

ADVANCES IN FOREST FIRE RESEARCH

2022

Edited by
**DOMINGOS XAVIER VIEGAS
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Large eddy simulations of the structure of spreading line fires at flame scale

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Keywords

Fire behavior; Flame spread; Particle burning rate model; Pyrolysis; Computational Fluid Dynamics

Abstract

Our general objective in the present study is to develop tools to better describe the coupling between solid phase and gas phase processes that control the dynamics of flame spread in wildland fire problems. We focus on a modelling approach that resolves processes occurring at flame scales, i.e., the formation of flammable vapors from the biomass vegetation due to pyrolysis, the subsequent combustion of these fuel vapors with ambient air, the establishment of a turbulent flow because of heat release and buoyant acceleration, and the thermal feedback to the solid biomass through radiative and convective heat transfer. The modelling capability is based on a general-purpose Computational Fluid Dynamics (CFD) library called OpenFOAM and an in-house Lagrangian particle model that treats drying, thermal pyrolysis, oxidative pyrolysis and char oxidation using a one-dimensional porous medium formulation that allows descriptions of thermal degradation processes occurring during both flaming and smoldering combustion.

The modelling capability is calibrated for pine wood and is first applied to simulations of fire spread across a surrogate vegetation bed corresponding to thin, monodisperse, cylindrical-shaped sticks of pine wood with prescribed particle and environmental properties (i.e., bed height, surface-to-volume ratio, packing ratio, moisture content, and wind velocity). While the model can be used in sloped terrain, the present simulations are limited to a flat ground surface. The current emphasis is on determining threshold conditions for successful spread, differences between the plume-dominated and wind-driven flame regimes, possible transitions to a steady or time-dependent flame structure, and differences in the relative weights of the flaming and smoldering regions.

1. Introduction

The dynamics of wildland fires involve multi-physics phenomena occurring at multiple scales. Computational Fluid Dynamics (CFD) models have the potential to provide detailed information on the interactions between physical phenomena occurring at all these different scales. However, because of computational cost, the domain of application of CFD models is typically limited to a particular range of scales. Thus, current CFD-based wildland fire models are scale-specific and belong to one of the following three classes: combustion solvers aimed at describing the coupling between pyrolysis, combustion, radiation and flow occurring at the vegetation and flame scales (Porterie *et al.* (2000), Morvan and Dupuy (2001), Morvan and Dupuy (2004), Fire Dynamics Simulator (FDS), Verma *et al.* (2022)); wildfire solvers aimed at describing the coupling between combustion and flow occurring at fireline scales and/or geographical scales (Linn and Cunningham (2005), Canfield *et al.* (2014), Mell *et al.* (2007)); and atmospheric boundary layer solvers aimed at describing the coupling between combustion and flow occurring at meteorological scales (Clark *et al.* (2004), Mandel *et al.* (2011), Kochanski *et al.* (2013), Coen *et al.* (2013), Filippi *et al.* (2009), Filippi *et al.* (2013)).

We focus in this study on the development of a combustion solver aimed at describing the physics of wildland fire spread at flame scale. The solver couples a one-dimensional, Lagrangian-based, solid particle model that describes the biomass vegetation phenomena (drying, pyrolysis, char oxidation) with a three-dimensional, Eulerian-based, CFD model that describes the gas phase phenomena (flow, combustion, radiative and convective heat transfer processes). The gas phase model uses a Large Eddy Simulation (LES) approach and is based on a general-purpose CFD library called OpenFOAM. The Lagrangian particle model uses an in-house solver developed both for fast one-dimensional simulations of flame spread (Forthofer *et al.* (2022)) and for

detailed LES simulations of the flame structure in wildland fire configurations. The model considers the particle as thermally-thick and composition-thick and includes descriptions of thermal degradation processes occurring during both flaming and smoldering combustion.

2. Numerical Model

The vegetation bed is treated as a population of porous particles, which can have different geometries and different sizes. Each porous particle is described as a system with a solid phase and a gas phase, which allows for a detailed treatment of the particle-to-external-gas outflow of volatile mass and the external-gas-to-particle diffusion of oxygen mass; this detailed treatment is required to account for in-depth oxidative pyrolysis and char oxidation. We consider here thermally-thick and composition-thick particles featuring in-depth variations of temperature and composition. The particles geometry can be modelled as rectangular (leaves or sticks), cylindrical (needles or stems) or spherical (embers or firebrands).

2.1. Lagrangian particle model

In the Lagrangian viewpoint, the thermo-chemical degradation of each porous particle is tracked individually in space and time. We consider each porous particle to experience four heterogeneous (gas/solid) reactions: a drying reaction; a thermal pyrolysis reaction; an oxidative pyrolysis reaction; and a char oxidation reaction. We follow the work of Lautenberger and Fernandez-Pello (2009) by describing the particle as a matrix of pores featuring a solid phase and a gas phase. We discretize the porous particle into a set of one-dimensional control volumes that contain information about the porosity, thermophysical properties, chemical composition, temperature and pressure. In the following case studies, we consider thermo-chemical degradation and flame spread of pine sticks. We combine the thermophysical properties of pine wood provided in Lautenberger and Fernandez-Pello (2009) with the reaction kinetic parameters provided in Anca-Couce *et al.* (2012); this combination was found to achieve a good fit of experimental data at both micro-scale and bench-scale, as shown in the next section.

The governing equations of mass, momentum, and energy conservation inside each control volume of the porous particle are solved numerically using an implicit approach that treats convection and diffusion through a second-order, Crank-Nicolson method and chemical reaction through a first-order, backward Euler method. An in-house object-oriented C++ solver of this Lagrangian particle model was developed. This code can serve as a stand-alone solver of thermo-chemical degradation of solids, or it can be implemented into larger frameworks to model fire spread over vegetation as discussed in the following section. This code also features an adaptive time-stepping technique (for speed, stability, and robustness) and a re-meshing capability (for deforming particles due to swelling or shrinking).

2.2. Vegetation bed model

In order to describe gas-solid mass, momentum and energy exchanges in simulations of fire spread across a given set of porous vegetation layers, ambient air conditions and a given terrain, we developed a LES solver that couples the open-source C++ library OpenFOAM and the Lagrangian particle solver presented in the previous section.

The LES solver adopts a multiphase formulation similar to previous work proposed by Porterie *et al.* (2000), Morvan and Dupuy (2001) and Morvan and Dupuy (2004). In the current work, the Favre-filtered reactive-radiative Navier-Stokes equations are solved using a low Mach number approach. Source terms are added to the governing equations to represent the contributions of solid particles to the mass production or consumption of gaseous species, the flow momentum through a drag force, and the energy exchange through radiative and convective heat transfer. These source terms are treated as subgrid-scale (SGS) terms using the Lagrangian particle model and are accumulated to account for multiple particles existing inside each elementary control volume of the vegetation bed. The number of particles is determined from the fuel loading and the geometric parameters of the vegetation bed. A three-dimensional representation of a typical computational configuration is shown in Fig. 1.

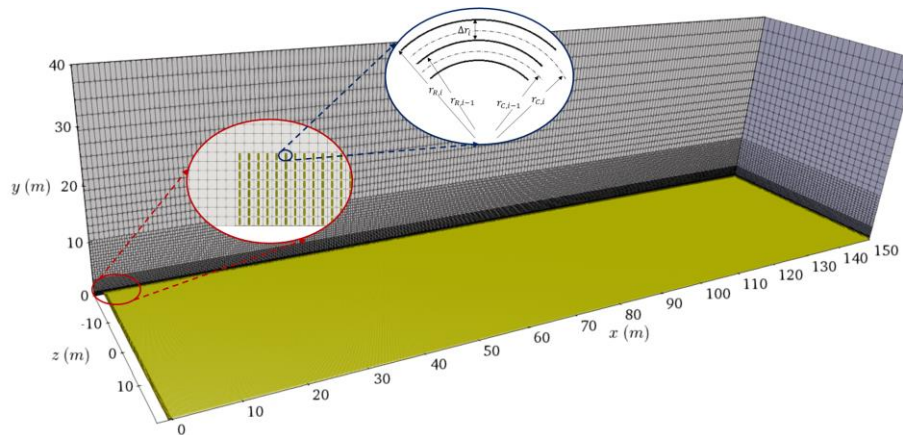


Figure 1- A view of the computational domain used in spreading line fire simulations. The solid particles are colored in yellow. A zoom into the 1D cylindrical mesh used for individual solid particles is shown.

The solver can leverage various SGS turbulence models implemented in the native OpenFOAM library. We use the WALE model proposed by Nicoud and Ducros (1999). The homogenous combustion of the gaseous fuel produced by pyrolysis reactions is treated by assuming a global reaction equation and using a modified version of the Eddy Dissipation Model (Magnussen and Hjertager (1976)) that we recently developed to account for the variations of the laminar diffusion characteristic time with LES filter size. The solver also features a radiation model based on a multi-phase radiative transfer equation (MRTE) that includes absorption/emission by the solid particles and by the gases (Consalvi *et al.* (2002)); the MRTE is solved using the finite volume Discrete Ordinate Method (DOM) implemented in the OpenFOAM library. The radiation absorption/emission by the gases is modeled by either a Prescribed Global Radiant Fraction (PGRF) approach or a Weighted-Sum-of-Gray-Gases (WSGG) model (Ahmed and Trouvé (2021)). The PGRF approach is adopted in the present study in the flame region, while the absorption and emission in the plume region are calculated using Plank-mean absorption coefficients of CO_2 and H_2O . Convective heat transfer is modeled using empirical Nusselt number correlations developed for a wide range of Reynolds numbers under no blowing conditions (Churchill and Bernstein (1977)). The blowing effect due to outflowing volatiles is accounted for through a Couette flow approximation (Lautenberger and Fernandez-Pello (2009)). The vegetation bed drag force is modeled using a drag coefficient that has been determined experimentally for isolated particles in crossflow (Mueller (2012)). It should be noted that there might be some uncertainties in the choices of the drag coefficient and the heat transfer coefficient, and more elaborate models that represent actual vegetation patches may be required.

3. Results and Discussion

3.1. Bench-scale validation of the Lagrangian particle model

We present here validation results of the Lagrangian particle model introduced in section 2.1. Numerical simulations were performed for a single particle exposed to prescribed heating conditions. The spatial resolution inside the particle is 0.1 mm. The first set of simulations corresponds to the experiment of Anca-Couce *et al.* (2012) in which a micro-scale pine wood sample is exposed to a heating rate of 5 K/min, while the second set of simulations corresponds to the experiment of Kashiwagi *et al.* (1987) in which a 3.8 cm-thick white pine sample is exposed to an irradiation intensity of 40 kW/m². Both sets of experiments consider different nitrogen-air atmospheres and thereby evaluate the ability of the model to correctly describe the contributions of oxidative pyrolysis and char oxidation. Figure 2 shows that the model predictions in terms of particle mass evolution and spatial distributions of temperature inside the particle are in very good agreement with the experimental data at both micro- and bench-scales.

3.2. Flame scale simulations of quasi-infinite line fires

We now turn to LES of a quasi-infinite line fire over a surrogate vegetation bed corresponding to vertical cylinders made of the same pine wood material tested in the previous section. A computational domain with periodic boundary conditions on the lateral sides is used to mimic quasi-infinite line fires. As shown in Fig. 1, the computational domain has a cross-section of 40 × 40 m². The vegetation bed of pine wood cylinders starts

at 2 m from the domain entrance and extends to a length of up to 150 m to achieve steadily-propagating line fires. Preliminary tests show that a shorter domain that extends to only 50 m is sufficient to achieve steadily-propagating plume dominated fires. The pine wood cylinders have a diameter of 2 mm and a total height of 0.4 m. The packing ratio and the surface-to-volume ratio of the vegetation bed are 0.005 and 2000 m⁻¹, respectively, which give a radiation absorption length-scale of about 0.4 m (Consalvi *et al.* (2002)). The initial moisture content of the fuel bed is 5%. The composition of the gaseous fuel produced from thermal and oxidative pyrolysis reactions is assumed to be C_{3.4}H_{6.2}O_{2.5} with a heat of combustion of 15.6 MJ/kg and a global radiant fraction of 0.35. External wind velocity is imposed at the domain's west boundary using a power-law profile with a nominal velocity evaluated at an elevation of 2.0 m. Turbulence fluctuations are introduced corresponding to 10% intensity. Ignition is achieved using a hot plate placed underneath the fuel bed. The plate has a length of 0.5 m and a temperature of 1600 K and is activated for 5 seconds.

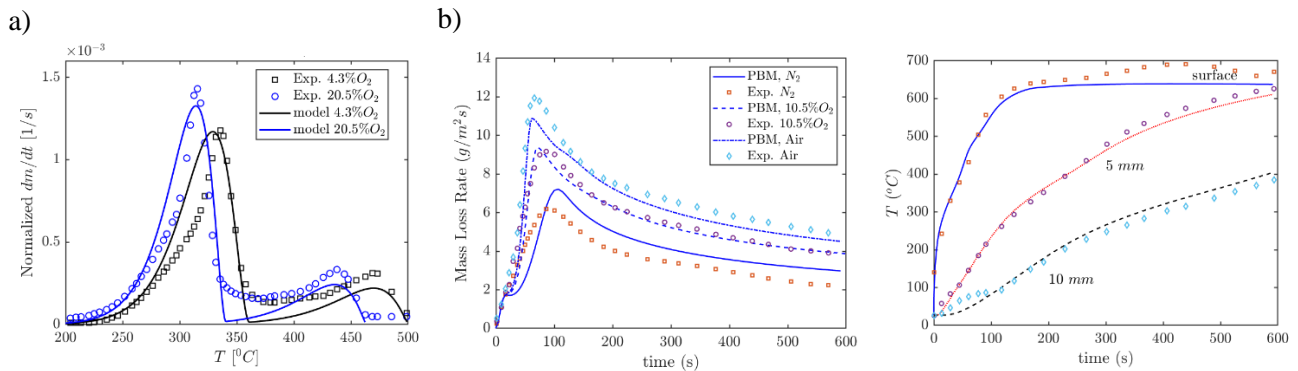


Figure 2- Series of validation tests of the Lagrangian particle model calibrated for pine wood: a) Mass loss rate in different atmospheres in micro-scale experiments taken from Anca-Couce *et al.* (2012) (5 K/min heating rate); b) Mass loss rate and surface/in-depth temperatures in different atmospheres in bench-scale experiments taken from Kashiwagi *et al.* (1987) (40 kW/m² irradiation).

The computational domain is divided into 4 regions with cells of equal size in the x - and y -directions: the grid resolution in the vegetation bed region from the ground to 0.8 m elevation is 0.1 m; the grid resolution in the flame region between 0.8 and 3 m elevation is 0.2 m; and the grid resolution in the plume region between 3 and 10 m elevation is 0.4 m; the grid resolution in the far-field region above 10 m elevation starts from 0.2 meters and is slowly decreased with elevation through stretching. The grid resolution in the span-wise direction (z -direction) is twice that in the x - and y -directions. The total number of grid cells is about 3.6 million with approximately 1.2 million particles. The time-step is controlled using a Courant–Friedrichs–Lewy condition and is of the order of ~ 0.001 s. The radiation field is updated every 5 time-steps using 144 solid angles. The simulations are carried out on a distributed-memory parallel cluster using Message Passing Interface (MPI) technique. A simulation of 60 seconds fire spread requires 96 hours using 160 processors (~ 15 kCPU hours).

We present here results from two cases corresponding to nominal wind speeds of 1.0 and 5.0 m/s. The corresponding Byram's convection number is 79 and 1.5, respectively. These two conditions are representative of the plume-dominated and wind-driven flame regimes. The corresponding values of the rate of spread (ROS) as predicted by the classical Rothermel model are 0.09 m/s and 0.34 m/s, respectively. A three-dimensional rendering of the simulated cases is presented in Fig. 3. The comparison between the left and right plots in Fig. 3 shows the expected differences between a low-wind-velocity flame that is vertical and develops above the vegetation bed and a high-wind-velocity flame that is horizontal, is attached to the ground and develops mostly within the vegetation bed. It also shows that the simulated fires feature a peak-and-trough structure (and a finger-like structure) similar to those observed in wildland fires.

Figure 4 shows the time evolution of the locations of the flame front (defined as the maximum x -location where the mixture fraction is greater than the stoichiometric mixture fraction), the back and front edges of the pyrolysis region (defined as the minimum and maximum x -locations where the pyrolysis reactions take non-zero values), and the smoldering front (defined as the maximum x -location where the char oxidation reaction takes non-zero values). The flame front location predicted by the Rothermel model is included for comparison. The simulation results show that the fireline intensity is 0.56 MW/m for the plume-dominated flame and 4.3 MW/m for the wind-driven flame; the corresponding values of the ROS are 0.082 and 0.52 m/s, respectively.

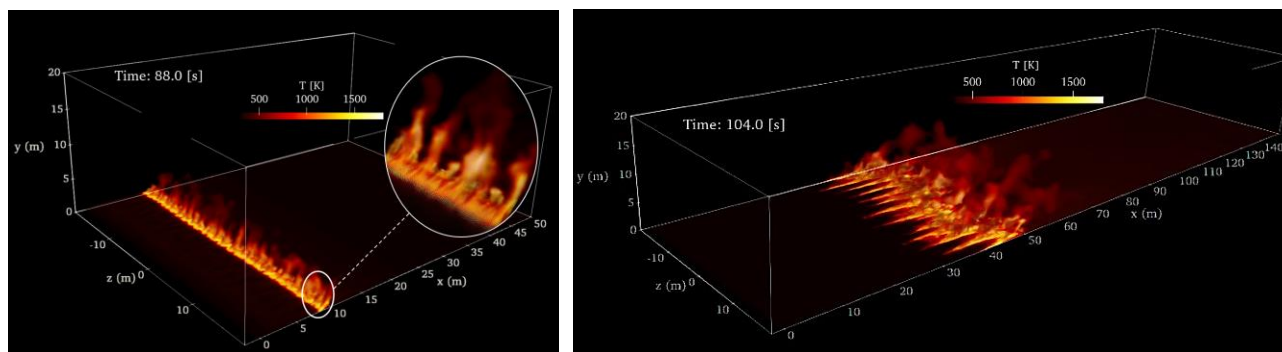


Figure 3- A 3D rendering of the structure of the line fire at a wind velocity of 1 m/s (left) and 5 m/s (right). The fire is visualized using an iso-volume of the region where the gas temperature is above 450 K.

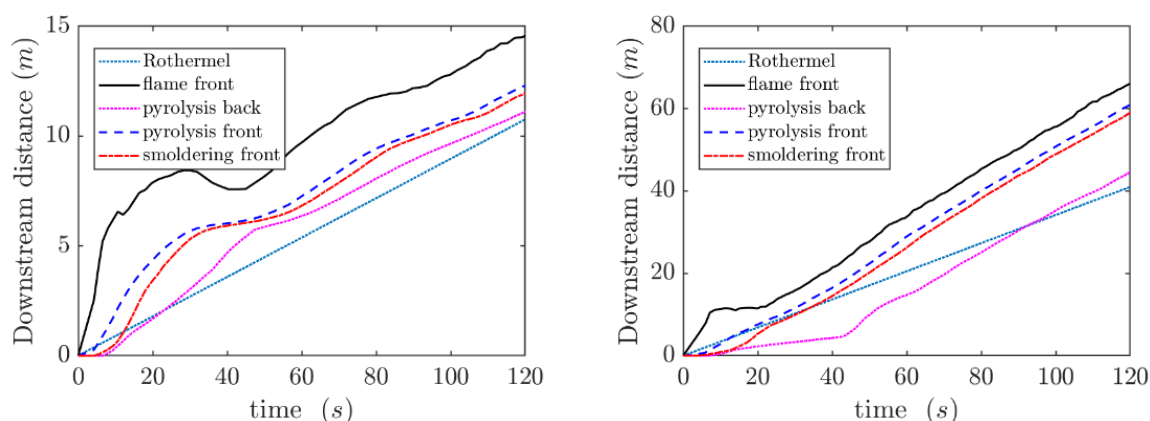


Figure 4- Time evolution of the position of the line fire at a wind velocity of 1 m/s (left) and 5 m/s (right).

4. Conclusion

This paper presents preliminary results obtained with a new modelling capability aimed at bringing fundamental information on the coupling between solid phase and gas phase processes that control the dynamics of flame spread in wildland fire problems. This modeling capability uses sub-millimetre-scale spatial resolution in the solid biomass solver and centimetre-scale spatial resolution in the gas phase solver and thereby resolves the exchanges of mass, momentum and heat associated with pyrolysis, combustion, radiation and flow at flame scales. The modeling capability is based on the OpenFOAM CFD library and an in-house Lagrangian model that treats particles as a one-dimensional porous medium and includes descriptions of thermal degradation processes occurring during both flaming and smoldering combustion.

5. Acknowledgements

This project is financially supported by the USDA Forest Service, Missoula Fire Sciences Laboratory. The project is also supported by supercomputing resources made available by the University of Maryland (<https://www.glue.umd.edu/hpcc/>) and by the US National Science Foundation (XSEDE Program, Grant #TG-CTS140046, <https://www.xsede.org>).

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