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Experimental and numerical investigation of the effect of heating modes and moisture content on pyrolysis and ignition of live fuels

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Abstract: The role and distribution of moisture during thermal degradation and gas phase combustion of a vertically oriented solid fuel subjected to convective and radiative heating is investigated experimentally and numerically. Manzanita (*Arctostaphylos glandulosa*) leaves were exposed to convective (flat flame burner at 1000°C) and radiative (50 kW/m²) fluxes and ignition characteristics were measured. The experiments were modeled using a three-dimensional computational model that simultaneously resolves both solid phase thermal degradation and gas phase combustion. The model uses Gpyro3D for solid phase degradation and FDS for gas phase combustion. A 12-step kinetic reaction scheme that accounts for evaporation of moisture and pyrolysis of solid fuel were incorporated. This reaction scheme was initially validated with experimental TGA results and computational results. We then simulated ignition of the solid fuel at three initial moisture contents (44, 65, 90%) subject to convective heating. The simulated ignition and burnout times were consistent with the experimental results. As initial moisture content decreased, time to the onset of pyrolysis and ignition decreased, resulting in higher mass loss and heat release rates. Local moisture evaporation and temperature rise were observed at the tip of the solid fuel in all three cases and a significant amount of moisture remained in the solid fuel during ignition, consistent with experimental findings. Enhanced heat flux present during combined radiative and convective heating led to accelerated burning and lower ignition times. The experimental and numerical results suggested that moisture content and heating modes influenced the pyrolysis and ignition of live manzanita leaves.

Keywords: *Live fuels, Wildland fuels, Pyrolysis, CFD*

1. Introduction

A large number of wildland fires occur in live fuels that contain significant moisture [1] and they often burn through smaller fuel elements such as leaves, twigs and branches. The live fuel elements in unburnt vegetation are exposed to both convective and radiative heat transfer. The relative importance of external heat transfer mechanisms in wildland fire has been a subject

of considerable debate for several decades. Furthermore, much of the experimental research that contributes to fire spread models focuses on dead and dried fuels. Hence additional research to quantify the contributions of moisture, radiation and convection is necessary to better understand burning characteristics of living vegetation.

When a solid fuel/biomass particle is heated to a sufficiently high temperature, it undergoes thermal degradation/pyrolysis. Hemicellulose, cellulose and lignin are the three main components of biomass and their proportions are 20-40, 40-60, and 10-25 wt.%, respectively. It was suggested by [2, 3] that the pyrolysis of any biomass can be considered as the superposition of these three main components. Pyrolysis reactions of biomass materials exposed to high temperature sources can be roughly classified as primary and secondary reactions. According to Di Blasi [4], primary reactions are concerned with the degradation of the biomass into char and numerous volatile products whereas secondary reactions are those undergone by primary volatile products. Miller and Bellan [5] used the extended Broido–Shafizadeh (BS) model of Di Blasi [4] as a skeletal model and formulated a superposed kinetic scheme for cellulose, hemicellulose and lignin kinetics. This superposed kinetic model was incorporated into our numerical investigation in which, the three primary biomass components are modeled with multi-step kinetics involving both competitive primary pyrolysis and secondary tar decomposition reactions.

The main aim of this investigation is to better understand the effects of heating modes and moisture content on pyrolysis and gas phase combustion of live fuels. The present work discusses mainly the results obtained from numerical simulations for a fuel moisture content (FMC, dry basis) of 44, 65, and 90%. Only a brief description of the experimental apparatus and conditions relevant to this paper is provided. The solid phase model uses Gpyro3D [6] for pyrolysis and the gas phase fluid dynamics and ignition are solved by Fire Dynamic Simulator (FDS) [7]. In the present study ignition was defined to be the time at which the first sustainable flame was observed in the experiments, and in the case of numerical investigation, ignition time was defined as the time at which the heat release rate (HRR) exceeded 200 kW/m^3 in the gas phase.

2. Experimental procedure and apparatus

Each month, combustion experiments (25 replicates) were performed on freshly harvested manzanita (*Arctostaphylos glandulosa*) in the flat flame burner (FFB) apparatus at Brigham Young University (BYU) (see fig. 1a). Video images, mass and temperature data were collected using the apparatus shown in fig. 1(a). Samples were individually weighed and placed within the apparatus. The water-cooled FFB produced exhaust gases at 1000°C and 10 mol% oxygen that flowed past the sample suspended on a holding rod using an alligator clip. The holding rod was connected to a Mettler Toledo XS204 Cantilever mass balance. Mass data were continuously measured using National Instruments Labview 8.6 Software. A glass cage surrounding the sample prevented ambient air from being entrained in the FFB exhaust gases. An Omega K-type thermocouple (0.013 mm diameter, 0.05 s response time) was used to measure the gas temperature. An Omega QH-101060 radiant panel was used to provide a 50 kW/m^2 flux at the sample location. Heat flux was measured using a Medtherm 64-series heat flux sensor.

3. Computational domain and model

The numerical investigation was carried out at The University of Alabama in Huntsville (UAH). The domain used to model the experimental apparatus is shown in fig. 1b. The solid fuel element had dimensions of $0.03\text{m} \times 0.002\text{m} \times 0.03\text{m}$ for Length \times Thickness \times Width. The effect

of convection and combined convection and radiation heating of the fuel was investigated in detail. During the convection-only case, the radiative heat source was absent in both experiments and the numerical simulations. The computational domain used for the gas-phase solver FDS is a rectangular cube of size $x = 0.18\text{m}$, $y = 0.25\text{m}$ and $z = 0.32\text{m}$. The grid resolution used in x , y and z directions was $120 \times 160 \times 216$, respectively. The solid fuel particle was oriented vertically and was centered in the gas-phase domain located at $z = 0.055\text{m}$. The initial temperature, moisture content, pressure, gaseous species mass fractions, and condensed phase species were set uniform throughout the solid. Fuel element is simulated as a separate region modeled by Gpyro3D with a grid spacing of 0.0006 m in x and y directions and 0.0003 m along the depth, resulting in 9600 grid cells. The fuel element for convection-only case was exposed to a modeled burner with a dimension of $0.18 \times 0.25\text{m}$, $L \times W$ from which heated air enters the domain at 1000°C and at a velocity of 0.6 m/s . In case of combined heating mode, it is exposed to a heated wall with dimensions $0.18 \times 0.32\text{ m}$, $L \times H$ providing 50 kW/m^2 input heat flux along with the convective burner. The center of solid fuel was located at a distance of 5 cm from the top surface of the burner and was 11 cm from the heated wall surrounded by solid walls on the sides with the top surface being open. All the computations were performed using the message passing interface (MPI) protocol on 60 processors of Dense Memory Cluster (DMC) located at Alabama supercomputer Authority. A typical simulation of 10 seconds of burning required a wall time of 48 hours and 120 GB of memory.

Significant variation in temperature and moisture content has been observed on the surface and depth of the fuel by McAllister *et al.* [1], Pickett *et al.* [8] and Prince *et al.* [9], indicating the three-dimensional nature of pyrolysis. A detailed description of the mathematical models with main assumptions and governing equations used in Gpyro3D and FDS are given in [6] and [7], respectively. Initially, the condensed/solid-phase domain consisted of moisture, cellulose, hemicellulose, and lignin. The gas phase within the solid fuel consisted of air (nitrogen and oxygen). Their respective initial mass fractions are given in Table 1. The initial mass fractions of other species were considered negligible. The initial temperature was set to the ambient temperature of 300 K .

The “skeleton” of the cellulose scheme outlined by Di Blasi [4] is shown in fig. 2. Reactions R1, R2, R3 are primary reactions and R4 is a secondary reaction. The primary reactions are concerned with the conversion of the virgin species to active state which later breaks down to lower molecular weight gases while the secondary reaction, which is an oxidation reaction, is concerned with tar breakdown to low molecular weight gases. The term “virgin” refers to reactants cellulose, hemicellulose and lignin which follow the same reaction pathway (R1-R4). In the current study, reaction R5 represented two evaporation reactions and was incorporated to account for moisture evolution based on free and bound state. Free moisture evaporation reaction was adopted from [10] and bound state evaporation was adopted from [9]. This 12-step reaction model has been incorporated in Gpyro3D. The reaction kinetics and thermo-physical properties for reactions R1-R5 are given in Tables 2 and 3 respectively. The thermophysical properties were assumed to be identical for cellulose, hemicellulose and lignin. Thermal conductivity was considered temperature dependent following correlation used for soft wood species in [11]. These correlations were used for the solid species for all the simulations invoking the coupled solver at various FMC cases (44, 65 and 90%). The properties for the gas species were assumed from the available data for air. A total of four numerical simulations (three for moisture + 1 for combined heating mode) were performed.

4. Results and Discussions

The 12-step kinetic model used in the numerical simulations was validated against the experimental and simulation data of Koufopoulos *et al.* [12] and Miller & Bellan [5], respectively. This validation was achieved using a zero-dimensional model of Gypro with similar heating rates. The reaction R5 was neglected during this exercise because the specimens were dry. Using the convection-only heating case shown in fig 1(b), the effect of FMC on solid and gas phase ignition will be discussed first, followed by the effect of combined convection and radiation by incorporating the heater into the computational setup shown in fig 1(b). During this discussion, the computational results were also compared with the experimental data obtained using the FFB burner. Although more detailed results pertaining to the experimental data can be obtained elsewhere [9], a few global results such as the mass loss rate and the normalized mass are presented here for the purpose of numerical validation.

4(a). Convection-only heating

The time history of mass loss rate (MLR) obtained for a case of FMC 65% during the simulation was compared with the experimental data as shown in fig 3(a). The time at which MLR values became positive can be treated as a point of initiation of evaporation, mainly due to formation of water vapor. For simulations, this occurred at 1.9s and for the experiments it occurred much earlier, at 0.5s. It is further observed that the simulation over predicts the peak experimental mass loss rate. This over prediction is believed to be due to the difference in the initial mass of the solid fuel considered in simulations and experiments. The initial mass in simulations was 1g whereas it was 0.38g in the experiments; this discrepancy was driven by computational limitations on the minimum thickness of the solid fuel. The time history of normalized mass is shown in fig 3(b). The burn out time in the simulation was close to 8s while it was close to 14s in the experiments. Also, the simulated residual mass was close to 40% while in the experiments it was 15%. This difference between numerical and experimental results is also attributed to a higher solid fuel thickness (2mm) considered in the simulations, which was because of computational constraints. Due to this higher thickness in simulations, the computed temperatures at the center of the fuel were low, potentially inhibiting pyrolysis in this region. The thickness of Manzanita leaves in the experiments was measured to be between 0.5 and 1mm.

The computational model was utilized to study the process leading up to ignition in detail. The evolution of overall MLR and HRR obtained from numerical simulations were plotted in fig. 4(a, b) for FMC's of 44, 65 and 90%. The initiation of evaporation occurred at 1.9s for FMC's of 44, 65 and 90%. It is noted that the MLR curves for each of these FMC cases exhibited two overall peaks. The first peak is caused by evaporation of the free water and the second peak is caused by the combined contribution of fuel vapor and water vapor from fuel degradation and bound water evaporation, respectively. Oxidation of the gaseous fuel vapors resulted in flaming combustion. In fig. 4(b), HRR quantifies the amount of heat generated due to combustion of fuel vapors in the gas phase. The fuel vapors were assumed to be methane and to react in stoichiometric proportion with air to cause ignition. For the 65% FMC case, ignition time was 3.3s in simulations and it was 3.1s in the FFB experiments. The ignition times were 3.2s and 3.4s for FMC of 40 and 90%, respectively, in simulations. Although the ignition times for various moisture contents were close to each other, there was a significant difference in the time at which HRR curves achieved the peak value.

The 65% FMC case was investigated in greater detail. The two-dimensional contours of temperature on a yz slice passing through $x = 0$ are for times $t = 2s$ and $t = 5s$ are presented in

figs. 5(a) and (b), respectively. In fig. 5(a), strong mixing between the ambient air and the hot air exiting the burner was observed. Since solid wall boundary conditions were used to model the glass cage used in FFB apparatus, boundary layers are also observed near the sidewalls. At $t = 5$ s in fig. 5(b), we observe that the tip of the solid fuel close to the burner ignited first and then fire propagated towards the trailing edge of the solid fuel. Two-dimensional contours of mass fraction of water vapor, are plotted on the same slice in the gas phase for times $t = 2$ s and $t = 5$ s in figs. 6(a) and (b), respectively. In fig. 6(a), observe that the water vapor was released into gas phase due to free moisture evaporation. This release occurred prior to ignition because of lower activation energy of 88 kJ/mol (Table 2). However, at $t = 5$ s when the fuel ignited, as seen in fig. 6(b), we observed water vapor close to the leading and trailing edge of the solid fuel. The vapor near the leading edge is primarily due to bound moisture evaporation. However, the vapor near the trailing edge is due to free moisture evaporation, which takes place earlier in time. It is evident in this figure that bound moisture evaporation front follows the free moisture evaporation during the ignition process. These observations in the simulation indicate the presence of water vapor in the region close to and away from the ignition zone, indicating that evaporation and ignition occur simultaneously in live fuels. This observation made through simulations is consistent with experimental observations of moisture release simultaneously with volatiles release.

4(b). Combined convection and radiation heating

The time history of MLR for FMC of 65% under combined heating mode is shown in fig. 7(a). It is seen that the simulation over predicts the experimental peak mass loss rate, as was noted in the convective heating case. Due to presence of radiation, the peak value of MLR in this case was 20% higher than that in convection-only case. The time history of normalized mass is displayed in fig. 7 (b). The fuel particle burn out time was around 7.1s and 10s in simulations and experiments, respectively. Due to the presence of radiation, the solid fuel was consumed approximately 1s earlier than when the mode of heating was convection.

5. Summary and Conclusions

The effect of heating mode and moisture content on pyrolysis and combustion of individual manzanita (*Arctostaphylos glandulosa*) leaves was investigated experimentally and numerically. The simulations were carried out by using a detailed 12-step kinetic model as the pyrolysis model. The kinetic model was first validated against the data obtained by other simulation and TGA experiments. Then, using a three dimensional computational model, it was compared with the experimental data obtained by the FFB apparatus for both convection-only and combined radiation-convection heating. The simulation and experimental results were consistent as far as ignition time, fire initiation and spread pattern were concerned. However, the peak MLR obtained experimentally was over predicted by the simulations. This difference is attributed to the larger initial mass of the solid fuel used in simulations. In the solid fuel, local evaporation of moisture and rise of temperature at a point closer to the burner was observed. Furthermore, a significant amount of moisture remained in the sample at the time of ignition, suggesting that different points in the domain pyrolyze at different times which has been observed qualitatively in other experiments. In the gas phase, high mass fraction of water vapor was observed in the regions close to and away from the combustion zone, indicating that that evaporation and combustion can occur at the same time. When FMC's of 44, 65 and 90% were considered, it was observed that the temperature response was higher for the case with 44% FMC and ignition occurred prior to the 65 and 90% FMC case; however, the MLR values were small for lower

FMC case. The additional radiative flux in the combined heating mode case increased the peak MLR by 20% and decreased burnout time by 1 s. While some adjustment needs to be made to the simulation to improve the MLR, we feel that this simulation setup can now be used to understand aspects of the effect of time of year and plant species on ignition which we were unable to measure in our experiments.

6. Acknowledgments

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7. References

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Table 1. Initial conditions

FMC	Cellulose	Hemicellulose	Lignin	Free moisture	Bound moisture	Oxygen	Nitrogen
44%	0.23	0.23	0.24	0.225	0.075	0.23	0.77
65%	0.198	0.198	0.204	0.3	0.1	0.23	0.77
90%	0.17	0.17	0.19	0.3525	0.1175	0.23	0.77

Table 2. Kinetic parameters pertaining to the 12-step mechanism

Cellulose		
Reaction	A (s^{-1})	E (kJ/mol)

R1	2.8×10^{19}	242.4
R2	3.28×10^{14}	196.5
R3	1.3×10^{10}	150.5
Hemicellulose		
R1	2.1×10^{16}	186.7
R2	8.75×10^{15}	202.4
R3	2.6×10^{11}	145.7
Lignin		
R1	9.6×10^8	107.6
R2	1.5×10^9	143.8
R3	7.7×10^6	111.4
Tar cracking		
R4	4.28×10^6	108
Free Moisture		
R5	2.8×10^{19}	88
Bound Moisture		
R5	2.8×10^{19}	166

Table 3. Thermophysical properties

	Cellulose	Hemicelulose	Lignin	Free moisture	Bound moisture	Char
Thermal Conductivity (W/mK)	$0.08124 + 0.003695 T$	$0.08124 + 0.003695 T$	$0.08124 + 0.003695 T$	0.56	0.56	0.10
Density (kg/m ³)	420	420	420	1000	1000	73
Specific heat (kJ/kgK)	2.3	2.3	2.3	4.2	4.2	1.1

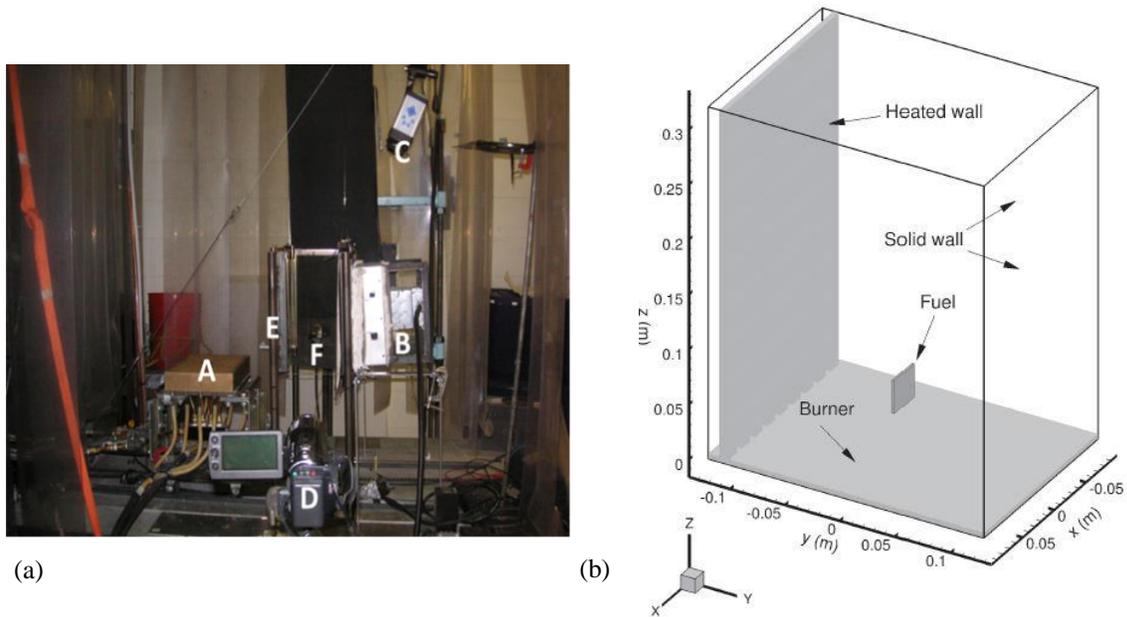


Figure 1: (a) Experimental apparatus: flat flame burner (A), radiant panel (B), IR camera (C), video camera (D), glass cage to prevent ambient air entrainment (E), sample location (F), mass balance (G) and sample holding rod (H); (b) Isometric view of computational domain showing a thin solid fuel subjected to combined convection and radiation surrounded by solid wall.

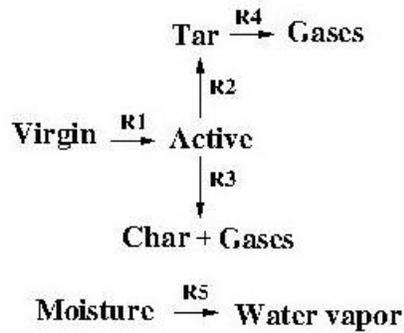


Figure 2: Generic reaction scheme used to model cellulose, hemicellulose and lignin pyrolysis (Miller & Bellan [6]) along with vaporization reaction of moisture.

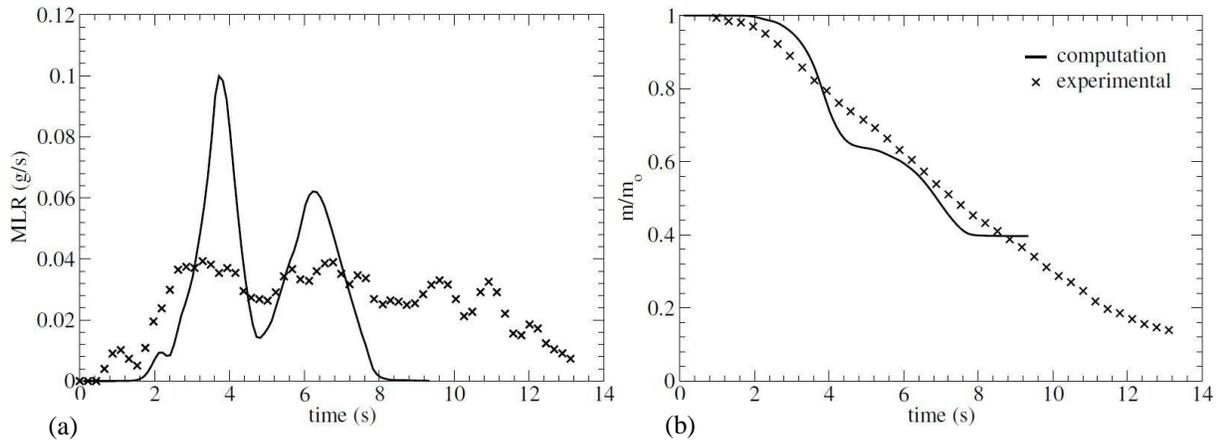


Figure 3: Comparison of time histories of (a) mass loss rate, (b) normalized mass (solid line) with experimental results of manzanita species (symbols) for an initial FMC of 65% using convection-only heating.

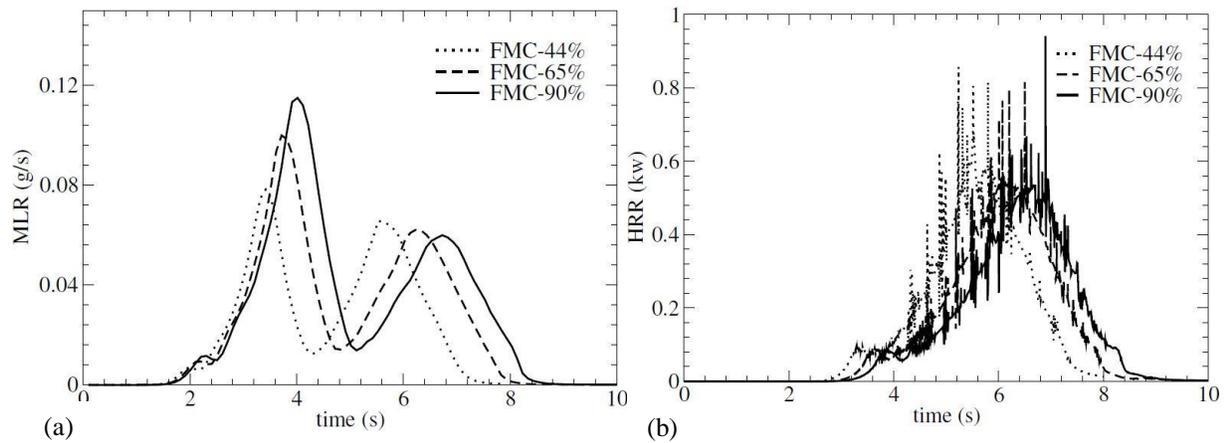


Figure 4: Time histories of (a) mass loss rate and (b) heat release rates for three cases with an initial FMC of 44%, 65% and 90% using convection-only heating.

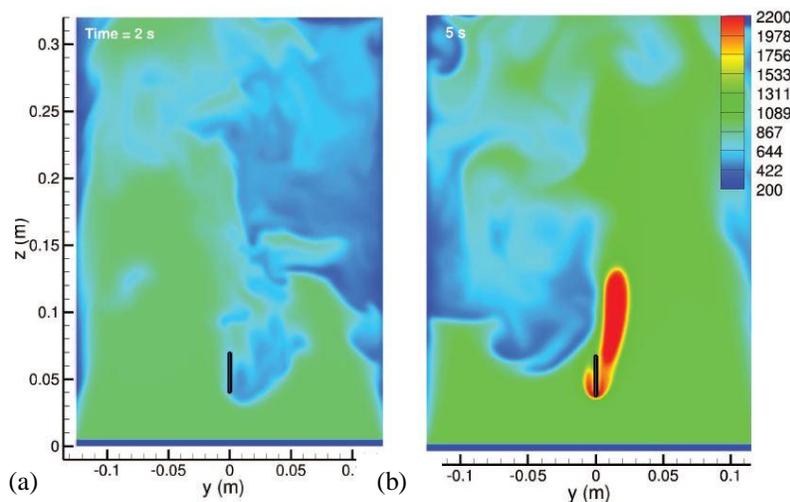


Figure 5: Contours of gas-phase temperature at times (a) $t = 2$ s, and (b) $t = 5$ s on an yz slice located at $x = 0$ for a case with an initial FMC of 65% using convection-only heating.

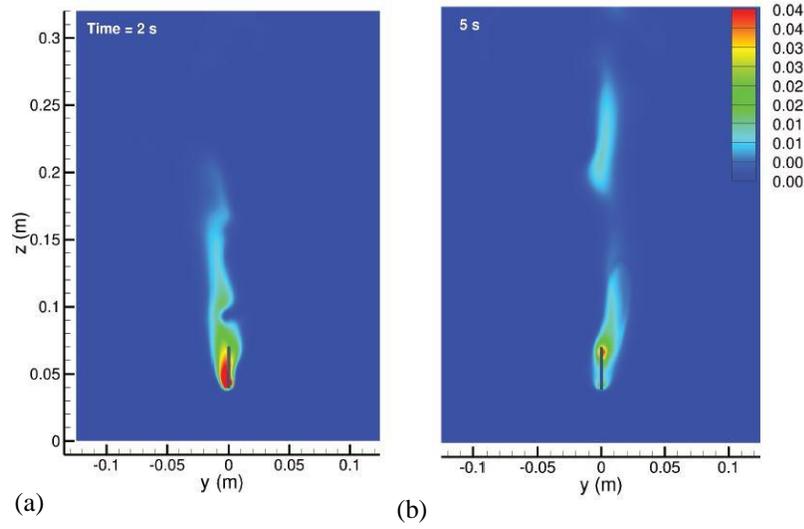


Figure 6: Contours of mass fraction of water vapor in the gas phase at (a) $t = 2$ s and (b) $t = 5$ s on an yz slice located at $x = 0$ for a case with an initial FMC of 65% using convection-only heating.

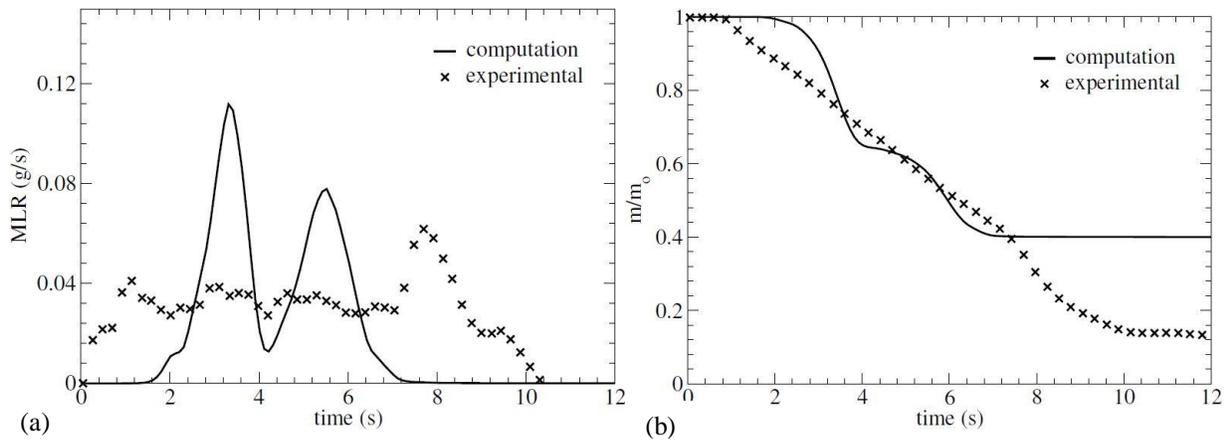


Figure 7: Time histories of (a) mass loss rate, (b) normalized mass (solid line) with experimental results of manzanita species (symbols) for an initial FMC of 65% using combined convection and radiation heating.