# Developments in Numerical, Artificial Intelligence and Machine Learning based Fire models of Lignocellulosic and other polymer-based composites – A Short Review

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**Abstract**

The ability of composite materials to withstand fire is a crucial factor in both construction and manufacturing. For centuries, different materials have been used to improve the fire-resistance properties of lignocellulosic materials and other composites. Several fire prediction models have been developed over the years as a result of efforts to model fire behavior, which begins in the 1970s. These models are useful for predicting the fire behavior of materials under different conditions and are helpful for choosing and refining next-generation fire-retardant materials. This study examines how fire prediction models have changed over the previous few decades, paying special attention to more recent developments made possible by machine learning (ML) and artificial intelligence (AI) technologies.

**Key words:** Fire modelling, Artificial Intelligence, Machine learning, Composites, Lignocellulosic

## Introduction

Fire resistance is an important aspect of the materials used in construction and manufacturing [1]. Over the years various developments have been made in this field. Research has been conducted on lignocellulosic materials as construction materials [2]. Considering the fire-prone behavior of wood, chemicals, barriers, and other methods, such as modification of fibers, are carried out to improve the fire resistance of lignocellulosic materials [3]. Technologies have been developed to check these improvements in fire behavior and to analyze the fire resistance properties of wood and wood-based composites through various tests and standards [1]. In addition to these standard tests, the heat release rate (HRR), limiting oxygen index (LOI), and calorimetry tests also provide insight into the fire behavior of materials.

Numerous physical and chemical changes happens in wood and its composites under heat or fire [4]. The chemical processes include softening, melting, pyrolysis, volatilization, growth, and oxidation of char. The physical processes include matrix cracking, delamination, internal pressure buildup during volatiles, thermal expansion, and contraction. The heat generated and absorbed from the breakdown of the polymer matrix, heat conduction through the composite, etc., are thermal processes in the fire event. Most of these processes are interconnected, and do not occur separately. Studying these changes enables detailed analysis of the fire resistance and reaction-to-fire characteristics of composite materials [5]. Different fire testing methods have been employed to evaluate the specific material characteristics that change when exposed to fire.

However, there are some challenges to traditional fire testing. All these tests are performed under laboratory conditions, and are expensive and time consuming [6]. Laboratory scale or full-scale fire testing is mostly limited to single scenarios, such as current weather conditions and, ventilation. It is also impossible to predict the fire behavior in different scenarios [7]. If fire-retardant materials are used, only the test results of the different compositions of these materials can provide insights into the fire resistance parameters. Furthermore, the composition of the fire retardant was optimized. In addition, fire testing can be harmful or dangerous.

Given the challenges associated with safety, performance under varying fire scenarios, optimization of fire-retardant materials, and time and cost constraints, fire prediction modelling offers a valuable alternative to address the limitations inherent in conventional fire testing methods [6]. A fire prediction model simulates different Characteristics of a material in various scenarios and predicts the fire behavior of the material. Various Machine Learning (ML) algorithms, including Support Vector Machines (SVM), Convolutional Neural Networks (CNN), and ensemble methods, have been employed to analyze fire behavior in lignocellulosic materials [8], [9], [10]. It uses physical, computational, and mathematical tools to predict fire behavior in a material. Fire modelling of composites involves simulating combustion parameters such as limiting oxygen index (LOI), heat release rate (HRR), and total heat release rate (THRR) [11]. The key challenges in modelling composites in fire are the complexity of the chemical, thermal, physical, and failure processes of polymer laminates. Some studies have been conducted on the fire modelling of wood-based composites [12]. Because pyrolysis is an important step in the degradation of lignocellulosic materials, several pyrolysis-based models have been developed to analyze fire models. However, there are other considerable changes that occur in composites during fire catching.

In earlier fire prediction models, numerical and analytical methods based on physics and materials science were used. These are physics-based equations (such as Fourier's Law, Arrhenius kinetics) and are governed by thermodynamics, heat transfer, and pyrolysis theory. Finite element methods (FEM) [13], ThermaKin are examples of such models. Analytical and finite element-based models were increasingly used in the 1970s when carbon fiber materials were used in different applications, and it was necessary to predict their performance under different fire scenarios, such as the application in the internal lining of solid rocket motors. In the 1990s, glass fiber-based composites required prediction models in various scenarios [1]. Computational Fluid Dynamics modelling) is another model used for numerical computational methods for predictions [14]. CFD methods have emerged as analytical tools for fluid flow problems, including fire. These partial differential equations assert conservation of mass, momentum, and energy within the fire and throughout the space surrounding it [15]. Over the past five decades, many efforts have been made to develop detailed pyrolysis models that can properly describe the concomitant effects of the main transport phenomena and relevant chemical kinetics. Di Blasi [16] reviewed the most important achievements in the modelling chemical and physical processes of biomass pyrolysis. More recently, Anca-Couce [17] highlighted the multi-scale nature of this problem, that is, in pyrolysis, understanding the physical and chemical changes of the material during the process is very important.

Currently, Artificial Intelligence (AI)/computer-based models are being developed for fire prediction. These are data-driven, based on machine learning algorithms such as Artificial Neural Network (ANN), SVM, XGBoost [18], and SISSO etc. [19]. These were trained with historical or material-specific datasets. Currently, ANN networks are widely used for this purpose. It has been suggested that the integration of optimization techniques with neural networks can lead to better predictive capabilities in the context of material ignitability [20]. In a recent study, a thermal model for wood pyrolysis that incorporates temperature-dependent thermophysical parameters were successfully developed. The Experimental model used finite element software (Abaqus 6.14) and finite volume software (OpenFOAM 5.0) to simulate the three-dimensional temperature profiles within the wood. This simulation helps to visualize the change in temperature of the wood during the thermal process [21]. A new computational framework (bioSMOKE) was developed using OpenFOAM software for advanced simulations of thermal decomposition models. This model addresses the anisotropic behavior of lignocellulosic materials and how the orientation of fibers affects the thermal behavior [22].

Accurate Fire modelling will be helpful for rapidly assessing the fire resistance of new design options. These models reduce the need for expensive fire testing. These models can be used to understand the fire behavior of in-use polymers and the development of new fire-resistant materials. However, experimental backing is required to draw conclusions about these models [1].

In this review paper, the development of fire prediction models throughout the last few decades is discussed from basic numerical and computational methods to current data-driven AI/ML-based models.

**Fire models based on Pyrolysis, Thermal Expansion and other Processes**

Pyrolysis is an important aspect that occurs during fire events. Polymer materials degrade and are reduced to carbon residues in this process. Earlier fire models considered charring as the main change in the material during a fire event. Owing to the limited research on other material transformations during fire exposure, pyrolysis-based models were predominantly used. Although some additional fire-related processes have been considered in predictive modelling, these approaches have not gained widespread attention. Some of these studies include thermal expansion-based models developed by Florio et al. [23], Sullivan et al.[24], McManus and Springer[25], and volatile flow-based models studied by Henderson et al. [26], [27], Dimitrienko [28], and Boyer & Thomas [29]. Some of the earlier fire models are discussed in this section.

A mathematical model was developed based on Darc's law of gas flow, mass and energy conservation, and kinetic expressions for the reaction involved in pyrolysis [30]. Wood samples were heated in a Pyrex reactor, and different heat flux levels of 80 kW/m2 and 130 kW/m2 were applied. Thermocouples assembled in the sample provided data on the change in temperature during pyrolysis. The developed mathematical model predicted that the temperature profiles and product yield were almost similar to the experimental data. It is notable that the most accurate prediction comes for low heat flux (80 kW/m2) applications [24]. The post-fire mechanical properties of the composites of carbon, Glass and Kevlar fibers with epoxy, polyester, and phenolics were analyzed using analytical equations. In this study, researchers combined the Charred and Un Charred properties of a composite [31].

Numerical modelling of the gas-phase combustion process (ignition, flame spread, and extinction) has been developed to understand the evolution of gas during combustion and its reaction with solid fuels [32]. The interaction between chemical reactions and physical processes on thermal degradation is vital for the accurate modelling of combustion using this method.

Kansa et al. [33] developed a one-dimensional mathematical model to simulate the charring pyrolysis of wood. This model includes various factors of pyrolysis, such as physical properties, time-dependent surface radiant flux, and global Arrhenius reaction. This model addresses how the direction of the heat flow relative to the wood grain affects the movement of gases within the wood by incorporating Darcy's law. The biochar, tar, and gas yields under different pyrolysis conditions were predicted using a simulation technique [34]. In comparison with the experimental data, this simulation showed high accuracy in the prediction of the pyrolysis process. The temperature dependence of the reaction rates and their influence on the overall pyrolysis behavior of wood was also analyzed in this study.

A numerical one direction model used to make a fire model of multilayer wood based composite contain PVC(Polyvinyl chloride)-Kydex (polymethyl methacrylate-polyvinyl chloride alloy) and wood[35]. Fire scenario in both pyrolysis and combustion are analyses in this study.

A detailed computational model showed that the pyrolysis rate of wood primarily depends on the radiant surface temperature and size of the wood particles. That is, a higher temperature and smaller particles led to faster pyrolysis rates. The moisture content also has an influence on pyrolysis, but it is secondary compared to the temperature and size of the wood particles. [36]. In another study, coupled simulations that integrated gas-phase fire phenomena (using computational fluid dynamics (CFD)) with solid pyrolysis were developed [37]. This dual approach allows for a more comprehensive understanding of the fire dynamics involving polymer composites.

A numerical model has been developed based on 3D finite element model for cross laminated panels (CLT) [38]. Abaqus software was employed for this study and user subroutine (custom routine for specialized task) "Umatht" has been implemented in Abaqus. Predicted results verified the effectiveness of "Umatht". A constitutive model (Wood$^{ST}$) developed by combining various mechanics based submodels used for making mechanical and fire prediction model [39]. This model is capable of simulating themo-mechanical response by fire and force on LVL beam and glulam connection. Modeling and testing results show only 10% difference.

An open-source platform OpenSees used for modelling of timber structures under realistic fire conditions [40]. Developed model has been validated by testing on cross laminated timber beams under ambient temperature and fire furnace. A concrete - timber composite also used for experiment in this model and OpenSees shows the suitability of making such models for timber-based construction materials.

Pyrolysis and fire behaviour of different wood composites like Oriented strand board (OSB), Plywood, particle board (PB), Low density fiber board (LDF), Medium-density fiber board (MDF) and high-density fiber board (HDF) are studied [41]. Cone calorimetry testing data of these composites are used to make a CFD fire modelling. Numerical, Kinetic model-based experiments based on TGA result are also conducted.

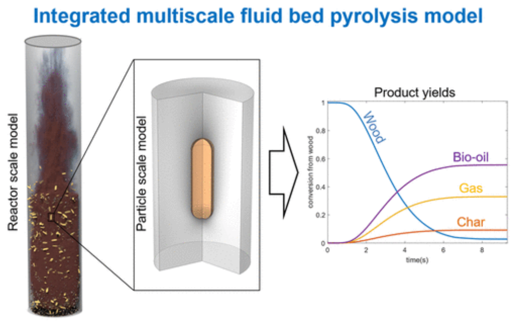
It is suggested that moisture content, wood density, and temperature are key parameters in the burning behavior of wood. Various scenarios were created to evaluate the effects of these parameters and changes in the combustion process. The simulation process was supported by experimental data [42]. Many previous models have not considered the variability and diversity of lignocellulosic materials that are inherently or process-induced [43].

**AI, ML and other data driven Models**

Artificial Intelligence and machine learning have been incorporated into different fields of scientific studies. Biology [44], Forest Fire prediction [45][46][47] etc., are some of the areas where AI has been successfully studied. Nguyen et al. [8] compiled the use of artificial intelligence and ANN to predict the performance of different construction materials, such as concrete [48], steel[49][50], and timber [51] etc. There have been some studies on fire modelling of lignocellulosic and lignocellulose-based composite materials. A Coupled fire structure model combining finite volume and finite element models to predict the structural performance of flax-PP-based beams has shown promising results [52]. Theoretical models of fire behavior on natural fibers have recently been developed [53].

An Artificial neural network (ANN) was developed to predict the decomposition behavior of rice husk sewage sludge during co-pyrolysis [54]. The TGA data were used to analyze the energy change during co-pyrolysis, such as enthalpy, Gibbs free energy, and change in entropy. The Coasts-Redfern method was employed to analyze the kinetic parameters of the co-pyrolysis process. In this method, the activation energy is calculated using mass loss data. Statistical data showing the reliability of artificial neural networks (ANNs) in predicting mass loss during co-pyrolysis.

A Two-fluid model (TFM) with predictions from a finite element method (FEM) simulation of heat and mass transfer and chemical reactions within pine pellet biomass particles was studied [55]. The experimental pyrolizer consisted of a fluidized bed reactor (FBR). combined TFM and FEM simulation results to predict net bio-oil and char yields in a reactor that align with the outcome of experimental observations [55]. Fire dynamics were simulated using “PyroSim,” which is a GUI (Graphical user interface), for computational fluid dynamics (CFD) solver “Fire Dynamics Simulator” (FDS) developed by th e National Institute of Standards and Technology (NIST), USA.




Pic 1: Graphical representation of FBR method used by Pecha et.al 2018

A self-enforcing deep neural network (SDNN) has been developed to predict the flammability of flame retardants in epoxy resins [19]. Limiting oxygen index (LOI), Peak Heat Release Rate (PHHR), and Total Heat Release Rate (THR) were used as parameters for this study. In this study, a small dataset was used for evaluation. Chen et al. [56] employed the SISSO algorithm to screen the performance of a flame retardant in a PP-based composite. Different Halogenated and Non-halogenated Fire retardants and parameters such as LOI were used for the analysis. The results show that data-driven analyses will be helpful in the optimization of flame-retardant use. Another study based on Machine learning showed how historical data analysis of LOI of epoxy resin-based composite can predict the performance of organo-phosphorus based fire retardants [57].

Machine learning algorithms are also used to predict the flame retardancy index based on cone calorimetry data, such as THR, pHHR, and Time to Ignition (TTI) [58]. The flame-retardancy index is a value based on a calculation that includes the above-mentioned parameters[59]. different types of algorithms were used simultaneously for analysis in this experiment. A mechanistic model was developed to predict the behavior of epoxy-based glass fiber composite materials under fire-loading conditions [60]. This model was combined with a standard diffusion model for heat transfer in the composite to predict the time-dependent failure of composites subjected to simultaneous one-sided heat flux and compression loading. Khalvandi et al. [61] employed a Deep neural network to predict the fire behavior of eco-friendly composites made of Abaca fibers. Predictions by this model of the heat release rate and total smoke production showed excellent results and effectiveness of the DNN network.

ANSYS commercial FEM software was used to simulate various physical phenomena of fire, such as the mass loss rate,HRR and THR of Vinyl ester-based glass fiber composites. It is Important to note that this is a three-dimensional model [62]. A heat-transfer modelling developed to predict the behavior of fiber-reinforced polymer-based structures under simultaneous fire and mechanical loads [63]. All these data-driven models show the potential of AL, Machine learning, and other methods to analyze the fire behavior of composites.

**Conclusion**

AI/ML methods have become important in scientific studies. Only a few studies have been conducted on Fire prediction models for lignocellulose-based composites using these techniques. Some studies have reported promising results. However, various studies have been conducted in earlier numerical-computational method-based studies. Similar to any new technology, it may take its own time to be adopted by a large number of scientists. Fire prediction models will be helpful for researchers to analyze the performance of fire retardance, its optimization, and the combination of different fire retardants and matrices. It is suggested that the interpretability of ML models in natural fiber composites can hinder their practical use [64] and the effectiveness of ML models is constrained by the availability and quality of training data, which is necessary for better predictions [65].

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Author Contributions

Nihal Basheer MC: Writing – original draft, Writing – review & editing, Conceptualization, Resources.
Pradeep K Kushwaha: Conceptualization, Resources, Supervision, Writing – review & Editing.

Both authors have read and approved the final manuscript and agree to be accountable for all aspects of the work.

Disclosure of Interest

The authors declare no competing interests.

Data Availability Statement

The authors declare that the data used for this study are available within the paper in the reference section. No original data has been generate in this study.

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