows the temperature distribution on the centered plane of the wooden table over time. During the fire, the gas temperature at head level can reach approximately 900°C , which is in accordance with actual building fires reported in the literature (Iringova & Vandlickova, 2021; Zou & Chow, 2005).

The capability to predict fire spread in buildings furnished with various wood species can serve as a guideline for selecting wood species while considering safety concerns. For example, the multiscale model can allow for the evaluation and comparison of fire risks associated

with different wood species and wood structures. Such information is crucial in the design and construction of safer buildings by facilitating informed decision-making on material selection and fire prevention measures and simultaneously contributes to enriching the dataset for deep learning applications addressing wood performance (X. Cheng et al., 2023; Qian et al., 2022). Additionally, our developed multiscale model can be coupled with finite element method (FEM) simulations to predict the thermo-mechanical properties of wood structures (A. Zhou et al., 2015; A. Zhou et al., 2020; Tam et al., 2017; X.Q. Wang et al., 2020). This integration enables a comprehensive analysis of the structural response under fire conditions. For instance, the multiscale modeling provides essential information such as the thermal boundary conditions, including the heat flux and temperature of the surface exposed to fire over time. These data can be extracted from the multiscale model and utilized as inputs for the coupled



thermomechanical FEM simulation. This simulation captures the time-dependent thermal and structural behavior of the wood structure, allowing for a detailed understanding of its response to fire. By combining the capabilities of the multiscale model and FEM simulation, engineers can assess the performance and integrity of wood structures during fire events, optimizing the design, implementing effective fire protection measures, and ensuring the overall safety of the structure.

4 | CONCLUSION

The widespread application of wood as a construction material is limited by safety concerns. Although various kinetic models have been proposed to simulate the fire properties of wood, the reaction kinetic parameters are still a challenge for accurate simulations, especially considering the influence of chemical components. This paper presents a novel multiscale model that can distinguish the fire properties of different wood species. In the multiscale model, the kinetic parameters of cellulose, hemicellulose, and lignin obtained from nanoscale simulations are incorporated into the FDS simulation to model the TGA test at the microscale and the cone calorimeter at the mesoscale. The validated multiscale model is then applied to predict the fire spread behavior of wooden furniture in a building at full-scale. The results can be summarized as follows:

1. The kinetic parameters, including the heat of reaction, heat of pyrolysis, activation energy, and pre-exponential factor of cellulose, hemicellulose, and lignin in the multiscale model, are calculated from MD simulations using the ReaxFF approach and underestimated, compared with experimental data deduced from TGA test.
2. The thermal decomposition of cellulose and hemicellulose, predicted using kinetic parameters obtained from MD simulations, exhibits better agreement with thermogravimetric experiments, compared with the predicted results when experimental data is used as the initial parameters for FDS simulations.
3. The reaction schemes and kinetic parameters of cellulose, hemicellulose, and lignin from MD simulations are implemented into the kinetic model with a parallel reaction scheme to predict the mesoscale fire test. The predicted HRR of oak, larch, and red cedar at the heat flux of 35 and 50 kW/m² by the multiscale model has higher accuracy than predictions by kinetic models where the kinetics parameters are deduced based on experiments.
4. The multiscale model enables a clear distinction of the effect of chemical components on the fire properties of wood. The disparity in fire properties between pre-

dictions and experiments is strongly influenced by the quantity of ReaxFF parameters and the kinetic model applied in FDS modeling.

Therefore, the developed multiscale model can predict pyrolysis and the effect of chemical components on it. The ability to predict fire properties of various wood species by the multiscale model enables to forecast realistic fire scenarios in high-rise timber buildings. Furthermore, understanding the burning behaviors of various wood species can provide a guideline for the evacuation model development, as well as the material design for woodworking facilities.

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