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Modeling High Heat Flux Combustion of Coniferous Trees Using Chemically Reacting Lagrangian Particles

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Abstract: Modeling ignition and burn in high heat flux scenarios at large scales can challenge predictive capabilities of the most up to date fire simulation codes. Sandia National Laboratories (SNL) has developed a reactive flow computational fluid dynamics code known as SIERRA/Fuego. The implementation of chemically reacting Lagrangian particles within the code provides the capability to model various forms of combustible matter. Due to the variety of problems the code has evolved to model, the code has been validated for a range of laboratory-scale fire and flow tests. Recent fire experiments at SNL's Solar Tower Facility have provided data for meter-scale, high heat flux ignition fire scenarios. As part of this test series, piñon pine trees were tested. The resulting experimental data from these tests are used to demonstrate and calibrate the capability of using SIERRA/Fuego as a modeling tool to simulate ignition of coniferous trees exposed to high heat fluxes. The calibrated model from the first experiment is further tested at providing insight to some of the later tests. This work presents the capability and some limits of using SIERRA/Fuego for modeling ignition and burn at the meter-scale for coniferous trees exposed to high heat fluxes.

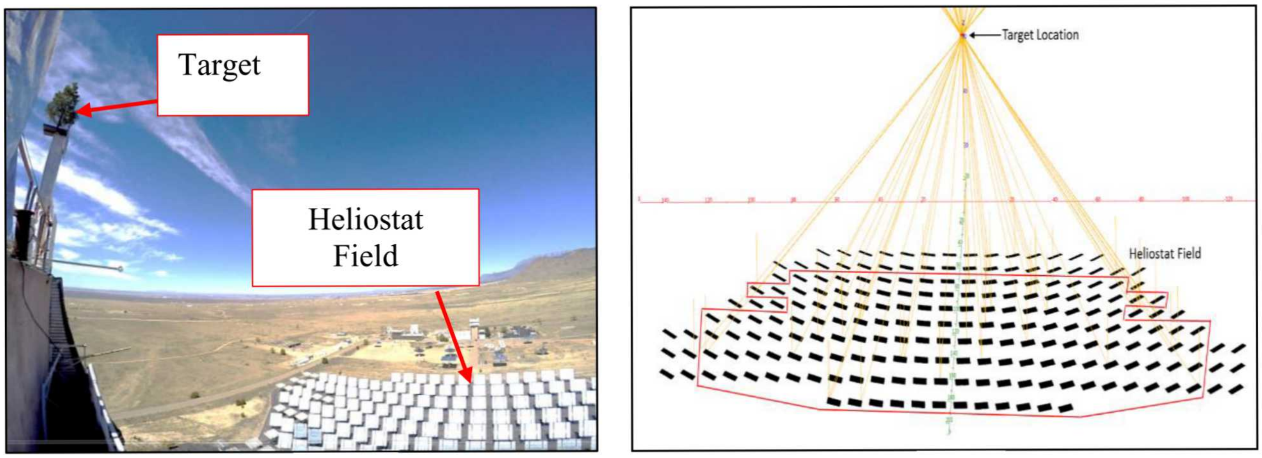
Keywords: Ignition, Fire, Coniferous Trees, Lagrangian Particles

1. Introduction

A capability of modeling ignition and burn of coniferous trees exposed to a high heat flux radiative source using Sandia National Laboratories' (SNL) tools is presented in this paper. Simulations were performed using SNL's low Mach number, reactive flow, computational fluid dynamics (CFD) code, SIERRA/Fuego. Calibration of the models was performed by comparing simulation results to experimental data where a piñon pine tree was exposed to similar heat flux and fluence profiles, also performed at Sandia National Laboratories. The results highlight key parameters to consider when attempting to properly capture the physics of a coniferous tree exposed to large radiative heat fluxes using a reactive flow CFD code. This paper begins by introducing the experimental work that provided the data set to calibrate the models presented in this paper. A general overview and key features of Fuego are subsequently presented, which is then followed by a discussion of the computational domain and boundary conditions used. Lastly, this paper ends with a discussion of the fully implemented model with respect to the experimental data.

2. Overview of Experimental Setup

The model presented here was calibrated using experimental data from high heat flux tests performed at SNL's Solar Tower, which is part of the National Solar Thermal Test Facility (NSTTF) [1]. The Solar Tower is a concentrating solar energy facility which consists of 214 heliostats that can concentrate a heat flux up to 3.5 MW/m^2 on a meter-sized spot. Figure 1 presents a layout of the facility, where Figure 1a shows an image taken from the top of the tower towards the heliostats, capturing a tree on its test stand with the heliostat field below. Figure 1b is a top view schematic of the grounds.



(a) (b)

Figure 1. SNL Solar Tower facility: (a) View from top of Solar Tower angled towards the heliostat field. (b) Ray trace schematic, where the red outline highlights active heliostats aiming at the target.

The series of high heat flux tests performed at the SNL Solar Tower were separated into Phase 0 and Phase 1. While multiple tests were performed per phase, only the tests on piñon pine trees are discussed here. The full details of all tests performed within these two test-series are not discussed in this work, but thorough discussions have been presented in separate publications [1] [2] [3]. In Phase 0, only one tree was tested, and it was used here for model calibration. In Phase 1, various trees were tested with various fluence conditions, but only the data from what is referred to as Tree #1 with fluence condition 1 is used, and it is referred to in this work as the Phase 1 tree data [1].

Figure 2 overlays the heat flux and fluence profiles imposed on the tree samples for both phases. The Phase 0 flux profile shows a gradual rise compared to Phase 1. This difference in flux profiles was a direct result of how the heat flux was imposed in each phase. In Phase 0, the heat flux was imposed as fast as the heliostats could be oriented on the target. Due to the various angular paths the heliostats take, there is a time lag before all heliostats point at the target location, and this effect results in the ramp seen on the heat flux curve in Phase 0. In Phase 1, a shroud was placed in front of the test specimen to shield it from the heat flux as the heliostats rotated to their target positions. As soon as all heliostats pointed at the target, the shroud was dropped with a gravitational acceleration plus some pneumatic assist to produce the sharper spike observed for the Phase 1 heat flux. At the end of their exposures, the overall fluence between the two phases varied by about 1 MJ/m^2. Further experimental details are discussed in subsequent sections in the context of the modeling work.

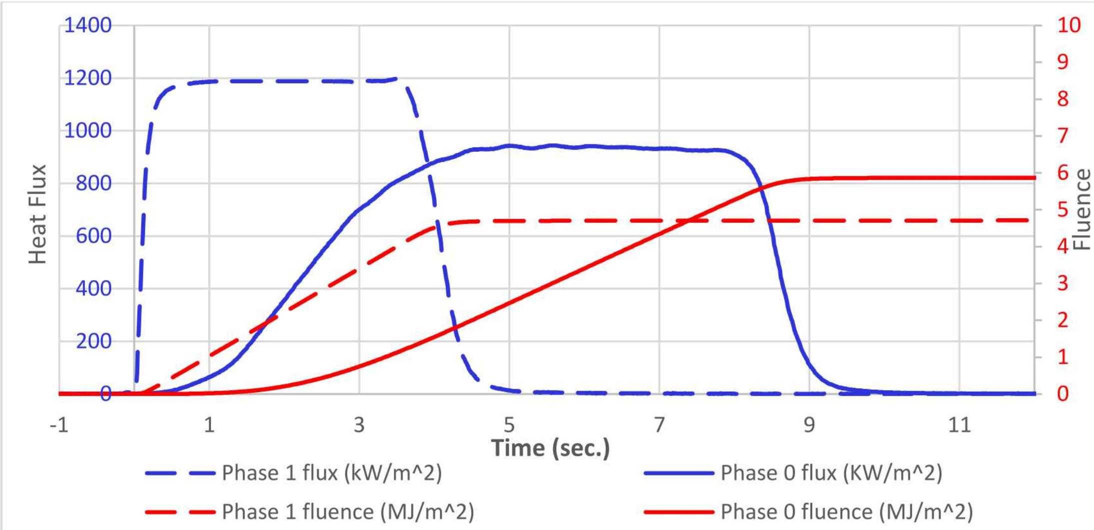


Figure 2: Heat flux (left y-axis) and fluence (right y-axis) profiles from Solar Tower tests.

3. Numerical Model

Fire simulation requires the solution of variable property, high Grashof number, turbulent, low Mach number flow. To comprehensively model combustion physics, fire modeling also needs to capture the effects of species/soot transport, radiation, and buoyancy. All of these phenomena are captured by the SIERRA multi-mechanics software development project within the Fuego and Syrinx modules, which are maintained by SNL [4]. For these reasons, Fuego and Syrinx were the computational tools used for fire simulation in this study.

To place the aforementioned tools into context, SIERRA is the SNL architecture in which Fuego and Syrinx are implemented, which is an architecture that allows for massive parallel computing, solution adaptivity, and mechanics coupling on unstructured grids. Fuego is the turbulent, buoyantly-driven incompressible flow, heat transfer, mass transfer, combustion, and soot low-Mach number CFD segregated Eulerian solver within SIERRA [4] [5]. As a segregated solver, Fuego sequentially solves the governing continuity, momentum, turbulence, and mixture fraction equations. For Time-Filtered Navier-Stokes (TFNS) simulations, as used in the work presented here, the solver repeats within a time-step in order to achieve time-step convergence. Unique to the Fuego solver is that, rather than employing the control volume (CV) method commonly used in fire CFD solvers, Fuego employs the control volume finite element method (CVFEM). In order to include soot participation in the radiation, Syrinx as adapted within Fuego is the portion that considers participating-media thermal radiation (PMR) mechanics by solving the radiative transport equation (RTE) with emission and absorption terms. In considering the angular dependence of the radiative intensity, Syrinx uses the method of discrete ordinates to numerically solve the RTE. To close the emission and absorption terms in the RTE, the Eddy Dissipation Concept (EDC) combustion model by Ertesvag and Magnussen is used for soot formation [5] [6] [7] [8]. Due to the current and future integration of Fuego and Syrinx within SIERRA, the two are referred to as just Fuego from here on.

Within Fuego, a capability exists to model chemically reacting Lagrangian particles that interact with the Eulerian domain. In order to couple the Eulerian region with the Lagrangian particles, Fuego uses a loose coupling mechanism between the two regions [4] [9]. Conservation of mass, momentum, and energy are respected for the coupled system, thus providing the capability to model combusting, evaporating and condensing particles. The loose coupling then allows the transfer of computed source terms (species, mass, energy, and momentum) between the two grids. By configuring Lagrangian particles in different arrangements, various forms of combustible matter can be modeled within Fuego. Thus, the combined features of the Lagrangian particles within Fuego were used to simulate coniferous trees. The configurations and geometries used to represent the trees studied in this work are discussed in the next sections.

For further details on the methods and models implemented within Syrinx and Fuego, specifics are found in the Fuego user and theory manuals [4] [5].

4. Computational Environment for the Model

4.1. Domain

The computational approach used for this work was to place tree representations composed of Lagrangian particles in the center of a cubic domain as shown in Figure 3. The figure also captures the mesh used for the modeling work presented here. The mesh is a hex mesh created with CUBIT 15.2 using a dual bias scheme along all edges [10]. The dual bias scheme provides the benefit of a higher mesh resolution towards the center of the domain, which is the region where the tree was placed. The mesh element-size ranged from 6 cm to 25 cm, producing a total of 98,000 elements on a cubic domain with a side length of 6.35 m. This scheme thus yielded a less computationally expensive domain by only refining near the principle region of interest.

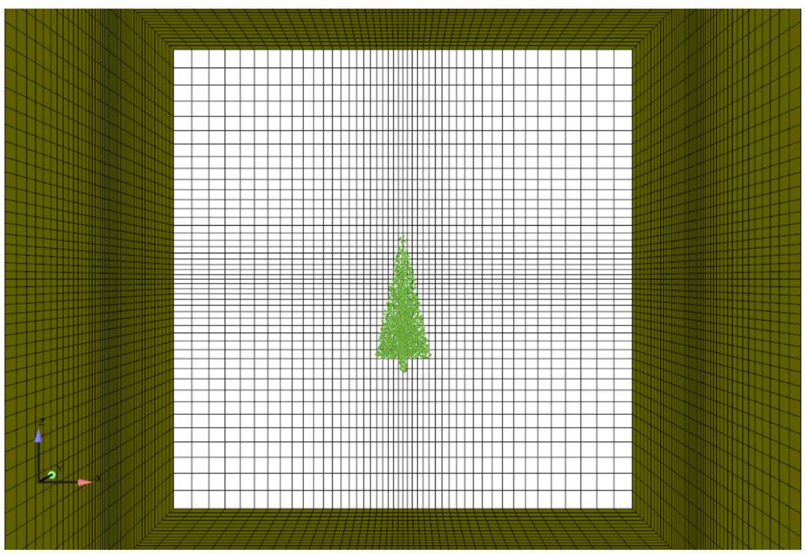


Figure 3: Interior of meshed domain showing with tree representation.

4.2. Boundary Conditions

To simulate the imposed heat flux in Fuego so that it resembled the configuration at the Solar Tower, Figure 4 shows a deconstructed domain with corresponding boundary conditions. Figure 4a shows how a hot wall boundary condition was used in the radiation solve to obtain a radiative flux on the test specimen. The remaining boundaries were set as non-absorbing/emitting. For the fluid solve, a no-slip boundary condition was always considered on the bottom wall. The remaining five sides of the domain were set as ambient temperature open boundaries.

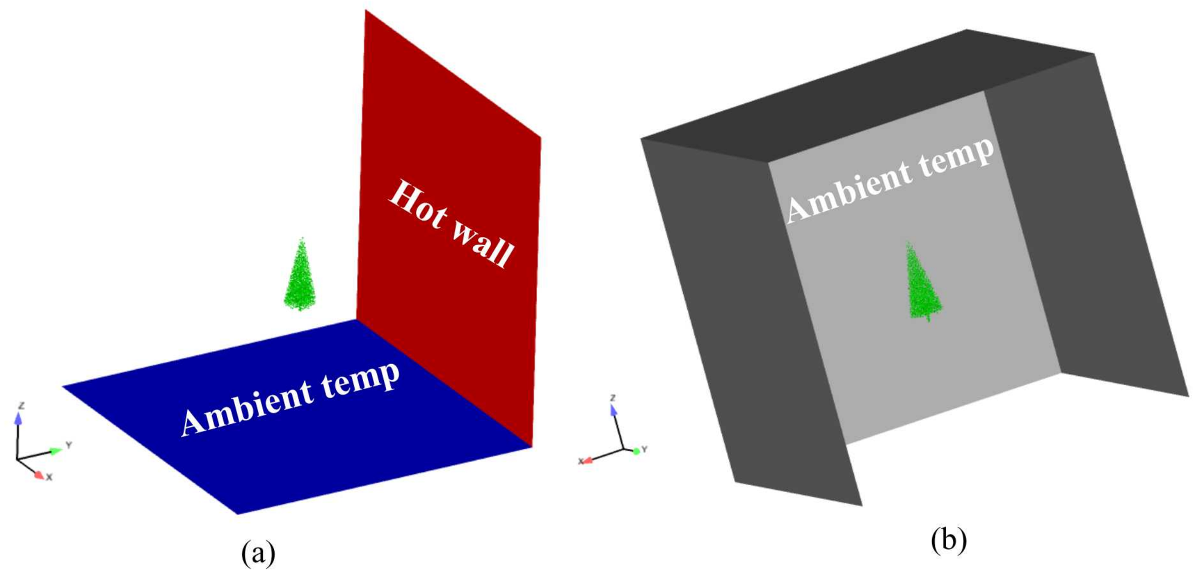


Figure 4: Radiation boundary conditions of computational domain.

In order to calibrate the heat flux profile imposed by the hot wall on the target to replicate the flux seen by the experimental trees, a 0.9 m by 1.5 m sheet was used as the calibration target area. Figure 5 illustrates this scenario, where the normal component of the incident heat flux on the target area was obtained as a function of the hot wall temperature. Consequently, for the tree simulations, the calibrated heat flux represented a normal flux that would be imposed on a rectangular plane at the center of the tree without interference from its branches. Due to how the incident heat flux was measured for the experimental setup (Figure 2), the computational flux and fluence were expected to be representative of the experimental flux and fluence.

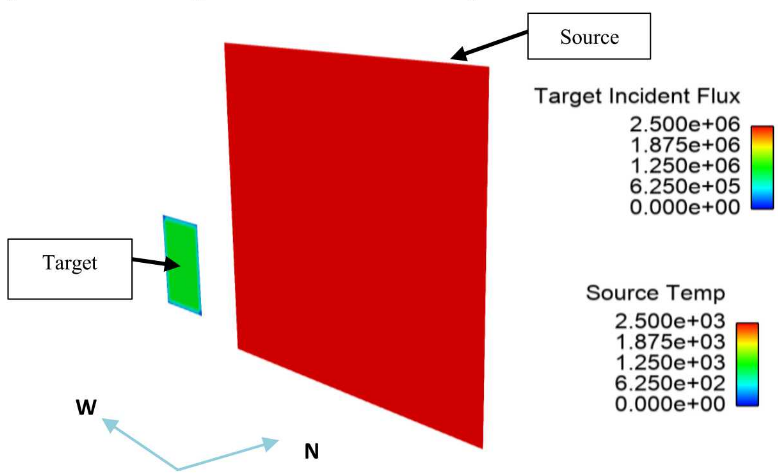


Figure 5: Sample calibration of computational model.

4.3. Tree Representations

The test specimens used in the experiments were piñon pine trees, where their physical diameter and height measurements were defined as shown in Figure 6a. To create the computational representations in Fuego, a specified number of Lagrangian parcels were dispersed within a conical volume. These parcels represented a prescribed number of particles in order to minimize computational expense. To capture the physical characteristics of the tree modeled for this analysis as best as possible to the experimental trees, the simulated tree was constructed using three main sections. As illustrated by the schematic in Figure 6b, parcels of different sizes filled three sections of the simulated tree: (1) A needles-section defined by parcels that fill a conical volume which conforms to the outer dimensions of the experimental tree's crown; (2) a branches-section defined by parcels that fill a conical volume with the experimental tree's height but with a radius that is 90% of the experimental tree's crown; and (3) a cylinder-cone combination to represent the trunk, where the diameter and height of the cylinder correspond to the experimental tree's base. A specified percentage of the volumes for each section are filled with parcels using a quasi-random number generator (Sobol sequence) to produce the parcel positions within the three sections. The needles cone and branch cone are distinguished from each other by the parcel size distribution; the needles cone is loaded with a relatively large number of smaller parcels, and the branches cone consists of a relatively small number of larger parcels, all sampled from a uniform distribution. Figure 6c shows the resulting computational representation for the tree, where needles are represented by the green parcels, and the branches and trunk are represented by brown parcels.

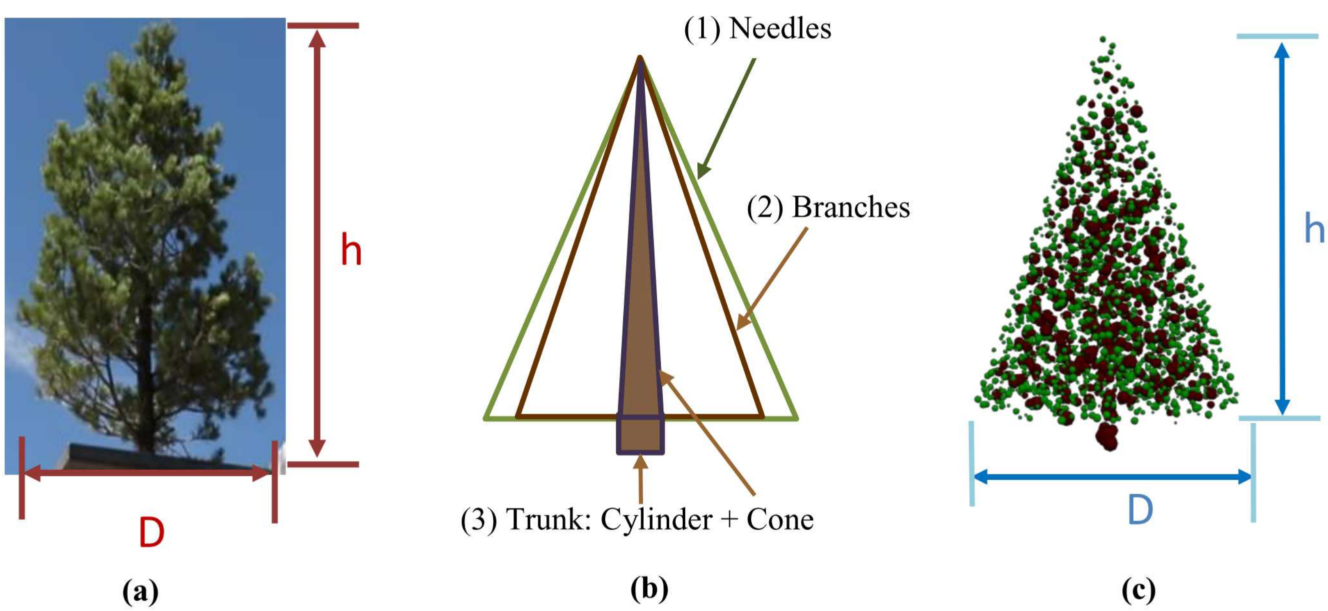


Figure 6: Tested trees. (a) Actual tree showing measured dimensions, (b) schematic of computational tree showing three primary regions, and (c) Lagrangian particle representation of tree as implemented in Fuego.

5. Discussion of Computation Model

5.1. Model Calibration

As previously mentioned, the Phase 0 Solar Tower tests were used to develop a calibrated model. Figure 7 shows the Phase 0 heat flux and fluence imposed on the trees, where the computational peak flux reached was ~940 kW/m^2 while the total fluence attained was ~5.7 MJ/m^2. Experimental fluence was ~5.8 MJ/m^2. A primary goal of developing a calibrated model was to arrive at an adequate representation of a tree using Fuego. Since the initial number of particles chosen to represent a tree was somewhat arbitrary, it also became of interest to understand the effect of modeling a given tree with varying numbers of particles as part of the calibration effort.

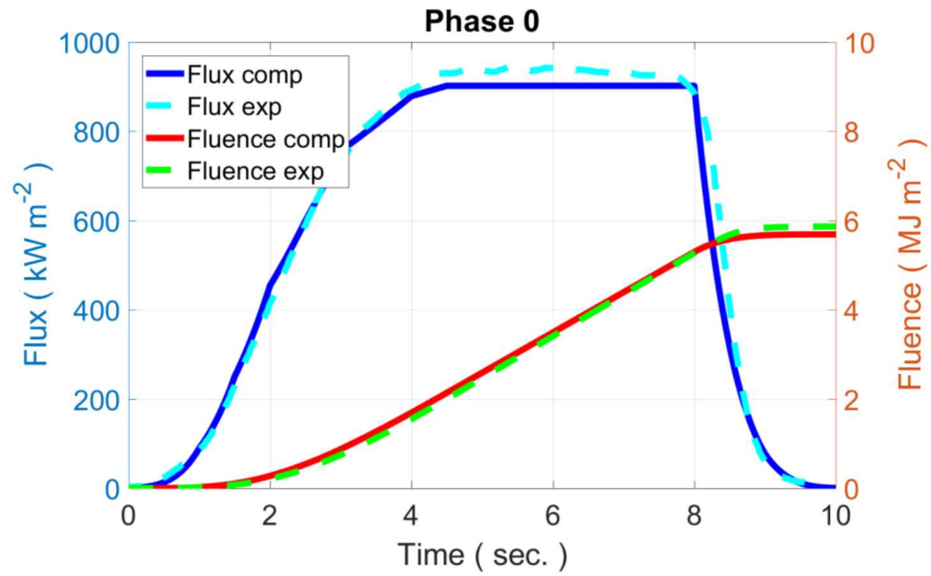


Figure 7: Computational and experimental flux (left y-axis) and fluence (right y-axis) profiles for Phase 0 test conditions.

To keep the computational and physical trees analogous, three characteristics were matched between the two: (1) The outer dimensions as outlined by Figure 6, (2) the ratio of the combustible surface area to the conical volume occupied by the outer dimensions of the tree, and (3) the total mass of the tree. The tree tested in Phase 0 measured 0.61 m in lower branch diameter and had a height of 1.47 m. The measured surface area to volume ratio was approximated to be 33 m^{-1}, and the total mass of the tree was 3.5 kg. These values were all maintained in the computational tree.

The Lagrangian particles used for the tree representations are implemented in Fuego as a combination of dry-fuel and water, where octane was used as the representative fuel source in this work. To simulate biomass pyrolysis of the particles, a multi-step reaction model [11] producing tar, char, volatiles, and moisture evaporation was used. To handle combustion of the pyrolysis gases, thermophysical properties of octane/air combustion gases were used as obtained from Cantera [12], an open-source chemical kinetics software. To further maintain consistency between the computational tree and the physical tree, the needles-particles and branches-particles were treated with different fuel/water compositions. A study by the U.S. Forest Service (USFS) on Ponderosa pine trees from the Sierra Nevada mountains shows that the water content of tree constituents varies throughout the year as well as spatially throughout the tree [13]. In this same study, the lowest moisture percentages observed for these pines were 45% and 50% for the twigs and needles, respectively. As a comparison, a post-test study done on combined branch-needle samples for the Phase 1 trees showed that the average moisture content for those piñon pines varied between 51%-57%. While the values from the USFS study were used as a starting point for dry fuel and water proportions in the model, the compositions were tuned to calibrate the model to match the extinguishing time of the experiment. The tuning was performed by iterating through various dry-fuel/water proportions for the branches and needles while maintaining the three physical characteristics mentioned in the paragraph above at constant values.

The general trends in this composition study were that larger proportions of dry fuel per particle resulted in longer burn times as determined by the $\gamma\chi$ parameter within the EDC ignition model. Generally speaking, $\gamma\chi$ is bounded between [0,1] and is an indicator of species (both reactants and products) concentrations in the reaction zone area. A $\gamma\chi$ value of 1 represents optimal species concentrations which will maximize the reaction zone area, and a value of 0 represents prohibitive species concentrations which would prevent reaction zone formation. Any values of the $\gamma\chi$ parameter greater than zero are indicative of ignition [4] [5]. Further details of the $\gamma\chi$ parameter and the EDC model are provided in the Fuego Theory manual [5].

After extensive exploration on the proportions of dry-fuel and water content for the different sections, the composition that most closely matched the extinguishing time of the Phase 0 experiment (~48 sec. after initial exposure) was 25.5% water for the branches and 30.5% for the needles when using the Phase 0 conditions (tree characteristics plus boundary conditions). While these percentages differ from what is suggested by the USFS study, variations were expected as the trees are modeled with randomly dispersed particles where conduction heat transfer from particle to particle is not considered in the model presented here. This identifies particle-to-particle conduction as something that could be implemented in future work since the capability has recently been developed within Fuego [9]. However, even though the composition calibrated for the computational tree didn't quite match the composition suggested by the USFS study, the computational model maintained the five percent moisture difference between the needles and twigs in order to respect the differences suggested by the study.

Once an initial model was obtained with a fixed number of particles, the effects of varying the total number of particles used for a single tree representation was studied. The metrics used in this particle study were similar to the initial calibration: (1) Extinguishing times as determined by the $\gamma\chi$ parameter within the EDC ignition model; and (2) mass loss, where Fuego's built-in capability of tracking particle mass was used.

Figure 8 shows mass loss results for a tree represented with anywhere between 45,000 and 80,000 particles. Several effects can be noticed from this analysis. First, it shows how the total mass loss was relatively similar between the various tree representations at about 28% (based on initial, full-tree mass), varying by only a fraction of a percent between the different representations. Furthermore, when studying the back portion (the south half) of the tree, a similar effect was shown with an approximate 9% mass loss (based on initial mass of back portion), where variations were also only a fraction of a percent. Ignition analysis for the different representations also showed similar results. For tree representations between 45,000 particles and 80,000 particles, extinguishing occurred near 48 seconds as determined by the $\gamma\chi$ parameter implemented in Fuego. These combined results were an indicator that the combustion physics of the tree were being captured in a similar fashion as long as: (1) the ratio of total parcel surface area to the volume of cone is maintained constant, (2) the tree mass and dimensions are preserved, and (3) the same flux/fluence and boundary conditions are imposed. Simulations modifying these latter parameters showed that modifying either one of them would produce different results. A preliminary study on the mesh resolution used also identified it as an important parameter. However, a formal mesh sensitivity study was not performed, but it is recommended as future work in order to better quantify its effect. From here on, the model discussed above, which was developed using data from the Phase 0 tree, will be referred to as the calibrated model.

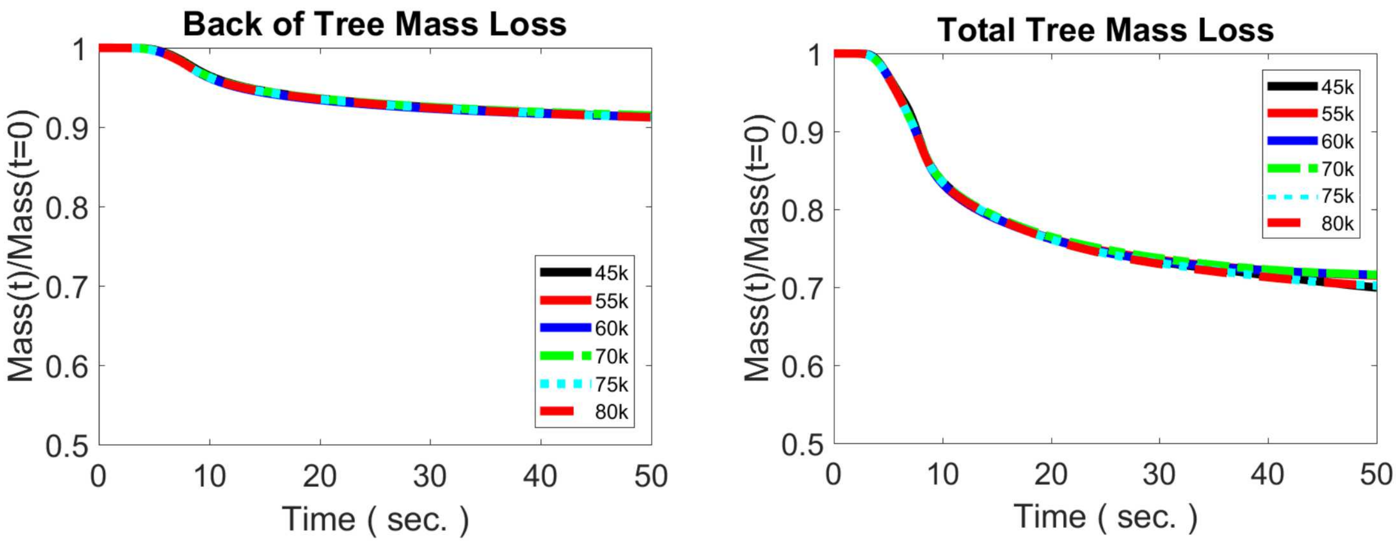


Figure 8: Mass loss on calibrated tree.

5.2. Using the Calibrated Model

Previous work from Martin et al. has shown that fluence thresholds for ignition decrease as the imposed heat flux increases [14] [15]. This correlation entails that, for a given fluence, the probability of sustaining ignition increases at higher heat fluxes. The Phase 0 tree used for the calibration model saw ignition and sustained it beginning at a fluence slightly under 2 MJ/m^2. Thus, when analyzing the flux/fluence profiles imposed on the Phase 1 tree (Figure 2 & Figure 9), sustained ignition would have been expected near the 2 second mark, at the latest. However, while some ignition was observed in the Phase 1 test, the tree did not experience prolonged ignition.

Due to the unexpected outcome of the test for Phase 1, the Phase 1 data were not used to test the calibrated model. Instead, the calibrated model was used to understand the Phase 1 outcome. Three main observations were noted in the Phase 1 test that were speculated to have caused the unexpected outcome: (1) Wind direction, (2) wind speed, and (3) a possible increased water composition in the trees. Therefore, the calibrated model was used on a tree with the Phase 1 tree dimensions to provide preliminary insight on these potential factors of influence.

Figure 10 shows the effects of varying wind and moisture composition on the Phase 1 computational tree by showing the incident flux experienced by the outer portion of the tree at its central height. To place this figure into perspective, all simulations had the imposed heat flux coming from the north end. For the no-wind condition, combustion and soot formation (participating media) due to ignition cause fluctuations on the flux observed by the tree surface. If a 2 m/s wind blowing in the south direction is considered, the imposed flux sees negligible fluctuations as participating media is blown away from the heat source. When the wind is switched to blow at the same speed but towards the north, significant attenuation is observed as soot blows towards the heat source. These results show how participating media, produced from the igniting tree, can directly reduce the heat flux experienced by the tree.

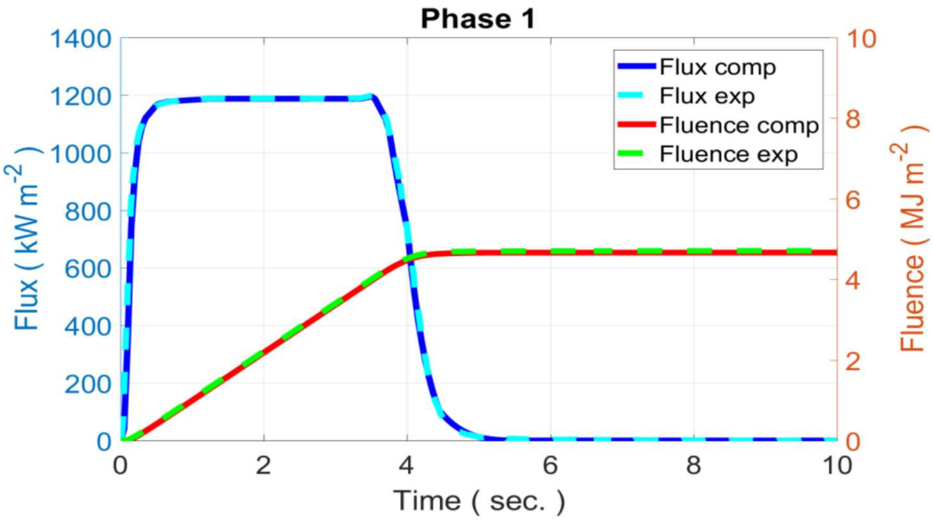
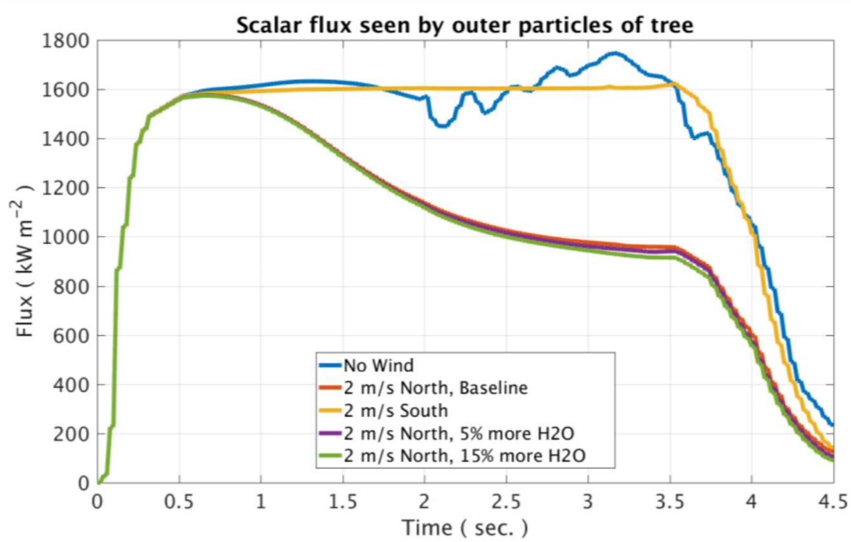


Figure 9: Computational and experimental flux (left y-axis) and fluence (right y-axis) profiles for Phase 1 test conditions.



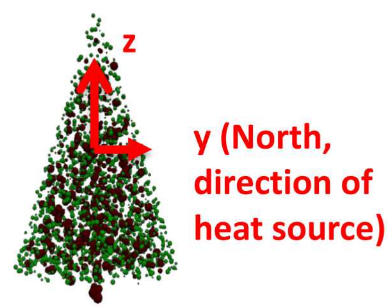


Figure 10: Study on the effects of wind and added moisture to particle composition.

The work of Martin and Dombrovsky et al., however, show that water droplets (suspected to be in the emitted products of the Phase 1 tree during testing) can attenuate radiation more effectively via scattering [16] [17]. While this modeling effort did not incorporate scattering by water droplets, the study shown in Figure 10 gives insight as to how active participating media blown in the direction of a radiative heat source can significantly attenuate the incident flux on a target, which was shown by the effect of soot as discussed above. It should also be noted that Fuego can overestimate drag and therefore skew the effect of wind due to how drag is calculated within the code. The overestimation of drag is further seen when extending these models of a single tree to a forest stand, but that effort is discussed separately [18]. In this work, however, the overestimation of drag is mitigated by studying cases with low wind velocities. Nonetheless, these wind and moisture studies, combined with the work of Martin and Dombrovsky et al., suggest that an increase in tree moisture composition, plus the effect of wind blowing towards the heat source, could explain the ignition discrepancy of the Phase 1 tests when compared to Phase 0. However, further testing would be needed to corroborate these arguments.

6. Conclusions

This paper outlines the capability of using SIERRA/Fuego as a tool for modeling meter-scale ignition and burn of biomass exposed to high heat flux scenarios, specifically in the context of coniferous trees. Calibration of using Fuego in this effort was performed by using experimental data for a piñon pine tree exposed up to a ~1 MW/m^2 heat flux, where the data was acquired from various high heat flux tests performed at SNL's Solar Tower facility. The computational trees used for the modeling effort presented here were created using arrangements of chemically reacting Lagrangian particles within Fuego. The studies discussed here show a methodology that highlight key parameters to keep in mind when modeling coniferous trees using Lagrangian particles, and they are: (1) The ratio of total particle surface area to the volume of a tree, (2) the tree dimensions along with total mass, and (3) the boundary conditions used (should be representative of the attempted scenario). These key parameters were identified from performing mass loss studies on different configurations. This paper ends with a discussion on how the calibrated model developed was further used to provide insight on subsequent testing that resulted in unexpected outcomes. This latter study showed how participating media produced from a combusting tree could significantly attenuate the effects of an incident radiative heat source. The work presented here helps motivate future efforts, and extensions of the model presented here should consider properly accounting for drag when using Lagrangian particles within Fuego. The work of Pierce et al. [9] could also be expanded to these models to capture the conduction between particles in order to more closely represent heat transfer within connected biomass such as tree branches. A mesh sensitivity study is also recommended to help identify any mesh dependencies.

7. Acknowledgements

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