An investigation of the heating, drying, and pyrolysis process of two separate moisturized cellulosic leaves

A. Edalati-nejad [a], **M. Ghodrat** [b] **and J.J. Sharples** [a]

[a] *School of Science, UNSW Canberra, Australia*
[b] *School of Engineering and Information Technology, UNSW Canberra, Australia*
Email: a.edalatinejad@adfa.edu

Abstract: Solid biofuel elements like leaves can play a significant role in the initiation of a wildfire that may escalate to a massive wildfire. As such, better understanding of the pyrolysis, ignition and combustion of individual leaves can provide insights into initial wildfire development and the way fire spreads from one plant to another. In the present investigation, the heating and drying process of two separate cellulosic leaves exposed to a convective heat source is numerically examined. Two moisturized leaves with fuel moisture content of 34% are stacked above a convective heat source which generates hot gas flow, as shown in Figure 1. The numerical results were validated against experimental measurements and showed an acceptable level of agreement with the experimental investigation of single leaf configurations of (Prince, 2014). The numerical modelling was conducted using FireFOAM, which is a large eddy simulation transient solver of the OpenFOAM platform. The wall-adapting local eddy-viscosity method is also applied. Combustion of the leaves was assumed to occur as a single step reaction with infinitely fast chemistry. Structured mesh is used to discretize the computational domain, which facilitates efficient and accurate numerical simulations. To capture the vortex flow near the leaves, a high-resolution area in the hot air entrance and in the vicinity of the solid leaves is considered.

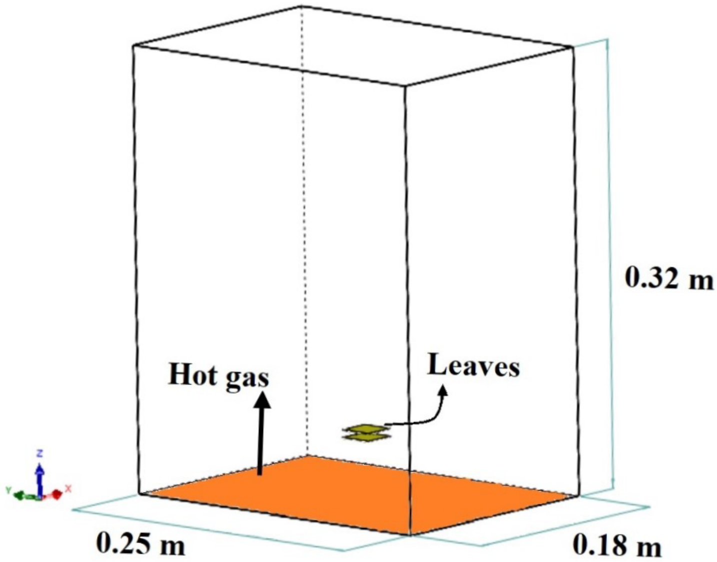

Figure 1. Schematic of the computational domain

The results showed that the edges and the corners of the square-shaped leaves start heating, drying and pyrolyzing earlier than the centre points. Hence, the ignition occurs at the corners of the leaf. It is also found that in this muti-leaf configuration, the lower leaf starts the heating process earlier than the upper leaf in that the lower leaf temperature starts rising after 0.6 seconds, while the upper leaf starts heating after 1.2 seconds. This is due to the fact that the lower leaf is more exposed to the direct hot gas flows and shields the upper leaf from the convective flow.

Keywords: *Large eddy simulation, FireFOAM, fuel moisture content, pyrolysis, drying process*

1. INTRODUCTION

Wildfires are experienced in many parts of the world, and often intersect with environmental and human socio-economic systems (Weise and Wright, 2014). Although wildland fire can be a natural phenomenon and a desired ecological disturbance in various regions, it also can have negative impacts on human lives and assets, natural and cultural resources and ecosystems, especially under more extreme conditions (Yashwanth et al., 2016).

Wildfires in wildland areas are primarily fueled by both live and dead vegetation, consisting of litter, foliage, and branches. Wildland vegetation comprises a variety plant types that exhibit a wide range of chemical and physical characteristics that affect the drying process, ignition, and pyrolysis, and ultimately wildfire spread. Fuel composition, structure, moisture content, and arrangement all play a critical role in the behavior of vegetation fuels during a wildfire. Additionally, environmental factors, such as temperature, humidity, wind, and topography, further affect the ignition and spread of wildfires. As such, understanding the complex interactions between these factors is crucial in developing effective wildfire management and prevention strategies. It is essential to consider and analyze these variables to mitigate the devastating consequences of wildland fires (Weise and Wright, 2014).

Expansion of the wildland-urban interface, due to increases in population and urban developments that encroach on wildland regions enhances the risk of wildfire to human systems and highlights a need to improve understanding of wildfire characteristics and the prediction of wildfire behaviour in different geographical and atmospheric conditions. A clear understanding of the complex factors that contribute to wildfires, including weather patterns, fuel availability, and ignition sources, is necessary for effective prevention and management strategies. Additionally, the prediction of wildfire behavior under different conditions is crucial for effective risk management and evacuation planning. Therefore, ongoing research and analysis of wildfire characteristics are vital for minimizing the devastating impact of wildfires and promoting sustainable urban development practices.

Although fire behaviour characteristics and related phenomena have been investigated for many years, our knowledge is still relatively limited (Finney et al., 2012). Wildfire behaviour and propagation involves a large number of very complex chemical and physical processes, and their interactions, which makes wildfire prediction an exceedingly challenging task (Verma, 2019).

At the most basic level, the propagation and intensity of a wildfire involves the combustion of leaves, twigs, foliage, and branches, across all structural layers of a vegetation stand. Individual leaves can play a critical role in the initiation of a wildfire that may escalate to a very large wildfire. As such, better understanding of the pyrolysis, ignition and combustion of individual leaves can provide insights into initial wildfire development and the way fire spreads from one plant to another (Borujerdi et al., 2020). Better understanding of these aspects of the flammability of leaves can be facilitated through detailed physical modelling of the complex physics of the problem, including the interaction and coupling of the driving processes (buoyancy induced flow, wind, thermal degradation of vegetation, thermal radiation, combustion, etc.).

One of the key parameters affecting the combustion of individual leaves and the subsequent behaviour of a wildfire, is the fuel moisture content (FMC) (Verma, 2019). FMC has a significant impact on the ignition, pyrolysis process, and rate of spread of wildland fires (Edalati-nejad et al., 2022; Weise and Wright, 2014). The effect of fuel moisture content on the combustion and pyrolysis of live fuels was numerically studied by Yashwanth et al. (2014), who investigated fuel moisture content values from 30 to 200% in live fuels. The dimensions of the fuel element they considered were similar to a typical Manzanita (Arctostaphylos glandulosa) leaf with the material of cellulose. They showed that the solid fuel with lower moisture content was ignited earlier than the cases with a higher amount of FMC and resulted in higher solid and gas phase temperatures. The effect of FMC on the spread of a surface fire in flat terrain was also investigated numerically by Morvan (2013), who used a detailed physical model to examine how FMC of a homogeneous vegetation layer impacts the behaviour of surface fire. Their results indicated that the impact of FMC on fire behaviour also depends on wind conditions; for lower wind speeds, the decrease in the rate of spread (ROS) was quite sharp, while for higher wind speeds, sustained fire spread could occur even for higher FMC. The effect of moisture content on fire propagation was also numerically investigated by Mulky and Niemeyer (2019). In their investigation, a one-dimensional model using Gpyro, an open-source software, was developed to study the smoldering combustion of cellulose and hemicellulose mixtures. Their results showed that in pure cellulose, by increasing moisture content from 0 to 30% the rate of fire spread increases about 4%. This is due to the expansion of the fuel when moisture is added, which decreases the density of fuel when the moisture evaporates. After that by increasing moisture content from 30% to 70%, the rate of spread decreases by about 1.4%. Awad et al. (2021) conducted a numerical investigation of the moisture content threshold under prescribed burning conditions. In the study, a physical multi-phase model with various parameters was used to understand the effect of fuel moisture content (FMC) on fire spread in a flat terrain with different wind speeds and fuel loads. The authors showed that increasing the FMC reduces the flame intensity and makes the flame and the fire plume more vulnerable to the action of the cross wind.

The ignition process and fire behaviour in burning leaves have also been investigated experimentally. For example, Prince (2014) investigated the convective heat transfer in burning shrubs through a series of experiments. Four different categories of dry dead (4% FMC), rehydrated dead (26% FMC), dehydrated live (34% FMC), and fresh live leaves (63% FMC) were considered. Their results showed that the dead leaves with 4% FMC released pyrolysis gas much faster than the live fuels.

While previous research has examined the effects of fuel moisture content on pyrolysis and ignition processes pertaining to individual leaves, less attention has been given to investigation of the effect of heating and drying processes on the ignition of solid fuels in multi-leaved configurations. In the present study, the heating and drying processes of two separate, vertically stacked, cellulosic moisturized leaves exposed to a convective heat source are examined using a multiphase CFD analysis. By examining the ignition behavior of these leaves, researchers can gain a better understanding of the physical and chemical processes that lead to solid fuel ignition, and ultimately contribute to the spread of wildfires. Such insights can inform the development of more effective fire prevention strategies and management techniques to mitigate the devastating impacts of wildfires.

2. PHYSICAL MODEL

This study considers two identical, square cellulose leaves, each oriented horizontally, but vertically stacked with a 0.005m vertical separation, as depicted in Figure 1. The leaves are considered as solid fuel with fuel moisture content of 34%, exposed to a vertically oriented convective flow (Yashwanth et al., 2016). The heated flow injects 10 mol% O_2 hot gases with a constant velocity of 0.6 m/s and a temperature of 1273K, which resemble the experimental conditions of (Prince, 2014). The size of the computational domain is 0.18 m (x)× 0.25 m (y) × 0.32 m (z) with the two leaves located in the center of the domain. The dimensions of the leaves are 23.7 mm in length, 23.7 mm in width, and 0.51 mm in height.

These dimensions are carefully chosen to ensure consistency with the experiments of Prince (2014). By using uniform leaf dimensions, one can eliminate the possibility of any confounding variables that may affect the results and ensure that any observed differences in ignition behavior can be confidently attributed to variations in the heating and drying process.

The computational domain used in this study is discretized using a structured mesh, which allows for efficient and accurate numerical simulations. A high-resolution area in the vicinity of the solid fuels and near the hot air entrance, is used to capture the vortex flow near the leaves. This allows for a detailed analysis of the flow field and heat transfer characteristics and ensures that the results obtained are reliable and accurate.

Three different mesh numbers of 324,000, 554,000, and 736,000 were considered to examine the grid dependency of the results. As shown in Figure 3, by increasing the grid number from 324,000 to 554,000 a significant change in the normalized mass of the solid fuel can be seen, but a further increment of the mesh number to 736,000 has less of an effect on the result. So, the simulations presented here used the medium grid numbers of 554,000 to optimise the computational costs.

3. GOVERNING EQUATIONS FOR REACTION AND FLUID DYNAMICS

In order to solve the complex governing equations that describe the heating and drying process of the cellulosic leaves with moisture content of 34%, the FireFOAM solver, which is an open-source computational tool developed within the OpenFOAM platform (Le et al., 2018), was used. This solver has been specifically designed to simulate pyrolysis reactions and fire dynamics, making it a powerful tool for studying the ignition of solid fuels in a wide range of scenarios.

In this work, the large eddy simulation (Wang et al., 2011) turbulence model is used and the wall-adapting local eddy (WALE)-viscosity method (Ren et al., 2013) is also employed. The infinitely fast chemistry model proposed by Mahle et al. (2006) was used as the combustion model. This model is widely used in the field of fire dynamics to simplify the combustion process, making it computationally efficient while still accurately representing the overall behavior of the system. Indeed, use of this model effectively captures the key features of the combustion process and permits accurate simulation of the ignition of the cellulosic leaves.

The governing equations for the pyrolysis and vaporization at the solid regions of the present investigation are as follows (Ding et al., 2015):

$$\frac{\partial(\rho_c Y_c)}{\partial t} = \dot{\omega}_c, \tag{1}$$

$$\frac{\partial(\rho_m Y_m)}{\partial t} = \dot{\omega}_m, \tag{2}$$

$$\dot{\omega}_c = \left[\frac{\rho_s Y_c}{(\rho_s Y_c)_0}\right]^n (\rho_s Y_c)_0 A_c \exp\left(-\frac{E_{a,c}}{RT}\right), \tag{3}$$

$$\dot{\omega}_m = \left[\frac{\rho_s Y_m}{(\rho_s Y_m)_0}\right]^n (\rho_s Y_m)_0 A_m \exp\left(-\frac{E_{a,m}}{RT}\right), \tag{4}$$

where and A_s and $E_{a,s}$ denote the activation energy and pre-exponential factor, respectively, of species s. Here the two species are cellulose, denoted by subscript "c", and moisture, denoted by subscript "m". $\dot{\omega}_s$ represents the mass consumption rate of species s, Y_s is the mass fraction of species s, T denotes the temperature and ρ_s is averaged density of species s. The subscript 0 indicates initial conditions, the parameter n denotes the reaction order, and R is the universal gas constant.

In the fluid domain considered here, the governing equations are as follows (Favre, 1983):

$$\frac{\partial\bar{\rho}}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial x_i} = 0, \tag{5}$$

$$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_i} = \frac{\partial}{\partial x_j}\left[\bar{\rho}(\upsilon + \upsilon_t)\left(\frac{\partial(\tilde{u}_i)}{\partial x_j} + \frac{\partial(\tilde{u}_j)}{\partial x_i} - \frac{2}{3}\frac{\partial(\tilde{u}_k)}{\partial x_k}\delta_{ij}\right)\right] - \frac{\partial(\bar{P})}{\partial x_i} + \bar{\rho}\, g_i, \tag{6}$$

$$\frac{\partial(\bar{\rho}\tilde{h})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{h})}{\partial x_j} = \frac{D\bar{P}}{Dt} + \frac{\partial}{\partial x_j}\left[\bar{\rho}\left(\alpha_t + \frac{\upsilon_t}{Pr_t}\right)\left(\frac{\partial\tilde{h}}{\partial x_j}\right)\right] + \dot{q}''' - \nabla.\dot{q}_r'', \tag{7}$$

$$\frac{\partial(\bar{\rho}\tilde{Y}_s)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{Y}_s)}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\bar{\rho}\left(D_c + \frac{\upsilon_t}{Sc_t}\right)\frac{\partial(\tilde{Y}_s)}{\partial x_j}\right] + \bar{\omega}_s, \tag{8}$$

$$\bar{P} = \bar{\rho}R\tilde{T}, \tag{9}$$

where ρ is the fluid density, u_i is the component of fluid velocity ($i = 1,2,3$), P is the static pressure, h denotes the total enthalpy, Y_s denotes the mass fraction of species s, g_i denotes the components of gravitational acceleration, and T denotes the temperature of the fluid. Pr_t represents the turbulent Prandtl number and $D_c, \upsilon, \upsilon_t, \mathrm{R}, \alpha_t, Sc_t$, and ω_s denote the laminar diffusion, laminar viscosity coefficient, the turbulent viscosity, gas constant, thermal diffusion coefficient, the turbulent Schmidt number, and production/sink rate of species s due to gas reaction, respectively. δ is the Kronecker delta, while the accents "¯" and "~" represent spatial averaging and Favre filtering, respectively.

As can be seen in equations (3) and (4), Arrhenius reaction kinetics are assumed. The kinetic parameters for the conversion of liquid water into water vapor, and the pyrolysis of cellulose are provided in Table 1.

Table 1. Arrhenius kinetic parameters for pyrolysis and moisture evaporation (Chaos et al., 2011). Here ΔHr is the enthalpy of the reaction, A denotes the pre-exponential factor, and E_a is the activation energy

Reaction	A (s^{-1})	E_a (J mol^{-1})	Reaction order	ΔHr (J g^{-1})
Moisture → Vapour	5.13×10^{10}	8.8×10^{4}	1	-2.44×10^{3}
Cellulose→ Char + Pyrolysate	7.83×10^{10}	1.27×10^{5}	4.86	-1.41×10^{3}

To validate the simulation results, the normalized mass profile of a single leaf with a fuel moisture content of 34% was compared with the experimental measurements of (Prince, 2014) under similar conditions and numerical findings of the authors' previous work (Edalati-nejad et al., 2022). The normalized mass profile provides insight into the time history of the leaf's drying and ignition, which is an essential characteristic for understanding the behavior of the solid fuels (see Figure 2). The comparison shows an acceptable amount of agreement between the experimental measurements and numerical results.

4. RESULTS

The time history of the area-weighted temperature of each leaf is shown in Figure 4. As can be seen, the lower leaf starts heating at about $t = 0.6$s, which is earlier than the upper leaf. From $t = 0.6$s to $t = 1.6$s, the temperature of the lower leaf is higher than the upper leaf, which is obviously because the lower leaf is more exposed to the heated flow. The upper leaf begins to heat up at around $t = 1.2$s, after which its temperature starts to steadily increase.

The temperature distribution contours for both leaves at $t = 1.6$s are shown in Figure 5, for several different views. Quite evidently, the lower leaf has the highest temperature, as was noted in Figure 3. Another point that deserves attention is that the edges of the leaves exhibit higher temperatures compared to the other regions, indicating non-uniform heating across the expanse of the leaves and this is because they are positioned in closer proximity to the source of convective heat, resulting in higher exposure to the hot gas. The highest temperature points on the lower leaf are located at its corners, which ultimately serves as the ignition point of the leaf, marking the beginning of its combustion.

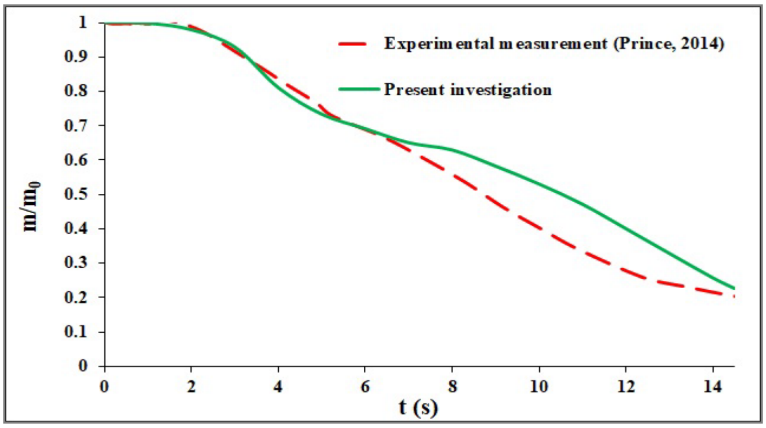

Figure 2. Normalized mass profile comparing the time history of the normalized mass of a solid fuel experimental study of (Prince, 2014) and the corresponding single leaf simulation

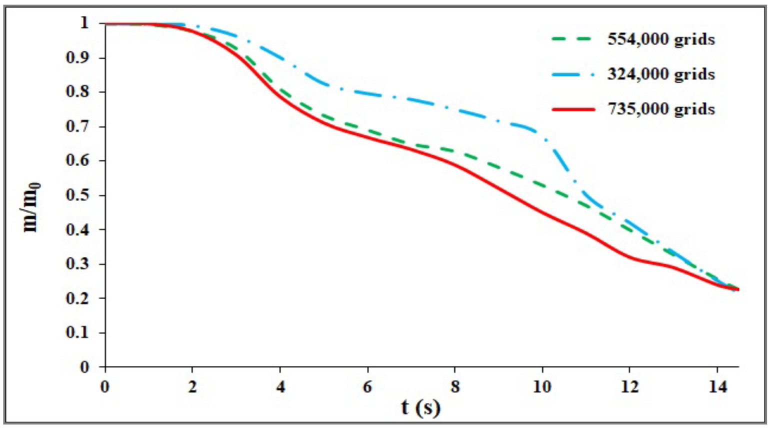

Figure 3. Normalized mass profile obtained from single leaf simulations using three different mesh numbers

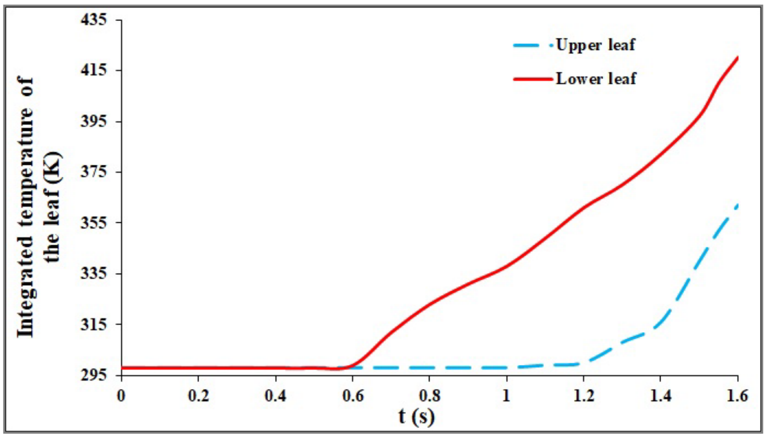

Figure 4. Area-weighted temperature of upper and lower leaf versus the time history

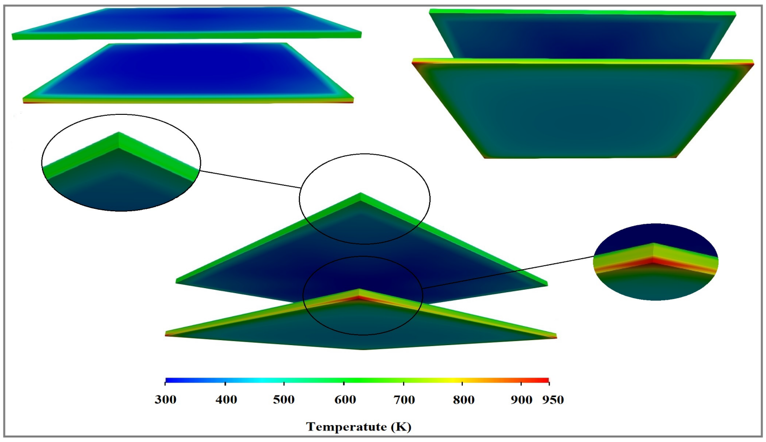

Figure 5. Temperature distribution of the two leaves for several different views, at $t = 1.6$s

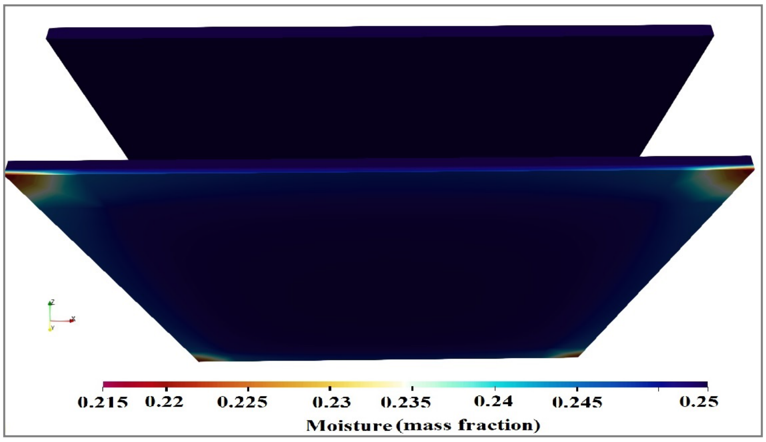

Figure 6. Contour of moisture distribution for two leaves at $t = 1.6$s

The moisture distribution across the two leaves at $t = 1.6$s is shown in Figure 6. Figure 6 indicates that the drying process starts from the lower leaf, at its edges, and especially at its corners. Comparison of Figures 5 and 6 confirms that the corners of lower leaf start heating, drying and then pyrolyzing, with ignition of the leaf later occurring at these points. In contrast, Figure 6 indicates that at $t = 1.6$s the upper leaf has exhibited very little moisture loss across its entire expanse.

5. DISCUSSION AND CONCLUSION

The current work considered the heating and drying process of two vertically stacked leaves with a fuel moisture content of 34%. The leaves were oriented horizontally to a convective heat source, and the heating and drying processes were investigated numerically. The research focused on understanding the dynamics of the pyrolysis reactions and combustion behaviour of solid fuels, as may occur in wildfires. The numerical investigation utilized the FireFOAM solver of OpenFOAM, which is a well-established open-source platform for simulating fire dynamics and pyrolysis reactions.

The main findings of the study can be summarized as follows:

- The numerical simulations exhibited an acceptable level of agreement with the experimental investigation of single leaf configurations.
- In the multi-leaf configuration, the lower leaf starts heating after about 0.6 seconds, earlier than the upper leaf that starts heating after about 1.2 seconds.
- The edges and the corners of the square-shaped leaves start drying, heating and pyrolyzing earlier than other parts of the leaf, so that ignition occurs at the corners of the leaf. This is consistent with experimental observations (S. McAllister, pers. comm.).

Although the current study has been somewhat preliminary, it provides a basis for examination of more sophisticated scenarios. Future work will consider multi-leaf configurations with different orientations and separations and will involve comparison with additional experiments to validate the simulation results.

ACKNOWLEDGEMENTS

The current work was supported by a PhD scholarship from the University of New South Wales and was conducted with the assistance of resources provided by National Computational Infrastructure at the Australian National University through the National Computational Merit Allocation Scheme supported by the Australian Government.

REFERENCES

Awad, C., Frangieh, N., Marcelli, T., Accary, G., Morvan, D., Meradji, S., ... & Rossi, J. L., 2021. Numerical study of the moisture content threshold under prescribed burning conditions. Fire Safety Journal, 122, 103324.

Borujerdi, P.R., Shotorban, B., Mahalingam, S., 2020. A computational study of burning of vertically oriented leaves with various fuel moisture contents by upward convective heating. Fuel 276 118030.

Chaos, M., Khan, M.M., Krishnamoorthy, N., de Ris, J.L., Dorofeev, S.B., 2011. Evaluation of optimization schemes and determination of solid fuel properties for CFD fire models using bench-scale pyrolysis tests. Proceedings of the Combustion Institute 33(2) 2599-2606.

Ding, Y., Wang, C., Lu, S., 2015. Modeling the pyrolysis of wet wood using FireFOAM. Energy conversion and management 98 500-506.

Edalati-nejad, A., Ghodrat, M., Sharples, J.J., 2022. Modelling the moisture effect on the rate of spread of fire in a leaf-like fuel element, 23rd Australian Fluid Mechanic Conference-23 AFMC: Sydney, Australia, p. 242.

Favre, A., 1983. Turbulence: Space-time statistical properties and behavior in supersonic flows. The Physics of fluids 26(10) 2851-2863.

Finney, M.A., Cohen, J.D., McAllister, S.S., Jolly, W.M., 2012. On the need for a theory of wildland fire spread. International journal of wildland fire 22(1) 25-36.

Le, D., Labahn, J., Beji, T., Devaud, C.B., Weckman, E.J., Bounagui, A., 2018. Assessment of the capabilities of FireFOAM to model large-scale fires in a well-confined and mechanically ventilated multi-compartment structure. Journal of fire sciences 36(1) 3-29.

Mahle, I., Mellado, J., Sesterhenn, J., Friedrich, R., de Ingenieros, S., 2006. LES of reacting turbulent shear layers using infinitely fast chemistry. Contribution to: Turbulence and Interaction.

Morvan, D., 2013. Numerical study of the effect of fuel moisture content (FMC) upon the propagation of a surface fire on a flat terrain. Fire Safety Journal 58 121-131.

Mulky, T.C., Niemeyer, K.E., 2019. Computational study of the effects of density, fuel content, and moisture content on smoldering propagation of cellulose and hemicellulose mixtures. Proceedings of the Combustion Institute 37(3) 4091-4098.

Prince, D.R., 2014. Measurement and modeling of fire behavior in leaves and sparse shrubs. Brigham Young University.

Ren, N., Wang, Y., Vilfayeau, S., Trouvé, A., 2013. Large Eddy Simulation of Turbulent Vertical Wall Fires, 7th International Seminar on Fire and Explosion Hazards.

Verma, S., 2019. A large eddy simulation study of the effects of wind and slope on the structure of a turbulent line fire. University of Maryland, College Park.

Wang, Y., Chatterjee, P., de Ris, J.L., 2011. Large eddy simulation of fire plumes. Proceedings of the Combustion Institute 33(2) 2473-2480.

Weise, D.R., Wright, C.S., 2014. Wildland fire emissions, carbon and climate: Characterizing wildland fuels. Forest Ecology and Management 317 26-40.

Yashwanth, B., Shotorban, B., Mahalingam, S., Lautenberger, C., Weise, D., 2016. A numerical investigation of the influence of radiation and moisture content on pyrolysis and ignition of a leaf-like fuel element. Combustion and flame 163 301-316.

Yashwanth, B., Shotorban, B., Mahalingam, S., Weise, D., 2014. A numerical investigation of the effect of moisture content on pyrolysis and combustion of live fuels.