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Understanding the role of moisture in live fuels subject to pyrolysis and ignition through radiation heat transfer

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The role of fuel moisture on eventual fire behavior is not very well understood in the context of live fuels. In this paper, the role and distribution of moisture during thermal degradation and gas phase combustion of a solid cellulosic fuel element representing living vegetation subjected to radiative heating is investigated numerically. The dimensions of a typical manzanita (*Arctostaphylos glandulosa*) leaf were used for the cellulose fuel. An improved three dimensional computational model that simultaneously resolves both solid phase thermal degradation and gas phase combustion (Lautenberger, 2014) is used. The model uses Gpyro3D for solid phase degradation and FDS for gas phase combustion. A 5-step extended Broido-Shafizadeh (Bradbury *et al.* 1979) model that accounts for evaporation of moisture is used to model moisture evaporation, and pyrolysis of cellulose. The model was validated against previous TGA experiments and computational results. Ignition of a modeled leaf-like fuel element at three initial moisture contents (5, 40, and 80%, dry mass basis) exposed to a 1500 K radiant source was simulated. Lower moisture content resulted in earlier onset of pyrolysis and ignition resulting in higher solid and gas phase temperatures. Local moisture evaporation and temperature rise were observed in all three cases and a significant amount of moisture remained within the sample during ignition. The numerical results confirm that moisture content not only affects the process of pyrolysis, but also influences the ignition and gas phase combustion of the solid fuel.

Keywords: *Live fuels, Cellulose, Wildland fires, Pyrolysis, CFD, Radiation*

1 Introduction

Fire burns in vegetation in many regions of the world; humans and ecosystems have evolved with this process. The vegetative fuel for wildland fire is a combination of the living plants and their dead, cast-off foliage and branches. Living plants actively regulate the water contained in their plants cells while the dead components absorb and desorb water passively like a sponge [1]. Current forest fire models are largely empirical ([2]) and are based on data from beds of dead vegetation. Therefore, improvement in modeling capabilities is sought by developing better kinetic models for the combustion of live fuels.

A solid fuel undergoes thermal degradation when heated to a sufficiently high temperature. For the purpose of modeling, thermal degradation is assumed to occur in two sequential steps. The first step is pyrolysis, which is usually an endothermic process that breaks down the forest matter into low molecular mass gases (volatiles), tars, carbonaceous char and mineral ash. The second

process is burning, which is an exothermic process known as combustion. Ignition is a transition process between the first and second step. Ignition criteria have been defined for solid phase, the gas phase or combined solid and gas phases [3]. In the present study, we defined ignition based on the gas phase. We defined ignition as the time at which the heat release rate (HRR) exceeded 200 kW/m^3 in the gas phase over the surface of cellulose element. Any value above this critical value would mean an active flame observed in the simulation over the solid fuel.

All plant/biomass matter consists of different polymers present in the organic fraction of the fuel. They are generally divided into cellulose, hemicellulose, lignin, moisture, mineral matter and a few other organic compounds [4]. Cellulose is the main component among all the constituents of plant matter [5]. Therefore, a better understanding of various physical and chemical processes during its thermal degradation is a first step towards the development of kinetic models of complex solid fuels. Chemical reactions of biomass materials exposed to high temperature sources can be roughly classified as primary and secondary reactions. Primary reactions are concerned with the degradation of the cellulosic fuel into char and numerous volatile products whereas secondary reactions are those undergone by primary volatile products [6]. The first kinetic models were proposed in the 1960s by Kilzer and Broido [7], Chatterjee and Conrad [8] and Shafizadeh [9], and are the basis of more recent kinetic models. Several investigators have developed multi-step kinetic models more or less derived from the original mechanism of Kilzer and Broido [7]. Bradbury *et al.* [10] reformulated Broido's reaction model by introducing active cellulose, as an intermediate species between native cellulose and reaction products and this reaction model is called as 'Broido-Shafizadeh model (BS)'. Blasi [6] in her numerical work used the BS model of cellulose pyrolysis and extended it to include secondary reactions concerning the tar cracking. This is known as the extended Broido-Shafizadeh model.

Fuel moisture content (FMC) present in the plant matter is an important factor that influences the burning behaviour of live fuels [11]. Water affects ignition processes involving both solid and gas phases. According to Pickett *et al.* [12], who investigated the burning of various live leaf samples in detail, ignition does not occur at the end of global evaporation, as predicted by conventional models, but possibly at the end of local evaporation. They also found that a significant amount of moisture (30–60%) remains in the sample for most species at the time of ignition. However, their experiments did not focus on pyrolysis and other physical processes inside the fuel while it pyrolyses.

The main aim of the present work is to better understand the effects of moisture content on pyrolysis and gas phase combustion in solid fuel composed of cellulose by taking into account multi-step thermo-physical processes occurring in the solid fuel and the associated combustion of the released gases using a three-dimensional solid-gas model. The solid model uses Gpyro3D [13] for pyrolysis and the gas phase fluid dynamics and combustion is solved using Fire dynamic simulator (FDS) [14].

2 Physical configuration

In a spreading wildland fire, unburnt vegetation that lies ahead of burning vegetation is exposed to varying combinations of convective and radiative heating. The heat fluxes associated with radiation are as high as 200 kW/m^2 [12, 15]. The focus of the present work is on an analysis of the effect

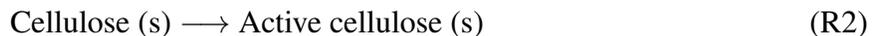
of FMC during ignition achieved via radiation heating of a thin, rectangular cellulose material. The fuel element we choose is a three-dimensional piece ($0.04 \times 0.04 \times 0.002$ m, $L \times W \times T$) of cellulose material with fixed thickness. The choice of this configuration is motivated by its similarity to experimental configurations studied by Pickett *et al.* [12] and Engstrom *et al.* [16]. A schematic of the physical domain along with the boundary conditions is shown in figure 1. The computational domain used for the gas-phase solver FDS, is a rectangular cube of size $x = 0.18$ m, $y = 0.18$ m and $z = 0.32$ m. The grid resolution used in x , y and z directions is $72 \times 72 \times 92$, respectively. The solid fuel particle is centered in the gas-phase domain and located at $z = 0.03$ m in the computational domain. 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 0.0008 m in the x and y directions and 0.0005 m along the depth. Here, 13824 grid cells are used for Gpyro3D. The fuel element is exposed to a radiant surface located at $x = -0.09$ m. The surface is maintained at 1500K through the entire simulation. Effects of wind are not considered here.

All the computations were performed using message passing interface (MPI) protocol using 36 processors of Dense Memory Cluster (DMC) located at Alabama Supercomputer Authority. A typical simulation of 30 seconds required a wall time of 72 hours and 64 GB of memory.

3 Reaction mechanism and computational models

A considerable amount of temperature and moisture variation was observed along the surface of fuel by Pickett *et al.* [12] and according to McAllister *et al.* [15] these gradients were observed along the depth of the fuel, indicating a three-dimensional nature of pyrolysis. CFD models such as FDS and FireFOAM resolve heat transfer only in the direction normal to the surface but not laterally in the directions parallel to the surface [13], which is important in the present context. Therefore, to investigate the three-dimensional effects during fire initiation and propagation on fuel elements where multidimensional heat and mass transfer effects are significant, a fully coupled Gpyro3D-FDS model is used. Detailed descriptions of mathematical models with main assumptions and governing equations used in Gpyro3D and FDS are given in [13] and [14], respectively. Initially, the condensed/solid phase domain consists of moisture and cellulose and the gas phase within the solid fuel consists 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 be the ambient temperature of 300K.

The reaction mechanism used in the current study is shown below:



Reactions R2-R4, known as Broido-Shafizadeh reaction model [10], are primary reactions and R5 is a secondary reaction included by Blasi [6] for pyrolysis of cellulose. The primary reaction are concerned with the breakdown of cellulose to lower molecular weight gases while the secondary reaction, which is an oxidation reaction, is concerned with the tar breakdown to low molecular weight gases. In the current study, reaction R1 is included to take into account the evaporation of the moisture [17]. The reaction kinetics and thermo-physical properties for reaction R1 is adopted from [17] and for reactions R2-R5, are adopted from [6].

As discussed earlier, FMC also affects the thermal properties of the material, it is therefore necessary to account for the material functionality in terms of FMC. When the FMC is more than the fiber saturation point (FSP) of that material, all the water is present in the lumen as free water since the cell walls are now saturated with bound water [18]. The FSP is usually considered to be around 30% (dry basis). In the current study, thermal conductivity and specific heat capacity was considered moisture dependent through the correlation of [18] for $FMC > 0$. On the other hand, thermal conductivity and specific heat capacities were considered only temperature dependent, following the correlations given by Yu *et al.* [19] and Bryden *et al.* [20] when the $FMC = 0$. Here, since no equations that correlates the thermo-physical properties of cellulose with temperature were found, such correlations which are available for wood were utilized for cellulose. The properties for the remaining species were considered constant.

4 Results and Discussions

The model has been validated initially with Gpyro, a one-dimensional version of Gpyro3D, for a configuration numerically studied by Di Blasi [6]. The results of the current study were in reasonably good agreement with Di Blasi's results [6]. Further the model was validated via the comparison of the modeling results against the experimental data of Reed and Posey [21]. They heated 6 mg of cellulose with a rate of $40^{\circ}\text{C min}^{-1}$ to generate experimental thermogravimetric analysis (TGA) data. In the current study, a zero-dimensional model of Gpyro was used to predict this experimental data. The first reaction R1 was neglected during this exercise since experiments and the numerical counterpart did not consider a moist specimen.

The classical combustion model assumes that all moisture will first evolve from the sample at a temperature near the boiling point of water. Ignition (according to the classical model) occurs when a combustible mixture of pyrolysis gases is obtained and follows shortly after moisture evaporation is complete [12]. In order to investigate this claim, for the main configuration considered in this work (fig. 1(a)), time history of temperature and mass fraction of moisture are plotted for a fixed point in figure 2. The point is noted as point A in fig. 1(b) which is located in the solid phase and is in proximity to the heat source. Figure 2(a) shows that the temperature slowly responds for the case involving higher FMC. This behaviour could be attributed to the higher thermal conductivity of water compared to cellulose. The decay of mass fraction of moisture is illustrated in fig. 2(b), and it is observed that the evaporation rate is low for the case with high FMC. In order to analyze the temperature and FMC in the solid fuel at a region away from the heat source, temperature and mass fraction of moisture have been plotted at time 5 s.

From fig. 3(a) and 3(b) we observed that temperature rise and evaporation of moisture were

confined to a local region close to the heat source. The temperature was higher by approximately 700 K for 5% FMC case at the leading edge of the solid fuel. The 40 and 80% cases differed in temperature by <50 K in this region and differed very little along the majority of the solid fuel. Similarly, the temperature for the 5 % FMC decreased by only 100 K over the majority of the solid fuel (-0.017 to 0.02 m). We also observed that a significant amount of moisture remained in the sample at the time of ignition for the 40 and 80% cases. In the area closest to the heat source (-0.02 to -0.016 m), the moisture mass fraction was 0; however, the mass fraction was unchanged in the region -0.012 to 0.02 m. In contrast, evaporation occurred in the 5% case along the majority of the fuel length.

The evolution of overall mass loss rate (MLR) is shown in fig. 4(a). Water vapor (from evaporation) and fuel vapor (pyrolyzates from active cellulose) comprised the gas species that diffused from the solid phase to the external gas phase domain. The time at which MLR values became positive can be treated as the initiation of evaporation, mainly due to formation of water vapor and this occurred at 2 s for FMC of 5%, 40% and 80%. Note that the MLR curves for each of these case exhibited two overall peaks. The first peak represented water vapor and the second peak represented fuel vapor. As FMC increased, the first peak value increased due to more water vapor being lost during the drying phase. The MLR associated with the second peaks did not differ greatly between FMC; maximum MLR of the second peak ranged from 0.09 to 0.12 g s⁻¹. Oxidation of the gas phase fuel vapors resulted in flaming combustion. Time histories of HRR are shown in fig. 4(b) for a FMC of 5%, 40% and 80%. HRR quantifies the amount of heat generated due to stoichiometric combustion of fuel vapors with oxygen in the gas phase. The fuel vapors in this work are modeled as methane. From fig. 4(b), it can be seen that FMC affected the time at which ignition occurred. Ignition occurred at 5.75, 8, 10 s for FMC of 5, 40 and 80 %, respectively.

Two-dimensional contours of temperature, mass fraction of water vapor are plotted at 5 s on an xz slice located at $y = 0$ in fig 5(a) and 5(b) respectively in the gas phase domain. The flaming combustion zone which is represented as the first ignition point in fig.5(a) was observed initially at the tip of the solid fuel located close to the heating source. Following this from fig. 5(b), the water vapor in the gas phase is predominant in the ignition zone as well as in the region away from it, clearly manifesting the point that evaporation and combustion occur together.

Figure 6, shows the relative importance of the convection and radiation heat transfer in igniting the solid fuel particle. The negative heat fluxes values observed in case of convection during initial time accounts for the heat transfer between the heated wall and the surrounding gas. However later in time when the solid fuel ignites, it undergoes cooling through natural convection which results in increased convective heat flux. The positive radiative heat flux observed during the initial time accounts for the radiation energy absorbed by solid fuel from the external gas phase domain. Later when the solid fuel ignites, it emits radiation back into the gas phase which results in negative heat flux as seen from the figure. The role of thermal radiation in causing gas phase ignition has also been investigated by considering many cases where in the solid fuel was being exposed to a heated surface maintained at different temperatures. Ignition was observed only when the temperature of the heated surface was more than 1100 K indicating that thermal radiation can ignite a live fuel without the use of a pilot source provided the temperature of the heating source is high enough.

5 Summary and Conclusions

The effect of moisture content on pyrolysis and combustion of a thin cellulose particle subject to heating by radiation has been investigated numerically. The thermal degradation reaction mechanism used for cellulose breakdown was initially validated with other simulation and TGA experiments. An FMC of 5%, 40% and 80% was considered during the study. The temperature response and thermal degradation rate was higher for the case with 5% FMC and ignition occurred prior to the 40% and 80% FMC case. The simulations also indicated that in the solid phase, water evaporated locally near the point of ignition and remained elsewhere indicating that different points in the domain evaporate and pyrolyse at different times. In the gas phase, high volume fraction of water vapor observed in the region close to the combustion zone as well as away from this region illustrated that evaporation and ignition can occur together in live fuels.

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Table 1: Initial mass fractions of solid and gas species within the solid fuel.

FMC	Moisture	Cellulose	N ₂	O ₂
80%	0.46	0.54	0.77	0.23
40%	0.22	0.78	0.77	0.23
5%	0.04	0.96	0.77	0.23

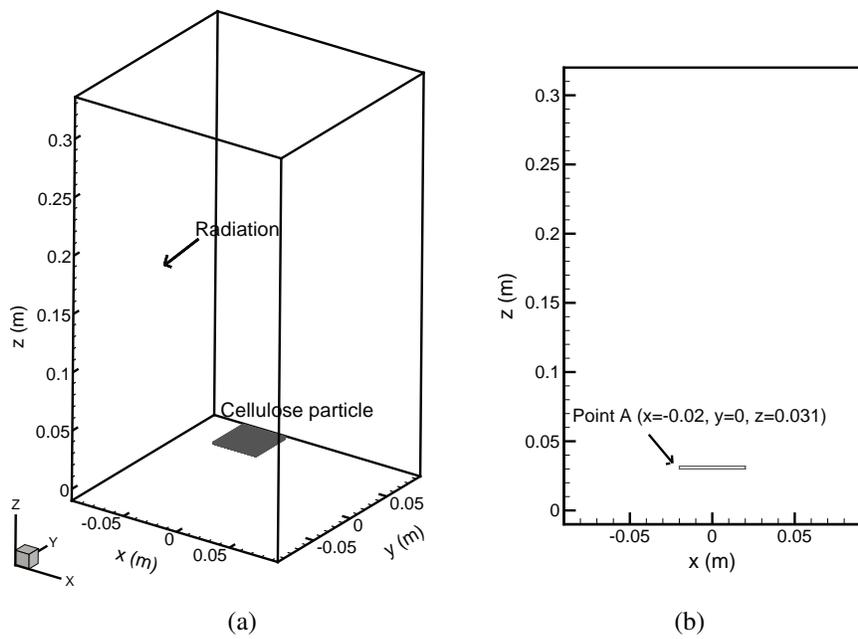


Figure 1: (a) Isometric view of computational domain showing thin cellulose particle subjected to radiative heating from surface at $x = -0.09$ m, (b) two-dimensional view of computational domain along the xz -slice at $y = 0$ m. Point A located at $x = -0.02$ m, $y = 0$, $z = 0.0315$ m is considered for analysis.

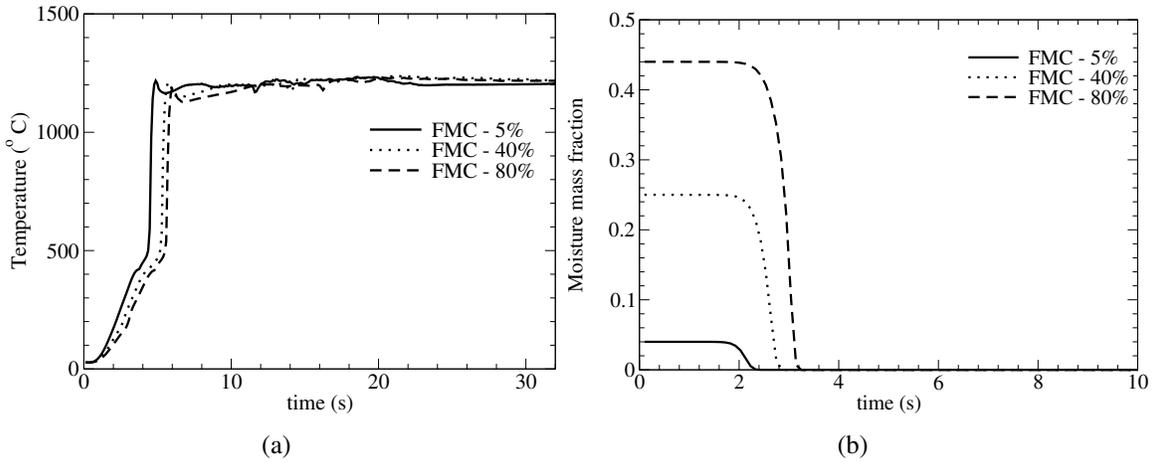


Figure 2: Time history of (a) temperature, and (b) mass fraction of moisture at point A (see fig. 1) for three cases with an initial FMC of 5, 40 and 80%.

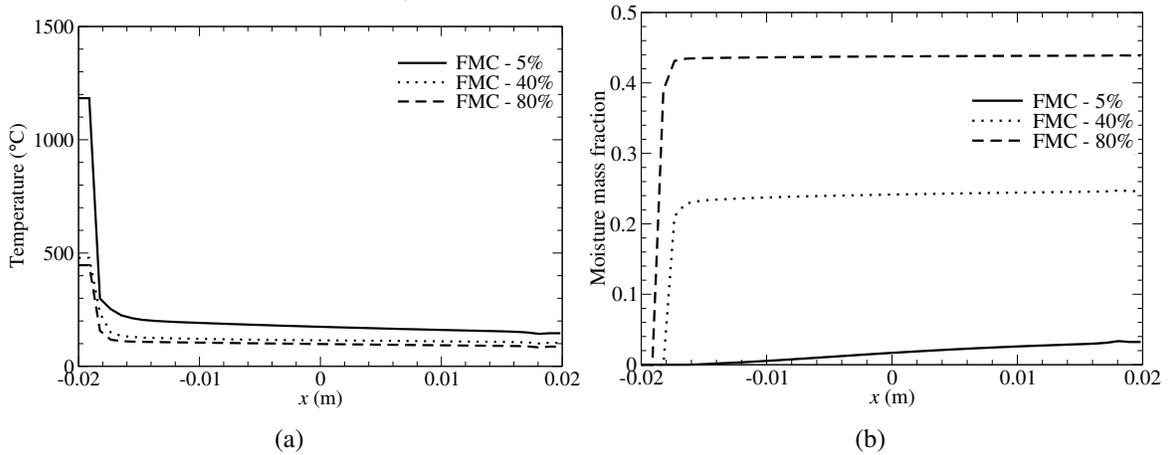


Figure 3: Variation of (a) temperature and (b) mass fraction of moisture along x at $y = 0$ and $z = 0.031$ m at time 5s in the solid phase for three cases with an initial FMC of 5, 40 and 80%.

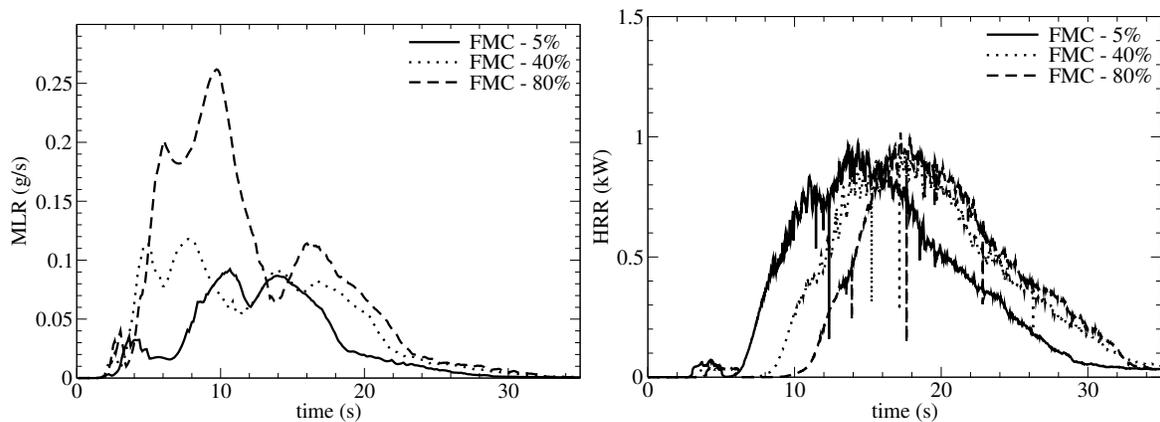


Figure 4: Time histories of (a) mass loss rate, (b) heat release rate for three cases with an initial FMC of 5, 40 and 80%.

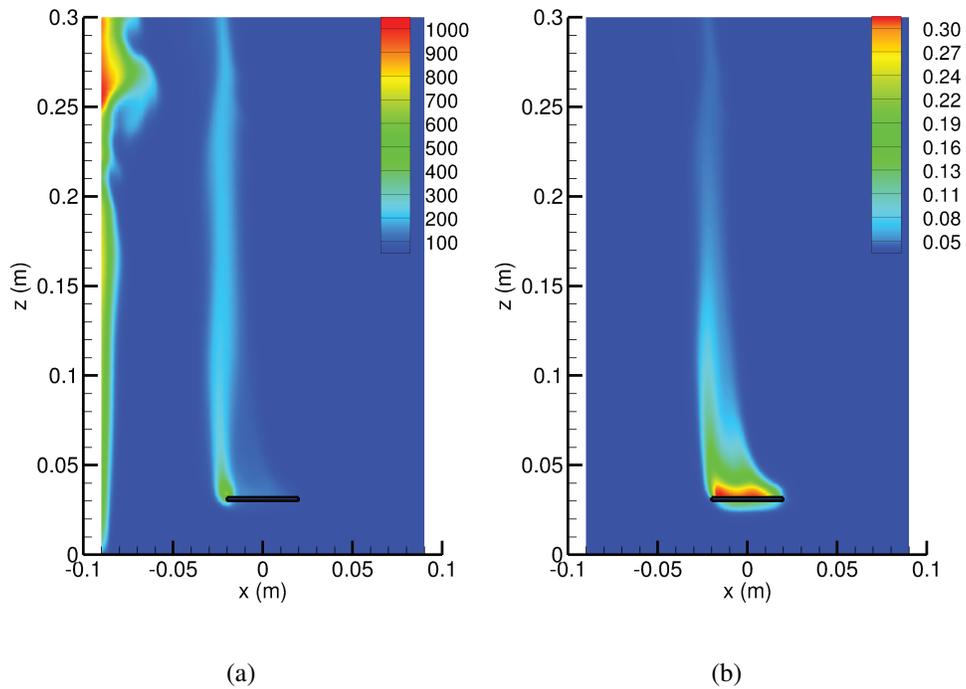


Figure 5: Color contours of (a) temperature (b) mass fraction of moisture at $t = 5$ s on an xz -slice located at $y = 0$ in the gas phase for a case with an initial FMC of 80%.

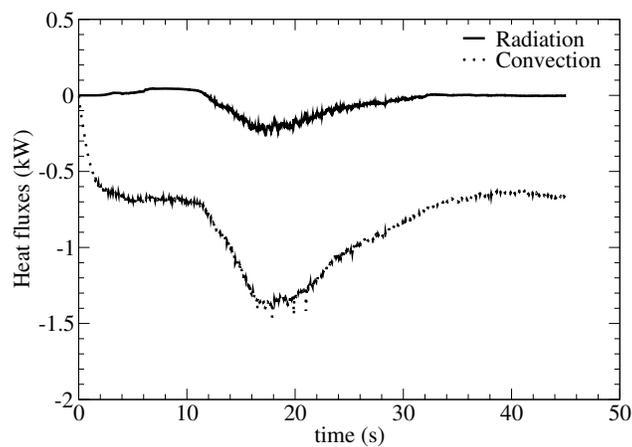


Figure 6: Time history of global radiation and convection fluxes for a case with FMC of 80%. Positive heat flux means heat is transferred from gas to solid particle and negative heat flux means vice versa.