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DYNAMICS OF SHRUB FIRES INVESTIGATED VIA
PHYSICS BASED MODELING

by

AMBARISH DAHALE

A DISSERTATION

Submitted in partial fulfillment of the requirements
for the degree of Doctor of Philosophy
in
The Department of Mechanical and Aerospace Engineering
to
The School of Graduate Studies
of
The University of Alabama in Huntsville

HUNTSVILLE, ALABAMA

2014
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Submitted by Ambarish Dahale in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Mechanical Engineering and accepted on behalf of the Faculty of the School of Graduate Studies by the Dissertation committee.

We, the undersigned members of the Graduate Faculty of The University of Alabama in Huntsville, certify that we have advised and/or supervised the candidate of the work described in this Dissertation. We further certify that we have reviewed the Dissertation manuscript and approve it in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Mechanical Engineering.

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ABSTRACT

School of Graduate Studies
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Degree: Doctor of Philosophy College/Dept.: Engineering/Mechanical and Aerospace Engineering

Name of Candidate: Ambarish Dahale

Title: Dynamics of Shrub Fires Investigated via Physics Based Modeling

A physics based model, capable of predicting fire spread through a multiphase porous media, is formulated and described in detail. The resulting governing equations of fluid dynamics, combustion, heat transfer and thermal degradation of solid fuel, are solved using discrete numerical methods. The burning of an isolated chamise (Adenostoma fasciculatum) shrub approximately 1 m in height, similar to previously reported experimental study, was investigated using this physics based model. Global quantities including burning time, total mass consumed, time history of mass loss rate and time to reach maximum mass loss rate are found to be in good agreement with experimental results. The model is then used to explore the importance of distribution of solid fuel bulk density, fuel moisture content, thermophoresis of soot particles and flame merging on the dynamical behavior of shrub fires in quiescent atmosphere.

Results from burning of an isolated shrub indicate that the local vertical fire spread rate within the shrub increases when the shrub bulk density is distributed along its height, the distribution being consistent with field measurements, as compared to that seen in a uniform bulk density shrub. Time required to initiate the burning of shrub and the amount of mass left unburnt increased by almost a factor of 1.5 and
10, respectively, when shrub moisture content is increased from 20% to 100%. With a two fold increase in moisture content, from 40% to 80%, the fire spread rate in vertical direction is seen to reduce by a factor 0.7. Soot thermophoretic velocities are found to be negligible compared to their convective counterparts. For this reason, global predictions of fire remained unaffected even if thermophoretic transport of soot was neglected.

Fire-fire interactions are investigated by considering two different shrub arrangements; (1) two shrubs placed adjacent to each other (two-shrub); and (2) three shrubs located on the vertices of an equilateral triangle (three-shrub). All shrubs are ignited simultaneously with the aid of separate ground fuels. The peak mass loss rate and the vertical fire spread rate within a shrub decreases with an increasing shrub separation distance. At zero separation distance, heat release rate, normalized by number of shrubs, is enhanced by 5% and 15%, for the two-shrub and the three-shrub arrangement, respectively. Generation of strong vorticity, due to higher magnitudes of gravitational torque, appears to be the cause for enhanced burning in the three-shrub arrangement. This phenomena is seen to be much weaker for the two-shrub arrangement. Interactions between the individual fires cease to exist for a center-to-center distance of 1.5 and 2 times the shrub diameter for the two-shrub and the three-shrub arrangement, respectively.
ACKNOWLEDGMENTS

I would like to thank my advisors, Dr. Babak Shotorban and Dr. Shankar Mahalingam, for giving me the opportunity to explore this fascinating field of fire modeling and providing the necessary guidance during the course of my research. This work has been greatly benefited by the useful discussions I had with my committee members, professors, and colleagues. I am also thankful to the extremely friendly office staff at my university for their help. I would especially like to thank my family members, friends and others for their moral support which allowed me to pursue higher education and has always helped me overcome obstacles in life.

I would like to acknowledge National Science Foundation (Grant number CBET 1049560) and the 2013 Individual Investigator Distinguished Research Program at The University of Alabama in Huntsville (UAH) for providing the required financial support. The high performance computing (HPC) resources are provided by the Alabama Supercomputer Authority (ASA), Extreme Science and Engineering Discovery Environment (XSEDE) and the High Performance Technical Computing (HPTC) facilities at UAH.
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\( g_i \)  Gravitational acceleration vector

\( \bar{F}_{L,i} \)  Gas-phase momentum equation source term accounting for drag

\( \tilde{h} \)  Total enthalpy of the gas-phase

\( \bar{q}_i \)  Gas-phase temperature diffusion vector

\( \bar{q}_{rad,i} \)  Gas-phase radiation source term

\( X_c \)  Fraction of enthalpy, generated from char combustion, distributed between solid- and gas-phase

\( \bar{Y}_K \)  Gas-phase \( K^{th} \) species mass fraction

\( \bar{q}_{K,i} \)  Gas-phase species diffusion vector

\( \bar{\omega}_K \)  Gas-phase species chemical source term

\( p_0 \)  Background pressure, assumed equal to 1 atm

\( R_u \)  Universal gas constant

\( W_K \)  Molecular weight of \( K^{th} \) gas-phase species

\( C_{D,L} \)  Drag coefficient between gas- and solid-phase

\( Re_{d_i} \)  Reynolds number based on solid fuel particle diameter

\( \mu \)  Dynamic viscosity of gas-phase

\( \Delta h^0_{f,K} \)  Formation enthalpy of \( K^{th} \) gas-phase species

\( \bar{c}_{p,K} \)  Heat capacity of \( K^{th} \) gas-phase species

\( N_K \)  Total number of gas-phase species considered
Pr  Prandtl number
Pr_t  Turbulent Prandtl number
Sc  Schmidt number
Sc_t  Turbulent Schmidt number
σ_{ij}  Sub-grid scale viscous stress tensor
C_R  Smagorinsky constant
Σ  Flame surface density
\tilde{Z}  Mixture fraction
P_L  Filtered probability density function
ρ_B  Bulk density; solid fuel dry mass per unit volume
\bar{m}_{L,H_2O}  Water mass of L^{th}-type solid fuel particle
\bar{m}_{L,pyr}  Pyrolysis mass of L^{th}-type solid fuel particle
\bar{m}_{L,char}  Char mass of L^{th}-type solid fuel particle
T_L  Temperature of L^{th}-type solid fuel particle
\bar{q}_{conv,L}  Convective heat transfer between gas- and solid-phase
\bar{q}_{rad,L}  Radiative heat transfer between gas- and solid-phase
\bar{q}_{mass,L}  Heat transfer between gas- and solid-phase due to phase change
\bar{c}_{p,L}  Heat capacity of L^{th}-type solid fuel particle
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Nu}_L$</td>
<td>Nusselt number for $L^{th}$-type solid fuel particle</td>
</tr>
<tr>
<td>$h_c$</td>
<td>Convective heat transfer coefficient</td>
</tr>
<tr>
<td>$I_i$</td>
<td>Radiation intensity in $i^{th}$ direction</td>
</tr>
<tr>
<td>$a_g$</td>
<td>Gas-phase absorption coefficient</td>
</tr>
<tr>
<td>$a_L$</td>
<td>Absorption coefficient of $L^{th}$-type solid fuel particle</td>
</tr>
<tr>
<td>$\tilde{f}_v$</td>
<td>Soot volume fraction</td>
</tr>
<tr>
<td>$\tilde{u}_i^{th}$</td>
<td>Soot thermophoretic velocity $i^{th}$ component</td>
</tr>
<tr>
<td>$W_{NSC}$</td>
<td>Nagle Strickland-Constable oxidation source term for soot</td>
</tr>
<tr>
<td>$t_{500}$</td>
<td>Time required by a horizontal ($xz$) shrub surface to reach average solid-phase temperature of 500 K</td>
</tr>
</tbody>
</table>
Dedicated to the men and women who lost their lives fighting wildfires.
In that moment of calm when the two counterwinds neutralize each other and so roughly eliminated wind as the major factor in determining the direction of Dodge’s fire, the hitherto lesser force of the steepness of the slope took over, and Dodge’s fire, now under the slope’s influence, burned straight or almost straight upslope. At that moment the survivors, the ground, the fires, and the winds were all in agreement—that is to say, testimony and nature were in agreement, and nature while seeming to act unnaturally was actually in agreement with all parts of itself.

—Norman Maclean

Young Men and Fire
CHAPTER 1

INTRODUCTION

1.1 Wildfires and Wildfire Control Strategies

Wildfire or wildland fire is an uncontrollable fire spread through combustible vegetation, the intensity of which is governed by the available fuel density, fuel physical parameters and the atmospheric conditions. Wildfires form an important part of our ecosystem having both pros and cons associated with it. Forest fires are important for various reasons such as maintaining an ecological balance for various plant species, creating a favorable habitat for some animal species, soil nutrition, killing diseases and insects that prey on trees, etc. [1]. At the same time wildfires can be a threat to human life and property if they occur in regions close to civilization. In 2012, wildfires in North America were responsible for burning more than 9 million acres of area, with 246,445 acres in the state of Colorado alone, causing tremendous loss to property and human life [2]. Recent studies indicate that changing climatic conditions, leading to global warming, are responsible for frequent occurrences of large wildfires [3]. In the period of past few decades the cost involved to counter wildfires has dramatically increased, seasonal expenditure of about $1.7 billion spent by the governmental agencies in United States alone [4].
Some of the strategies for controlling fire spread include, adding fuel breaks in the path of fire, creating back fires to eliminate the fuel, etc. [5]. Another approach to deal with wildfires is to prevent their occurrence in the first place by avoiding the over accumulation of fuel. For this purpose, land management agencies use prescribed burning as a tool [6]. In prescribed burning a low intensity fire is established under marginal burning conditions, to remove the accumulated fuel without running into the risk of starting a large uncontrolled fires [7]. Fire control planning and resource management in this situation is a complex task which requires understanding of fire behavior under given conditions [8]. Therefore, before carrying out prescribed burns or any kind of resource management activity associated with it, the land management agencies usually use predictive tools that can provide guidance on expected fire behavior under specified conditions. They are also used to obtain data in case of an actual wildfires to plan strategies used to control the fire. These predictive tools are based on mathematical models which require inputs, such as, wind velocity, vegetative loading, fuel moisture content, etc. Useful insights on fire behavior can then be obtained from the outputs, such as, fire spread rate (velocity at which the fire front propagates), time required to burn certain amount of vegetation, etc., [9]. In Section 1.2 some of the approaches adopted to construct these mathematical models are discussed.

1.2 Wildfire Modeling Approaches

One of the first reports on the state-of-the-art wildfire modeling approaches, developed during the period of 1940 to 1970, was written by Albini (1976) [10]. The
models discussed in this work were mostly empirical in nature, i.e., these models aim to establish a direct relationship between physical and chemical properties of the fuel and the resulting fire behavior, such as forward fire spread rate, etc. Later, Weber (1991) [11] classified modeling approaches based on their treatment of heat transfer mechanisms into three broad categories, namely, statistical, empirical and physical. Although statistical and empirical models were discussed, the focus was mainly on the physical models developed during the period 1965 to 1990. Following the a similar concept of model classification, Sullivan (2009) [12–14] published three review articles on models developed during the period of 1990 to 2007. Based on the work of Karplus (1977) [15], he classified the models into three broad categories covering the spectrum of modeling approaches, which are, physical and quasi-physical models, empirical and quasi-empirical models, and simulation and mathematical analogue models. At one end of the range are the empirical models, solely based on observations from system input and output, and on the other end are the physical models, derived from basic principles governing the behavior of the system. Most of modeling approaches fall within the range of these two extreme cases. The simulation and mathematical analogue models are based on mathematical concepts such as wave propagation, which provides an analogue of fire spread, and coincidentally describe the fire behavior.

Here, models from two major categories, viz., empirical and physical, are briefly described. By highlighting major differences between them, motivation for using a physics based model in this work is provided.
1.2.1 Empirical and Quasi-Empirical Models

Following the definition of Sullivan (2009) [12], an empirical model is one which is purely statistical in nature, i.e., no physical description of the phenomena involved is required to derive the model. On the other hand, a quasi-empirical model has some physical basis using which a statistical model is derived. The objective behind developing empirical or quasi-empirical models is to obtain global predictions of fire propagation, such as, rate of fire spread, intensity of flame front, etc. Empirical models are derived from experimental data using techniques such as curve fitting. The model proposed by Nobel et al. (1980) [16], for predicting fire spread rate through grassland type fuels, falls under the category of empirical models. Zhou et al. (2005) [17] proposed an empirical model for probability of fire spread, under marginal burning conditions in chaparral like fuels, through laboratory experimentation. While conducting experiments, different fuel species with varying moisture content were considered. The effect of these variables on model formulation was accounted, but it had no physical basis. Empirical models perform satisfactorily in circumstances under which they are derived, but due to the lack of physical basis they cannot be readily extended to other circumstances [11].

One of the most famous quasi-empirical model used widely for fire management purposes in United States, was proposed by Rothermel (1972) [9], based on the previous work of Frandsen (1971) [18]. The model is developed by applying the energy conservation principle to a unit control volume, lying inside the fuel bed with homogeneous solid properties, ahead of flame front moving in one direction. This
model takes into account the amount of heat flux required for igniting given amount of fuel, fraction of radiant heat flux emitted by the flame and received by the solid fuel surface, effect of external wind on flame tilt, moisture content of the solid fuel, intensity of reaction, etc., while calculating the fire spread rates through a homogeneous porous media. The various constants involved in the model were evaluated by conducting several series of laboratory scale experiments under varying conditions. The Rothermel model also forms the basis of the fire behavior prediction tool BEHAVE, proposed by Andrews (1986) [19]. The BEHAVE system, collection of fire propagation models, essentially consists of two parts, first deals with modeling of the fuels (FUEL sub-system) and second accounts for the fire behavior (BURN sub-system).

The limitations of these models are due to the assumptions that are made while deriving the set of governing equations. For example, it is assumed that fire propagates through a matrix of dead fuel particles, diameters of which are less than one-fourth of an inch, limiting the application of model to relatively low moisture containing fuels. Another important assumption is that fire front is described to spread through a surface fuel (height of which can be about 6 feet from ground), due to which model cannot be used in situations where crowning (transition of surface fire to crown fire) is expected.

Because of the simplicity of these (empirical and quasi-empirical) models and the low operational costs involved, in predicting important wildfire parameters (like rate of spread, etc.), they are still widely used for operational purposes by various agencies across the world [13]. But due to their inherent shortcomings these models cannot be applied to complex problems, such as, blowup fires, fire spread through
heterogeneous fuel beds, transition of fire from ground to crown, ignition of new fires due to transport of burning embers, generation of fire whirls, etc. Physics based models, which seek numerical solutions to the governing physical equations, though much slower than real-time, can be applied directly to a wide variety of scenarios.

Fire propagation involves large number of physical processes which are intricately linked to one another. The important mechanisms consists of; decomposition of solid fuels into pyrolysis gases due to externally supplied heat (some ignition mechanism is always required), oxidation of these pyrolysis gases which represents the gas-phase combustion, transfer of heat from gaseous flames back to unburnt solid fuels, formation of soot from both gas phase and solid phase combustion, turbulent flow field generation due to buoyancy effects (which further aids heat transfer), etc. Therefore to study such complicated phenomena a physics based model which explicitly accounts for the coupling between different physical processes is required.

Henceforth in this dissertation the category of empirical and quasi-empirical models will be referred to as empirical models since there is only a small difference between these two subcategories in comparison with the physics based models.

1.2.2 Physics Based Models

The fire propagation models which differentiate between the various heat transfer mechanisms such as, conduction, convection and radiation, were classified into the category of physical models by Weber (1991) [11]. To accommodate broader categories of modeling approaches, Sullivan (2009) [12] further classified the physical modeling category into two parts, namely, physical and quasi-physical models. Phys-
ical models are those that account for both physics and chemistry involved in the fire spread problem, whereas, the quasi-physical models account only for the physics of the problem. Recently, Morvan (2010) [20] introduced a new terminology to classify physical models. According to him, models that explicitly account for the coupling between the vegetation and the surrounding atmosphere are called “fully physical models”. The criteria used for defining this category of models, was; governing equations based on multiphase formulation and use of physical models to represent small scale phenomena, such as the structure of the flame, flow at the Kolmogorov scales, burning of the individual solid particles, etc.

Following the definition of Morvan (2010) [20], except referring to this class of models as physics based models instead of “fully physical models”, a brief description of some of the existing models is provided.

For the review purpose, the starting point will be considered as the monograph published by Grishin (1997) [21] on fire propagation through a forest layer using a multiphase modeling approach, since most of the current physics based models share similarities with this work. Grishin (1997) [21] describes the forest as a multi-layered porous media, with each layer describing a certain characteristics of the forest, for example, the lower most layer represents the forest floor made of needle and leaf litter, a layer above that represents the barks of trees and small shrubs, etc. The solid-phase layer is described using concepts from continuum multi-phase mechanics. This includes describing the distribution of solid fuel particles using volume fractions in a control volume, whereas, neglecting the internal structure and porosity of individual
fuel particle. Thus, the thermo-physical properties of an ensemble of particles in a given control volume are constant.

Larini et al. (1998) [22] developed a general formulation based on weighting average procedure that took into account existence of multiple species of solid fuel (characterized by their physical and chemical properties), to describe the behavior of fire-induced flow through a radiative, reactive, multiphase media. A reduced order model based on simplification of the general formulation (neglecting the effects such as char oxidation, fuel particle motion, etc., called as the “zeroth-order model”) was proposed. The sensitivity of the “zeroth-order model” to various input parameters, such as, moisture content, chemical composition of pyrolysis gases, etc., was studied. Porterie et al. (2000) [23] extended this model for studying the propagation of wind-aided fires through pine needle fuel beds. A $k - \epsilon$ RANS (Reynolds Averaged Navier Stokes) model was adopted for turbulence closure and the simulations were performed on a two dimensional domain.

A similar model, for fire propagation through porous media, based on multiphase formulation was developed at the Los Alamos National Laboratory (LANL) by Linn (1997) [24]. Fully compressible form of Navier Stokes with a local averaging procedure was used to derive the set of governing equations. Unlike previous studies, this model was applied to simulate three dimensional flows. Stricter restrictions on time step size, due to the fully compressible form of the governing equations, were observed to reduce the efficiency of the model in predicting large scale fires [25]. Later the model was simplified by reducing the complex combustion chemistry to a single
step reaction, and used to simulate the wildfire spread through an inhomogeneous vegetation in complex terrain by Linn et al. (2002) [26].

To model the fire spread through chaparral like fuel beds under marginal burning conditions, Zhou et al. (2005) [27] proposed a model based on multiphase formulation. Turbulence was modeled using a $k - \epsilon$ RANS approach, where the governing equations were two dimensional. Solid-phase was described as consisting of two distinct species, namely, branches and foliage. Models for moisture evaporation, decomposition of solid fuel to pyrolysis gases and char oxidation were included to describe the evolution of solid-phase. This model was validated against a set of laboratory scale experimental results. Later, Zhou et al. (2007) [28] extended the model to three dimensional domain where large eddy simulation (LES) was used to capture turbulence.

Mell et al. (2007) [29] described the formulation of WFDS (Wildland Fire Dynamics Simulator), an extension of FDS (Fire Dynamics Simulator) for wildland fires, developed by the National Institute of Standards and Technology (NIST). WFDS uses a 3-dimensional formulation for the gas-phase proposed by Rehm and Baum (1978) [30] for buoyancy-driven low Mach number flows. Large eddy simulation, with Smagorinsky sub-grid scale model, is used to capture the effects of turbulence. The combustion model used is based on mixture fraction approach and the effects of unresolved heat flux on thermal degradation of solid fuel is neglected. Due to the difference in dimensionality of the flames (in gas-phase) and the depth of the fuel bed, computational grids of different resolutions are used to track the evolution of solid- and gas-phase. Later, Mell et al. (2009) [31] validated the WFDS model through a series
of laboratory scale experiments on burning Douglas fir trees of different heights. The effect of firebrand generation on mass loss of the trees was accounted, by removing fully pyrolyzed solid fuel particles, which improved the model predictions for drier vegetation.

1.3 Motivation

The Mediterranean like climatic conditions in parts of southern California gives rise to long, hot and dry summers. Hence this region is extremely affected by the occurrences of wildfires [32]. Rapid economic development in this region has lead to an increase in population in the vicinity of wildland forests [33]. Such areas are identified as wildland-urban-interface areas. The increasing proximity of humans and property in areas prone to wildfires has renewed the interest of various researchers and government agencies, in this region, to study the behavior wildland fires and develop tools to predict them [34]. In these regions chaparral is found in abundant quantities. Chaparral represents a mix of species like chamise (Adenostoma fasciculatum), red shanks (Adenostoma sparsifolium), manzanita (Arctostaphylos spp.), Scrub oak (Quercus berberidifolia), California juniper, etc., [35]. Among these, chamise is the most commonly found chaparral species covering over 70% of California chaparral [36]. Typically chamise shrubs are around 0.6 to 3 m tall, grow very close to the ground, have needle like sharp pointed leaves with diameter of about 0.2 inches, diffusively branched structure with slender branches and have the ability to continuously grow and spread [37]. The characteristics of chamise, its high surface area to volume ratio, presence of high energy ether extractive in foliage, and its ability to hold large
amount of dead material, makes it a highly flammable shrub species [38]. For these reasons, burning of a chamise shrub is studied in this work. Ignition of this crown like shrub, where the fuel is at some distance above the ground, is achieved by distributing surface fuel beneath it and igniting the surface fuel.

1.3.1 Bulk Density Distribution

Bulk density is defined as the amount of dry mass per unit canopy volume, which essentially represents the volume fraction of dry fuel in a given control volume. Grishin (1997) [21] differentiates forest fires into three broad categories depending on the physical characteristics of the fuel burnt. The first category is soil forest fires, occurring in the lower most layer of the forest, where the fuel like moss, lichen, litter, etc., is consumed. The rate at which soil fires spread is extremely slow and they are hard to detect as they do not appear on the surface. If small shrubs and the lower barks of the trees are consumed during fire propagation, then it is classified as a surface fire. A nearly uniform rate of spread is seen for the surface fires (depending on the wind velocity and vegetation properties). If the intensity of the surface fire is large it has the tendency to start a crown fire. When top layer of the forest, consisting of the tree crowns is ignited the fire is classified as crown fire. Crown fires have highly unpredictable characteristics and usually are associated with high spread rates [39]. Transition from surface to crown fires is an important phenomena which cannot be captured by the empirical models discussed in Section 1.2.1.

Van Wagner (1977) [40] proposed a criteria, based on the combustion zone intensity in surface fires and heat transfer into the crown fuels, for the initiation and
spread of crown fires. The two important assumptions made in this work were: first, variation of ambient temperature has negligible effect on crowning phenomena and second, vertical fire spread inside the crown is independent of its bulk density. Based on the work of Van Wagner, Scott and Reinhardt (2001) [41] developed parameters called “Torching Index” and “Crowning Index” to describe the transition from surface to crown fire. These two indices accounted for the effects such as surface fuel characteristics, fuel moisture content in both surface and crown fuels, canopy bulk density, canopy base height, etc., in determining the crown fire hazards. Cruz et al. (2006a) [42] proposed an empirical model based on heat transfer between the surface and crown fuels to predict the initiation of fire in tree canopy. Using sensitivity analysis and experimentation Cruz et al. (2006b) [43] concluded that intrinsic crown fuel properties such as bulk density, surface area-to-volume ratio and foliar moisture content have a minor impact on crown fuel ignition.

The models proposed so far were mainly developed for predicting crowning phenomena in forest fire scenarios and hence did not give a satisfactory performance while describing crown fire initiation in shrub fires. The important reason is attributed to the difference in the fuel arrangement between tree canopies and shrub canopies [44]. The tree canopy height, defined as highest height above which the bulk density decreases below 0.011 kg/m$^3$ [41] is much larger for the trees as compared to shrubs. Similarly, the crown base height, defined as distance from the ground where bulk density exceeds 0.011 kg/m$^3$, is much smaller for the shrubs than trees. Also the bulk density values encountered for the tree canopies are considerably different than those seen in shrubs fuels. Using laboratory scale experimentation and physics
based modeling, Tachajapong (2008) [45] studied the characteristics of transition of surface to crown fires for shrub canopies. Important findings include: increase in bulk density of the shrub increased the chances of crowning due accumulation of hot gases inside the shrub canopy, higher base height of the crown reduced the chance of crown fire initiation and external wind speed was a critical factor in determining the crown fire behavior.

A laboratory-scale fire study has been recently reported by Mell et al. (2009) [31] who conducted experiments on the burning of isolated Douglas fir trees to validate WFDS. The tree was modeled with a constant bulk density throughout the canopy volume and char oxidation was neglected. Li (2012) [46] conducted experimentation and used physics based modeling approach to highlight the role of crown fuel bulk density on crown fire initiation. Even though different crown fuels were used, during the computational study, distribution of bulk density inside the canopy volume was considered constant. Most of the investigations conducted, using physics based modeling, have considered the bulk density of the fuel elements to be constant across its volume [23,27–29,47]. Some exceptions, like the work of Grishin (1997) [21], described fire propagation through a forest fuel layer (surface fire) having a non-uniformly distributed mass along the depth of the fuel bed.

In this work we investigate, the role of spatial variation of crown fuel bulk density, in determination of fire behavior. The crown fuel bulk density refers to oven dry mass of foliage and small twig (less than 3 mm in diameter) per unit volume of canopy [45]. Recent experimental measurements reveal that the bulk density of a chamise shrub, for instance, varies as a function of vertical height from its base.
and this variation is approximated with a cubic polynomial fit [46]. The impact of two types of modeling of a solid fuel matrix on fire spread rates is studied here. In first modeling approach, no spatial variation for the bulk density within a shrub is considered, i.e., fixed bulk density (FBD), while in the other, the spatial variation of the bulk density is accounted for, i.e., a distributed bulk density (DBD).

1.3.2 Moisture Content

The second focus of this work concerns, effect of fuel moisture on fire spread rates. From numerous field studies and experimental work [48–51], it is well known that solid fuel moisture content, formally defined as the mass of moisture per unit mass of dry solid fuel, influences fire behavior considerably. Foliar moisture content is shown to be an important parameter in determining the quantity of heat required to initiate ignition in crown fuels [40]. Countryman (1964) [52] described moisture content of the fuel as an important factor in analyzing interactions between multiple fires, in a wildland fire scenario. Rothermel (1972) [9], in his semi-empirical model on fire spread through porous fuel bed, defined moisture of extinction as a threshold value of moisture content beyond which self-sustained combustion cannot occur inside the solid fuel matrix.

Dimitrakopoulos and Papaioannou (2001) [53] conducted flammability tests on various Mediterranean forest fuels under varying fuel moisture content and expressed the relationship between ignitability of the fuel and its moisture content with a linear regression fit. This model has been used to demonstrate that variation of time-to-ignition for different fuel samples can be explained through only one parameter, fuel
moisture content. Zhou et al. (2005) [27] identified the fuel moisture content as a critical parameter determining the success of a prescribed burn. From experiments and computations they concluded that above a critical moisture content value of 70% fire did not spread through the chaparral fuel bed.

Babrauskas (2008) [54] using experimentation, studied the effects of fuel moisture content on burning of Douglas fir trees. Important findings reported by him can be summarized as follows: samples with moisture content less than 30% were reported to burn completely with a rapid fire spread through the crown after ignition; samples with moisture content in the range between 30% and 70%, even though ignited successfully, were only partially consumed by the fire; and for samples with moisture content larger than 70%, only a small portion of crown mass was burned beyond what is supported by the ignition mechanism. Manzello et al. (2007) [51] conducted experiments to determine size distribution of fire brands generated from burning of Douglas fir trees. They observed firebrand generation only if the moisture content of the trees was less than 30%. Further, Mell et al. (2009) [31] conducted a validation of WFDS model using same experimental setup, involving Douglas fire trees and bottom ignition. Incomplete consumption of vegetation, foliage and roundwood less than 10 mm in diameter, was observed in trees 5 m tall with moisture content of 49%. Baker (2011) [55], through his experimental work on fire spread in Douglas fir trees, identified moisture content less than 30% as the vigorous burning regime characterized by higher heat release rates and larger flame heights.

In this work a systematic investigation on the effect of fuel moisture content on dynamics of shrub fires is performed. The range of moisture content considered
varies between 20% to 100%, which is typically seen for live chamise shrubs. Moisture
content variation along with distributed bulk density is also considered, to gain further
insights on the role of moisture in fire spread phenomena.

1.3.3 Soot Thermophoresis

The third focus of this study is to explore the importance of soot particle
thermophoresis on fire predictions. In wildfire modeling, predictions of soot are im-
portant from two standpoints. First due to the harmful effects it has on human
health [56] and second due to its role in fire propagation. In this research we are
concerned about soot due to the second effect mentioned above, i.e., effect of soot
evolution on behavior of fire. Radiative energy involved in combustion process plays
an important role in fire propagation [57]. It is one of the important mechanisms by
which the unburnt fuel ahead of the flame front is heated and thus flame propagation
takes place. Experimental and observational data suggests that, flames generated due
to burning of typical wildland fuels (chaparral found in southern California region)
generates considerable amounts of soot [58]. Soot affects the radiative heat transfer
in gas phase [59]. Thus it can be seen that even though soot is not directly corre-
lated to fire propagation, it indirectly affects the overall behavior of flames. Due to
this strong coupling between fire propagation, radiation, and soot, it is important to
obtain accurate predictions of soot.

In general, soot particle evolution models for non-premixed flame simulations
can be classified into two categories. The first approach is to solve two transport
equations, one for the number density of soot particles and another for the soot mass
fraction, wherein the effects of nucleation, oxidation and surface growth are included using source terms [60]. Using this approach an average particle size, representative of an ensemble can be obtained. The second approach is based on solving the moment transport equations, which assumes that having the knowledge of infinite set of moments is equivalent of knowing the PSDF (particle size distribution function) itself [61]. The soot transport is based on the small particle (i.e. negligible mass) assumption. This assumption basically ensures that the particle will be transported with the flow without any lag. In turbulent flame simulations, generally, it is assumed that the only forces acting on the soot particles are the stokes force and the thermophoretic force [60–64].

Rosner et al. (1992) [65] showed the relative importance of various forces such as photophoretic (arising due to uneven radiation absorption at particle surface) and other phoretic forces (which arise due to thermal non-equilibrium between particle surface and surrounding gas) in transport of small particles suspended in gas. Neglecting the transport of particles due to bulk motion, they suggested that particles undergoing radiative cooling (particle temperature higher than surrounding gas) coagulate faster to form larger particles due to their thermophoretic motion. A similar observation was made by Mackowski et al. (1994) [66], specifically in the context of combustion generated particles. They also mentioned a significant change in local particle number density, due to the thermophoretic motion caused by externally applied temperature gradient in the gas-phase.

Due to the lack of knowledge on soot nucleation process, in the context of wildfires, physics based models account for soot particle transport by solving a single
transport equation for volume fraction [23,27–29,31,47,67]. Most of these models have considered transport of soot due to thermophoresis, assuming that the diffusion of soot is negligible. In this dissertation, the effect of soot thermophoresis on fire behavior is investigated to highlight the relative importance of this transport mechanism as compared to convective transport.

1.3.4 Flame Merging

The final focus of this work is to investigate the effects of neighboring shrub fires on burning of individual shrubs. Fire-fire interactions and the subsequently generated mass fires have been a topic of interest in fire research for a long time, not only due to the peculiar characteristics associated with it but also the varied circumstances under which they are seen [68]. A mass fire is described as a scenario where individual fires interact and exhibit a unified behavior [52]. During a wildfire, interactions between two or more fires are routinely observed which has the potential of creating a mass fire [69].

Countryman (1964) [52], under the sponsored project “Interaction of Mass Fire and its Environment”, developed a comprehensive report on characteristics of mass fires, generated due to merging of small individual fires and its effects on military and civilian safety. The classification of fire as “mass fire” was based on the energy release rate, although no quantitative information was provided, rather than the overall size of the fire. Mass fires were further classified into two broad categories as firestorms and conflagrations. Firestorms, identified as most violent type of mass fires, are formed when several individual fires coalesce quickly into a single fire. Conflagrations
are generally formed in the presence of strong winds and have definite moving fronts, where the terrain topology is also identified as an important factor.

While developing a new method for carrying out prescribed burns, which involved dropping of ignition sources from air, Rothermel (1984) [70] raised concerns over generation of merged fires. It is mentioned that when two initially separated fires approach each other, heat will be accumulated between them, resulting into intense heating and subsequent faster combustion of the fuel in this region. Accelerated burning can lead to higher flame heights and in some cases leads to torching of the tree crowns, if present. Occurrence of merging phenomena was considered hazardous, leading the prescribed fires out of control. Baum and McCaffrey (1989) [71] studied the flow field induced by pool fires ranging over four orders of magnitude in size, through theory and experimentation. They concluded that, the velocity of the horizontally induced draft, even though less compared to those observed in plume for isolated fires, can exceed the net vertical plume velocity in presence of large number of surrounding fires.

Several critical parameters and correlations (functions of flame height, spacing between individual fires, etc.) have been defined in the literature to identify the onset of fire interactions. Baldwin (1968) [72], by using experimental data from free burning fires (without any external wind) arranged in square arrays, defined a criteria for the onset of flame interaction based on increase in flame height. Interactions between individual fires were observed when separation distance between them was about 0.22 times the merged flame height. Sugawa and Oka (2003) [73] conducted experimental study on flame merging between fires generated by circular LPG-gas burners arranged
in 2 by 3 (2 parallel lines each consisting 3 fire sources) arrays. Flame merging was observed, based on visual observations of flame tilting, till the distance between the fires was about three times the burner diameter.

Several researchers have studied configurations consisting of propane burners arranged in square arrays to analyze the effects of flame merging on overall behavior of fire [74–76]. Studies were conducted using both experimental and computational modeling approach. A dimensionless heat release rate and flame height was used to identify the effects of flame merging. Important observations are: the fire intensity of merged fire was seen to be substantially larger as compared to the individual fires, flame height increased with increasing number of individual fires and for separation distance varying from 0 to 30 mm, the relationship between dimensionless flame height and dimensionless heat release rate remained the same.

Satoh et al. (2007) [77] conducted computational modeling and experimentation on pool fires, generated from circular pans filled with liquid fuel, arranged in square arrays. Large number of pool fires (15×15, 17×17 and 19×19) were considered to increase the overall surface area of fire. The simulations were performed without combustion by specifying only the heat release rate over the base area of pool fire. Visual observation was used as a criteria in experiments, to identify flame merging, whereas, thermal iso-surfaces of 313°C were analyzed to identify flame merging from simulation results. The critical merging distance, largest distance between two fires where flame merging is observed, was reported to decrease with an increase in heat release rate of individual pool fire. Later, Satoh et al. (2011) [78] conducted a CFD based analysis on flame interactions from huge oil depot fires. Creation of a negative
pressure zone at the center of the merged fires was reported, which in turn caused the flame heights to increase.

Morvan et al. (2013) [79] recently studied the interactions between two fire fronts (a head fire and a back fire) propagating through a fuel bed, using a computational approach. The motivation behind this research was from a fire fighting standpoint, where a back fire is used to eliminate the fuel ahead of the main propagating fire front. Total heat release rate from the fires was used as a criteria to identify the onset of flame merging phenomena. When the two fire fronts were in close proximity, the back fire was pulled towards head fire due to the nature of induced drafts. Flame merging led to a considerable increase in total heat release rate. The buoyancy driven flow field generated by the head fire acted as a screen, shielding the effects of external wind on backfire.

The occurrence of fire merging phenomena becomes extremely hazardous from a fire fighting standpoint and thus it is important to study the physical nature of these interactions. Here we highlight the important mechanisms responsible for fire-fire interactions and flame merging in the context of shrub fires. Two different shrub arrangements, consisting of two shrubs and three shrubs ignited simultaneously, are considered. These cases can be considered as a starting point for investigating the simultaneous burning of multiple shrubs.

1.4 Outline

Following the introduction and motivation presented in current Chapter 1, detailed formulation of the physics based model is presented in Chapter 2. The numer-
ical methods used to solve the governing equations are described in Chapter 3. The effect of physical parameters such as, distribution of mass and fuel moisture content; and thermophoretic mechanism of soot transport on behavior of isolated shrub fires is highlighted in Chapter 4. Fire-fire interactions and their effects on burning of individual shrubs are studied in Chapter 5. Summary of the work, important conclusions and some recommendations for future work are proposed in Chapter 6. Appendix A and Appendix B contain additional details of the formulation and additional figures, respectively.
CHAPTER 2

PHYSICAL MODELS

2.1 Introduction

The problem at hand consists of propagation of fire through porous media. The overall burning process of solid fuel is shown in Figure 2.1, which also highlights the important physical mechanisms involved and the way they are coupled. As can be seen from Figure 2.1, to initiate the burning an external ignition mechanism is always required. In real life wildfires the ignition can occur by various causes, such as lightning, arson, spotting from another fire source, etc. [80]. While conducting experiments on fire spread, the ignition zone is usually replicated in such a way that it closely mimics the real ignition mechanisms. The region in the solid fuel where ignition takes place is referred to as ignition zone. The external heat supplied to the ignition zone, when enough, causes the solid fuel to undergo decomposition. As the temperature of the solid fuel starts to rise, the drying process initiates and the moisture content of the solid is converted into water vapor. With a further increase in temperature the solid fuel undergoes phase change and is converted into pyrolysis gases. The composition of the pyrolysis gases is an extremely complex mixture of various hydrocarbons and varies for different species of solid fuel [81]. Finally, with
Figure 2.1: Important physical and chemical phenomena involved in the burning process of solid fuels and their coupling.

A further rise in temperature the solid media is converted into char, which is solid carbon. The pyrolysis gases undergo mixing with the ambient air, the process usually being turbulent, resulting into gas-phase combustion. Similarly, the oxidizer from the ambient directly reacts with the solid-phase, resulting into char oxidation. The heat released from gas- and solid-phase combustion is transferred to the surrounding unburnt solid fuel through the mechanisms such as convection, radiation and diffusion.
This cycle will thus continue, either, till all the solid fuel is consumed or till the heat feedback mechanism to unburnt fuel is strong enough [82].

A physics based model should capture all these important mechanisms and adequately account for the coupling between them. Formulation of one such model is presented, describing various sub-models accounting for the different blocks shown in Figure 2.1.

Governing equations, derived from the conservation principals need to include the multiphase nature of the flow due to the coexistence of gas and solid phases in the control volume. The solid fuel matrix is thus modeled as a porous medium with gas phase porosity $\xi$ and a packing ratio $\beta$ characterizing the solid phase [22]. Since the solid-phase contains multiple species, e.g., foliage and branches, we define $\beta = \sum_{L=1}^{N_L} \beta_L$, where $\beta_L$ denotes the fractional volumes occupied by the $L^{th}$ solid-phase species and $N_L$ is the total number of solid-phase species. For a given typical control volume,

$$\xi + \sum_{L=1}^{N_L} \beta_L = 1,$$  \hspace{1cm} (2.1)

ensures the conservation of volume and forms the bases of multiphase formulation. The specific wetted area per unit volume, $A_L$, for the $L^{th}$ solid phase is defined as $A_L = \beta_L \sigma_L$, where $\sigma_L$ is the surface area to volume ratio for $L^{th}$ solid phase. In case of cylindrical fuel elements, $\sigma_L$ can be approximated via $\sigma_L = 4/d_L$ [83], where $d_L$, denotes diameter of fuel particles from $L^{th}$ solid phase.

A Wide range of spatial and temporal scales exists in the fire phenomena. For example, chemistry occurs at the molecular length scales whereas the convective
heating can occur at the length scale of meters or even kilometers (depending on the size of fire). The difference between largest and smallest scales in practical fires can be up to ten orders of magnitude [84]. Therefore, the existence of wide range of scales prohibits solving the governing equations in their direct form (leading to Direct Numerical Simulation). This prohibition is due to the lack of sufficient computational resource required to resolve all the scales involved in the fire problem. Some sort of averaging procedure is thus needed. The classical time averaging procedure, that leads to Reynolds Averaged Navier-Stokes (RANS) equations [85], cannot be used due to an inherently unsteady nature of the flow generated by burning of the solid fuel. A variation of RANS known as Unsteady-RANS (URANS), wherein the time averaging is conducted over eddy turnover time associated with the largest eddy [86], has been used by researchers to model fire propagation problem [47]. Although URANS is capable of capturing the largest scales associated with unsteadiness of the flow, more of the smaller scales need to be resolved in order to better predict the turbulence and its interaction with other phenomena such as combustion [87]. For these reasons, Large Eddy Simulation (LES) is the method of choice to deal with turbulence in this study.

In LES, only the large scale motion of the flow is captured, whereas its interactions with small scales are modeled [88]. Given a generic field variable \( f(x, t) \), which is a function of position vector \( x \) and time \( t \), application of spatial filtering,

\[
\bar{f}(x, t) = \int f(x', t)G(x, x'; \Delta)d{x'},
\]

(2.2)
decomposes the variable into large scale \((\bar{f})\) and small scale \((f' = f - \bar{f})\) contributions \([89]\), respectively. The quantity \(G\), is a filter kernel function satisfying \(\int G(x, x'; \Delta)dx' = 1\), with parameter \(\Delta\) denoting filter width, and the integration is performed over the spatial domain of interest. In this work a top-hat filter function, in physical space, is used to perform the filtering of transported quantities. The filter size is given by, \(\Delta = \sqrt[3]{\Delta V}\), where \(\Delta V\) is the volume of computational cell. For compressible flows, it is more convenient to work with density-weighted or Favre-filtered field quantities \([90]\), defined with a tilde as follows,

\[
\tilde{f}(x, t) \equiv \rho \bar{f} / \bar{\rho}.
\] (2.3)

By using the density-weighted averaging, occurrence of, unclosed terms in continuity equations and higher order correlations in other transport equations is avoided.

With multiphase aspect of the control volume and averaging procedure described, the governing equations for gas- and solid-phase are presented in next section.

### 2.2 Gas-phase Governing Equations

The mathematical model for turbulent, compressible (low Mach number), multiphase, reacting flow, in the context of LES, includes the following set of governing equations;

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i}{\partial x_i} = \sum_{L=1}^{N_L} \bar{S}_L, \tag{2.4}
\]
\begin{align}
\frac{\partial \tilde{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} &= \frac{\partial}{\partial x_j} \left\{ -\tilde{\rho}(\tilde{u}_i \tilde{u}_j - \tilde{u}_i \tilde{u}_j) \right\} - \frac{\partial \tilde{p}}{\partial x_i} + \frac{\partial \tilde{\tau}_{ij}}{\partial x_j} + \tilde{\rho} g_i - \sum_{L=1}^{N_L} \tilde{F}_{L,i}, \quad (2.5)
\end{align}

\begin{align}
\frac{\partial \tilde{\rho} \tilde{h}}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_i \tilde{h}}{\partial x_j} &= \frac{\partial}{\partial x_j} \left\{ -\tilde{\rho} \left( \tilde{u}_j \tilde{h} - \tilde{u}_j \tilde{h} \right) \right\} - \frac{\partial \tilde{q}_i}{\partial x_i} + \frac{\partial \tilde{q}_i,\text{rad}}{\partial x_i} \\
&- \sum_{L=1}^{N_L} \tilde{q}_{\text{conv},L} + \sum_{L=1}^{N_L} (1 - X_c) \tilde{m}_{\text{char},L} \tilde{E}_{\text{char}} + \sum_{L=1}^{N_L} \tilde{h} \tilde{S}_L, \quad (2.6)
\end{align}

\begin{align}
\frac{\partial \tilde{\rho} \tilde{Y}_K}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_i \tilde{Y}_K}{\partial x_j} &= \frac{\partial}{\partial x_j} \left\{ -\tilde{\rho} \left( \tilde{u}_j \tilde{Y}_K - \tilde{u}_j \tilde{Y}_K \right) \right\} - \frac{\partial \tilde{q}_{K,i}}{\partial x_i} + \sum_{L=1}^{N_L} \tilde{S}_{L,K} + \tilde{\omega}_K, \quad (2.7)
\end{align}

\begin{align}
\tilde{p}_0 = \tilde{\rho} T R_u \sum_{K=1}^{N_K} \frac{\tilde{Y}_K}{W_K}. \quad (2.8)
\end{align}

Here equations (2.4) to (2.7), are the filtered conservation equations for; mass, \(i\)th component of momentum, energy and \(K\)th gas-phase species, respectively. Equation (2.8) is the state equation for multicomponent system of ideal gases, where \(\tilde{p}_0\) is the background pressure [30], which is assumed constant and equal to one atmosphere, \(R_u\) is the universal gas constant, \(W_K\) denotes the molecular weight of the \(K\)th gaseous species and \(N_K\) is the total number of gaseous species. In the above set of equations, \(\tilde{\rho}\) is the filtered gas mixture density, \(x_i\) is the component of the position vector in \(i\)th direction, \(\tilde{u}_i\) denotes the component of Favre-filtered velocity along \(x_i\).
and $t$ denotes time. In equation (2.4), the source term $\bar{S}_L$, is the filtered mass production rate resulting from decomposition of $L^{th}$ solid-phase to gas-phase. Term $\bar{S}_L$ is non-zero only within the solid fuel matrix.

In equation (2.5), $\bar{p}$ denotes the filtered first order pressure [30], $g_i$ is the gravitational acceleration vector, $\bar{F}_{L,i}$ is the filtered $i^{th}$ component of the drag force resulting from the interaction between the gas- and $L^{th}$ solid-phase; it is nonzero only within the fuel bed. A simple model for the drag force, of the form

$$F_{L,i} = 0.5 \, C_{D,L} \bar{p} A_L |\bar{u}| \bar{u}_i,$$

(2.9)

applicable to cylindrically shaped solid particles, is used. The drag coefficient $C_{D,L}$ for $L^{th}$ solid-phase is approximated as proposed by Clift et al. (1978) [91],

$$C_{D,L} = \frac{24 \left(1 + 0.15 \, Re_{dl}^{0.687}\right)}{Re_{dl}}.$$

(2.10)

where, $Re_{dl}$ is the Reynold number defined in Section 2.3. The quantity $\bar{\tau}_{ij}$ in equation (2.5), represents the filtered viscous stress, which is modeled using the standard Newtonian model based on filtered quantities as,

$$\bar{\tau}_{ij} = -\frac{2}{3} \mu \frac{\partial \bar{u}_k}{\partial x_k} \delta_{ij} + \mu \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right),$$

(2.11)
Here $\mu$ is the dynamic viscosity of the gaseous mixture evaluated using a power law based on filtered temperature as \[92\]

$$
\mu = \mu_0 \left( \tilde{T}/T_0 \right)^{0.6756},
$$

(2.12)

where, $\mu_0 = 1.983 \times 10^{-5} \text{kg/(m.s)}$ and $T_0 = 300K$.

In the filtered gas-phase energy equation (2.6),

$$
\tilde{h} = \sum_{K=1}^{N_K} \bar{Y}_K \left( \Delta h_{j,K}^0 + \int_{T_0}^{T} \bar{c}_{p,K}(\tilde{T})d\tilde{T} \right),
$$

(2.13)

is the gas mixture enthalpy. Here, $\Delta h_{j,K}^0$, $\bar{c}_{p,K}$ and $\tilde{T}$ is the standard enthalpy of formation of the $K^{th}$ gaseous species, heat capacity of the $K^{th}$ gaseous species and the Favre-filtered gas temperature, respectively. $N_K$ is total number of gaseous species considered. Curve fit coefficients given in Kee et al. (1991) \[93\], are used to calculate $\bar{c}_{p,K}$ values. The quantity $\bar{q}_i$ is the filtered heat flux vector modeled using the standard Fourier law based on filtered quantities as

$$
\bar{q}_i = -\frac{\mu}{Pr} \bar{c}_p \frac{\partial \tilde{T}}{\partial x_j},
$$

(2.14)

where $Pr = 0.7$, is the Prandtl number and

$$
\bar{c}_p(\tilde{T}) = \sum_{K=1}^{N_K} \bar{Y}_K \int_{T_0}^{T} \bar{c}_{p,K}(\tilde{T})d\tilde{T},
$$

(2.15)
is the specific heat of the gas mixture. The filtered source term $\bar{q}_{\text{conv}, L}$ denotes the convective heat transfer rate per unit volume between gas- and the $L^{th}$ solid-phase, and $\bar{q}_{i, \text{rad}}$ is the radiative heat flux. The last two terms on the RHS of equation (2.6) describe, the heat released from the heterogeneous combustion of char with oxygen and enthalpy associated with gases generated from thermal degradation of solid fuel, respectively. These terms are non-zero only within the solid fuel matrix. Here, $\bar{m}_{\text{char}, L}$ is the rate of char mass consumption per unit volume, $E_{\text{char}}^L$ denotes the specific enthalpy associated with char combustion for the $L^{th}$ phase and $X_e$, assumed 0.5 [94] for all $N_L$ solid phases, is a fraction denoting the distribution of enthalpy of char combustion between the solid and gaseous phases.

In equation (2.7), $\tilde{Y}_k$ is the mass fraction of the gas-phase species $K$, $\tilde{S}_{L,K}$ is the filtered production rate of the gas-phase species $K$ resulting from the decomposition of the $L^{th}$ solid-phase, and $\bar{\omega}_K$ is the filtered production rate of the gas-phase species $K$ due to gas-phase chemical reaction. In equation (2.7), $\bar{q}_{K,i}$ is the species diffusion flux modeled with the standard Fick’s law

$$\bar{q}_{K,i} = -\frac{\mu}{Sc} \frac{\partial \tilde{Y}_K}{\partial x_j},$$

(2.16)

where Sc is the Schmidt number with a constant value of 0.7 for all species. Finally, the constraint

$$\sum_{K=1}^{N_K} \tilde{Y}_K = 1,$$

(2.17)
is imposed to solve for the mass fraction of the $N^K$ species, assumed to be gaseous nitrogen, $N_2$. Model for $\bar{\omega}_K$ is described in Section 2.2.2.

### 2.2.1 Subgrid-scale Diffusivity Model

The first terms on right hand side of equations (2.5)-(2.7) represent the unresolved scales of respective transported quantities, arising due to the filtering operation involved in LES. In equation (2.5), $\sigma_{ij} \equiv \bar{\rho}(\bar{u}_i\bar{u}_j - \bar{u}_i\bar{u}_j)$ is the subgrid-scale stress, calculated according to the Smagorinsky model [95]:

$$\sigma_{ij} = -2C_R\Delta^2\bar{\rho}\Pi \left( S_{ij} - \frac{1}{3} S_{kk}\delta_{ij} \right) + \frac{2}{3} C_I\Delta^2\bar{\rho}\Pi\delta_{ij}. \quad (2.18)$$

The second term on the RHS of equation (2.18), containing model constant $C_I$, is neglected here due to its negligible contribution in low Mach number flows [96]. The resolved rate of strain tensor is

$$\tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial\bar{u}_i}{\partial x_j} + \frac{\partial\bar{u}_j}{\partial x_i} \right), \quad (2.19)$$

the magnitude of strain tensor is $\Pi = (2\tilde{S}_{ij}\tilde{S}_{ij})^{1/2}$, and the subgrid-scale eddy viscosity is

$$\mu_t = C_R\Delta^2\bar{\rho}\Pi. \quad (2.20)$$

Here, the model constant $C_R$ is evaluated using a dynamic procedure proposed by Germano et al. (1991) [97]. The calculation procedure involves another filtering operation called test filtering, that uses a test filter of size $\tilde{\Delta}$ (larger than the grid
size), performed on the grid filtered momentum equation (2.5). The test filtering operation results into an additional stress term, called as the subtest-scale stress, given by \( T_{ij} = \hat{\rho} \left( \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j \right) \). The important assumption made in the dynamic procedure is the existence of scale similarity between the subgrid-scale stress and the subtest-scale stress. Therefore, \( T_{ij} \) can be modeled using the same functional form as that used for \( \sigma_{ij} \) (Smagorinsky model equation (2.18)) as follows,

\[
T_{ij} = -2C_R \hat{\Delta}^2 \hat{\rho} \hat{\Pi} \left( \hat{S}_{ij} - \frac{1}{3} \hat{S}_{kk} \delta_{ij} \right). \tag{2.21}
\]

The resolved turbulent stresses can now be obtained by using the algebraic relationship

\[
L_{ij} = T_{ij} - \hat{\sigma}_{ij} = -\hat{\rho} \left( \hat{u}_i \hat{u}_j - \hat{u}_i \hat{u}_j \right), \tag{2.22}
\]

where, \( L_{ij} \) represents the test-window stresses. Using the functional form of \( \sigma_{ij} \) and \( T_{ij} \), from equations (2.18) and (2.21), respectively, in equation (2.22)

\[
L_{ij} = 2C_R M_{ij} + \frac{1}{3} L_{kk} \delta_{ij}, \tag{2.23}
\]

where

\[
M_{ij} = -\hat{\rho} \left( \hat{\Delta}^2 \hat{\Pi} \hat{S}_{ij} - \hat{\Delta}^2 \hat{\Pi} \hat{S}_{ij} \right). \tag{2.24}
\]
The model constant $C_R$ can now be obtained by solving equation (2.23). Here we use the approach proposed by Lilly (1991) [98], which involves obtaining the solution of equation (2.23) using the least squares technique as follows,

$$Q = \left( L_{ij} - 2C_R M_{ij} - \frac{1}{3} L_{kk} \delta_{ij} \right)^2 .$$

(2.25)

Here $Q$ is the square of the error which is minimized by setting $\partial Q / \partial C_R = 0$ to obtain $C_R$, given by

$$C_R = \frac{L_{ij} M_{ij} - \frac{1}{3} L_{kk} M_{ij} \delta_{ij}}{2M_{lm}M_{lm}} .$$

(2.26)

In this work, the ratio of the test filter size to the grid size is set to $\Delta / \hat{\Delta} = 2$ [97]. A detailed procedure for the calculation of $M_{ij}$ and $L_{ij}$ can be found in Lilly (1991) [98] with an extension made by Ghosal et al. (1995) [99] to the statistically inhomogeneous flows.

In equation (2.6), the subgrid-scale energy flux is modeled, using the gradient diffusion hypothesis, as

$$\bar{\rho} \left( \bar{u}_j \bar{h} - \bar{u}_j \bar{h} \right) = - \frac{\mu_t}{Pr_t} c_p \bar{T} \frac{\partial \bar{T}}{\partial x_j} ,$$

(2.27)

similarly, in equation (2.7), the subgrid-scale mass flux is modeled as

$$\bar{\rho} \left( \bar{u}_j \bar{Y}_K - \bar{u}_j \bar{Y}_K \right) = - \frac{\mu_t}{Sc_t} \bar{Y}_K \frac{\partial \bar{Y}_K}{\partial x_j} ,$$

(2.28)
where $Pr_t$ and $Sc_t$ are subgrid-scale Prandtl and Schmidt numbers, respectively; both are assumed to be equal to 0.7 [100].

### 2.2.2 Gas-phase Combustion Model

Combustion in gas-phase requires the interaction of the pyrolysis gases and oxidizer at molecular level. In LES, the length scales to which the flow is resolved is much larger than the molecular mixing length scales. Thus, the entire combustion process occurs in the subgrid-scale region due to which the filtered reaction rate terms ($\bar{\omega}$) need to be modeled [101]. Various modeling procedures are adopted to close these terms, which inherently assume that time and length scales associated with combustion are separated from those of turbulence in inertial subrange. An excellent review on turbulent combustion models, in context of both RANS and LES, can be found in Peters (2000) [102].

The filtered chemical reaction rate terms appearing in the gas phase species transport equation, equation (2.7), are modeled using the flame surface density based approach proposed by Zhou and Mahalingam (2002) [103]. Briefly, this filtered reaction rate is modeled as

$$\bar{\omega}_K = \dot{M}_K \Sigma,$$  \hspace{1cm} (2.29)

where $\dot{M}_K$ is the production/consumption rate of the $K^{th}$ species per unit flame surface area, per unit time, i.e., the flamelet consumption rate and $\Sigma$ denotes the available flame surface area per unit volume, i.e., the filtered flame surface density. The flamelet consumption rate is pre-computed for a steady, laminar, opposed flow,
diffusion flame of pyrolysis gas and air, for various strain rates using the OPPDIF code [104] and stored in a lookup table which can be used while performing large eddy simulation. A one-step global reaction, described as follows,

\[
aCH_4 + bCO + cCO_2 + dH_2 + e(O_2 + 3.762N_2) 
\rightarrow (a + b + c)CO_2 + (2a + d)H_2O + e3.762N_2,
\]

(2.30)

where \( e = 0.5(4a + b + d) \), is used as gas-phase chemistry model [105].

The flame surface density \((\Sigma)\) can be obtained by solving a separate transport equation [106]. But this equation contains several unclosed terms for which modeling is required. For turbulent combustion, Vervisch et al. (1995) [107] showed a similarity between the flame surface density (FSD) and a probability density function (PDF). Therefore the term \( \Sigma \), is modeled by

\[
\Sigma(x, t) = |\nabla Z(x, t)|_{st} P_L(Z_{st}; x, t),
\]

(2.31)

where \( Z \) is the mixture fraction [105]. Here, \( |\nabla Z|_{st} \) is the conditional filtered value of the mixture fraction gradient along the stoichiometric isosurface and \( P_L(Z_{st}; x, t) \) is the filtered PDF (FDF) [108] of \( Z \), defined according to its mean \( \langle Z \rangle \), its sub-grid scale variance \( \langle Z'^2 \rangle \) and assuming a beta function distribution. The FDF essentially models the subgrid-scale distribution of flame surface density, thus capturing the turbulence-chemistry interactions. Further description and details on modeling of these quantities can be found in Zhou et al. (2004) [109].
2.3 Solid-phase Governing Equations

For simplicity, the solid-phase fuel is considered stationary, before, during, and after the flame front has passed. The mass balance equation for $L^{th}$ solid phase is given by,

$$\frac{d\bar{m}_L}{dt} = -\bar{m}_{L,H_2O} - \bar{m}_{L,pyr} - \bar{m}_{L,\text{char}}, \quad (2.32)$$

where, $\bar{m}_L$ is the filtered mass per unit fuel bed volume of the $L^{th}$ solid phase species, which in turn includes, the filtered mass per unit fuel bed volume of water ($\bar{m}_{L,H_2O}$), pyrolysis gases ($\bar{m}_{L,pyr}$) and char ($\bar{m}_{L,\text{char}}$). The corresponding filtered mass loss rate terms are denoted by $\bar{m}_L$ with appropriate subscripts, and are deduced from Arrhenius type laws. Since no data is currently available for burning of chaparral fuels, models proposed for pine needle combustion [23] are used as follows:

$$\frac{d\bar{m}_{L,H_2O}}{dt} = -\bar{m}_{L,H_2O} = -6.0 \times 10^5 T_L^{-0.5} m_{L,H_2O} \exp \left( \frac{-5800}{T_L} \right), \quad (2.33)$$

$$\frac{d\bar{m}_{L,pyr}}{dt} = -\bar{m}_{L,pyr} = -3.63 \times 10^4 m_{L,pyr} \exp \left( \frac{-7250}{T_L} \right), \quad (2.34)$$

$$\frac{d\bar{m}_{L,\text{char}}}{dt} = -\bar{m}_{L,\text{char}} = -\frac{1}{r_1} 430 A_L \rho_{O_2} \exp \left( \frac{-9000}{T_L} \right), \quad (2.35)$$

where $r_1$ is the oxygen to carbon stoichiometric mass ratio and $\rho_{O_2}$ is the density of oxygen. The filtered production rate of $K^{th}$ gaseous species, $\bar{S}_{L,K}$ (for water, and other gases released as a result of drying, pyrolysis and char combustion), present in
equation (2.7) are given by

\[ \bar{S}_{L,H_2O} = \bar{m}_{L,H_2O}, \quad (2.36) \]
\[ \bar{S}_{L,CO_2} = \bar{m}_{L,pyr} \gamma_{CO_2} + \bar{m}_{L,\text{char}} r_2, \quad (2.37) \]
\[ \bar{S}_{L,O_2} = \bar{m}_{L,pyr} \gamma_{O_2} - \bar{m}_{L,\text{char}} r_3, \quad (2.38) \]
\[ \bar{S}_{L,K} = \bar{m}_{L,pyr} \gamma_K, \quad (2.39) \]

where \( \gamma_K \) is the fraction of the \( K^{\text{th}} \) gaseous species released via pyrolysis. The quantities \( r_2 \) and \( r_3 \) denote respectively the mass of gaseous \( CO_2 \) formed and \( O_2 \) consumed, per unit mass of solid carbon burnt via char combustion, modeled using a reaction \( C + O_2 \rightarrow CO_2 \). Note that production of \( CO_2 \) and consumption of \( O_2 \) during char combustion is accounted for in equation (2.35). The filtered conversion rate of solid mass to gaseous mass \( \bar{S}_L \), appearing in equation (2.4), is given by

\[ \bar{S}_L = \sum_{K=1}^{N_K} \bar{S}_{L,K}. \quad (2.40) \]

The difference in \( \sigma_L \) for foliage and branches with different size is pronounced and hence it is reasonable to model the solid fuel matrix (shrub) as consisting of two phases: foliage (higher value of \( \sigma_L \)) and branches (lower value of \( \sigma_L \)). In the current work, 53\% of the total solid mass per unit volume is that of foliage and 47\% of the total solid mass is due to branches, as reported in Tachajapong (2008) [45] for chamise shrubs. Surface area to volume ratio for foliage is taken to be 8000 m\(^{-1}\) and that for branches is 1800 m\(^{-1}\); physical density for foliage and branches are 500 kg/m\(^3\) and
600 kg/m³, respectively [83]. At the subgrid scales, the solid fuel mass is assumed to have a uniform distribution. All $N_L$ solid-phase species in a given fuel matrix are assumed to have same moisture content.

Assuming that the solid fuel particles are thermally thin [110], the energy balance equation for $L^{th}$ solid phase is,

\[
\frac{d (\bar{c}_{p,L}\bar{m}_L\bar{T}_L)}{dt} = \bar{q}_{\text{conv},L} + \bar{q}_{\text{rad},L} + \bar{q}_{\text{mass},L},
\]

(2.41)

where $\bar{c}_{p,L} = 1.3 \text{ kJ/(kg K)}$ [111], denotes the filtered specific heat of the $L^{th}$ solid phase (assumed equal for all $N_L$ phases) and $\bar{T}_L$ represents the filtered solid phase temperature. In equation (2.41),

\[
\bar{q}_{\text{conv},L} = A_Lh_c(\bar{T} - \bar{T}_L).
\]

(2.42)

The heat transfer coefficient appearing in above equation is deduced from the Nusselt number for the solid phase as

\[
\text{Nu}_L = \frac{h_c d_L}{\lambda} = 0.683\text{Re}_{d_L}^{0.466},
\]

(2.43)

where $\lambda$ is the gas phase thermal conductivity, and the Reynolds number $\text{Re}_{d_L}$, is based on the diameter of the $L^{th}$ fuel particle, the filtered gas-phase velocity and kinematic viscosity.
In equation (2.41), $\tilde{q}_{\text{mass},L}$, is modeled as

$$
\tilde{q}_{\text{mass},L} = -\tilde{m}_{L,H_2O}E^{H_2O} - \tilde{m}_{L,\text{pyr}}E^{\text{pyr}} + X_c\tilde{m}_{L,\text{char}}E^{\text{char}},
$$

(2.44)

where $E$’s with appropriate superscripts denote the associated enthalpies for the process of vaporization, pyrolysis, and char combustion. The values used for these parameters in the present study are; $E^{H_2O} = 2250 \text{ kJ/kg}$, $E^{\text{pyr}} = 0.418 \text{ kJ/kg}$ [21], and $E^{\text{char}} = 32740 \text{ kJ/kg}$ [111]. Here, $\tilde{q}_{\text{mass},L}$ represents the amount of heat exchanged between gas- and the $L^{th}$ solid-phase due to phase change.

The quantity $\bar{c}_{p,L}$ is deduced from the constant values for dry wood material and water ($c_{p,\text{dry}}$, $c_{p,H_2O}$), and the filtered mass fraction of moisture $\bar{Y}_{L,H_2O}$, in the $L^{th}$ solid phase,

$$
\bar{c}_{p,L} = (1 - \bar{Y}_{L,H_2O})c_{p,\text{dry}} + \bar{Y}_{L,H_2O}c_{p,H_2O}.
$$

(2.45)

Model for $\tilde{q}_{\text{rad},L}$, in equation (2.41), is described in Section 2.4.

### 2.4 Radiative Heat Transfer Model

It has been well established that the accurate modeling of thermal radiation is an important feature in description of a heavily sooting turbulent diffusion flame generated from hydro-carbon fuels [112, 113]. Radiative heating is also one of the important heat transfer mechanisms responsible for fire spread [114]. Radiation can be predicted if the radiative properties of the participating media and the temperature distribution in the flow field is known. But usually temperature itself is an
unknown quantity which needs to be determined as the part of calculation procedure, giving rise to a coupling between energy conservation equation and thermal radiation conservation equation.

When an averaging procedure is used for the governing flow field equations the radiation source term appearing in the energy conservation equation needs to be evaluated in an average sense. When using a RANS type of averaging procedure, several authors [115–117] have found that radiative emissions from turbulent diffusion flames can increase by 50-300% (depending on fuel type) if calculated using instantaneous values, compared to those calculated based on mean temperature and absorption coefficient. Only the mean values of variables are explicitly resolved in RANS approach whereas entire fluctuating part needs to be modeled. Because of this proper modeling of thermal radiation, and its interaction with turbulence, plays an important role in RANS approach.

There are a very few studies conducted on effects of turbulence/radiation interactions (TRI) in context of LES. Although it should be noted that in case of large eddy simulation (LES) the turbulent scales above the filter size are explicitly resolved and only the sub-grid part needs to be modeled. Coelho (2009) [118] conducted an a priori study of Sandia flame D, which is considered a lightly sooting non-luminous flame, to highlight the relevance of TRI. The required flow field data was generated using a stochastic method. It was concluded that effects of sub-grid scale TRI are small in the studied flame. Due to these facts, the radiation model in the current study is completely based on filtered quantities, i.e., the effects of subgrid-scale fluctuations on radiation intensity have been neglected.
The conservation equation for thermal radiation, also known as the radiation transport equation (RTE), can be obtained by applying the principles of conservation to a monochromatic bundle (pencil) of radiation traveling along a straight line through an emitting, absorbing and scattering medium [119]. For a multiphase media, the RTE can be written as (neglecting scattering) [22]

\[ \mu_{i,j} \frac{\partial \xi \tilde{I}_i}{\partial x_j} = \xi a_g \left( \frac{\sigma \tilde{T}^4}{\pi} - \tilde{I}_i \right) + \sum_{L=1}^{N_L} a_L \left( \frac{\sigma \bar{T}_L^4}{\pi} - \tilde{I}_i \right), \]  

(2.46)

where \( \tilde{I}_i \) denotes the filtered radiation intensity per unit time per unit solid angle per unit area normal to the direction \( \vec{\Omega}_i \) and \( \mu_{i,j} \) denotes the direction cosines associated with this direction with respect to the Cartesian coordinate directions \( x_j \). Here we have invoked the grey gas assumption, to eliminate the functional dependence of radiation intensity on wavenumber, which is appropriate for fires from vegetative fuels [29] due its highly sooting character. The total radiation intensity per unit time and unit normal area is then computed via,

\[ G = \int_{4\pi} \tilde{I}_i d\Omega_i. \]  

(2.47)

Using \( G \) from this equation, the radiation heat source term in the energy equations of the \( L^{th} \) solid- and gas-phases, viz., equations (2.6) and (2.41) are computed as

\[ \frac{\partial \tilde{q}_{i,rad}}{\partial x_i} = \xi a_g (G - 4\sigma \tilde{T}^4), \]  

(2.48)

\[ \tilde{q}_{rad,L} = a_L (G - 4\sigma \bar{T}_L^4), \]  

(2.49)
where \( a_g \) and \( a_L \) denote the absorption coefficients for the gas- and the \( L^{th} \) solid-phase, respectively and \( \xi \) is the gas-phase porosity as defined in equation (2.1). For propagation of a surface fire through pine needles or excelsior fuel beds, experimental measurements of the heat fluxes received by a radiometer have shown that the model, \( a_L = \beta_L \sigma_L / 4 \) is appropriate [120]. In the case of \( a_g \), we make the gray gas assumption and use the empirical model proposed by Kaplan et al. (1996) [113], as follows,

\[
a_g = 0.1(\bar{X}_{\text{CO}_2} + \bar{X}_{\text{H}_2\text{O}}) + 1862 \tilde{f}_v \tilde{T},
\]

in units of \( \text{m}^{-1} \), noting that temperature is in degrees Kelvin. Though gas phase species contribute negligibly to \( a_g \) as compared to soot, they are retained for the sake of generality. The soot phase absorptivity shown in the last term of equation (2.50), is that used in RadCal package [121].

2.5 Soot Transport and Chemistry Model

As discussed in the previous section (Section 2.4), proper modeling of soot is important to obtain accurate predictions of radiation heat transfer. In a highly sooting flame the gas-phase consists of multiple species of gases and soot exists as a solid-phase. Soot particle size varies in the range of 200 to 400 \( \text{A} \) (at nucleation) to a few \( \mu\text{m} \) (for soot aggregates) [122]. The number density of soot particles (total soot particles in a unit volume) is relatively high, therefore to predict soot evolution an Eulerian approach is generally adopted, i.e., soot particle particle transport equations have same form as the gas-phase species transport equations. Soot formation in
flames specially turbulent flames, is a complex processes involving rich set of physical phenomena, such as, nucleation, coagulation, surface growth, agglomeration and oxidation, which makes experimental and computational investigations challenging [64]. Some of the difficulties involved in developing a comprehensive soot model for wildfire simulations are:

- Soot chemistry involves a complex set of reaction mechanism from nucleation to surface growth. Notably, formation of high molecular weight species like PAH’s is considered responsible for soot inception [123].

- The time scales of soot formation are longer than typical combustion time scales, resulting in overlap of soot chemistry and large-scale flow features [124].

- Pyrolysis gas generated due to decomposition of solid fuels varies a lot in composition for different fuel species [125]. Therefore identifying the precursor species required for soot nucleation and surface growth is difficult.

- As wildfires involve a broad range of spatial and temporal scales, resolution required for comprehensive soot model cannot be attained due limited computational power available.

Sophisticated models for soot particle evolution, have been developed and used in the context of hydrocarbon-air turbulent jet flames [126, 127]. Due to the lack of information on generation of soot from cellulosic fuels, we have retained a simple model in this work, which only accounts for evolution of soot volume fraction along with existing semi-empirical models, as described below. The soot volume fraction is
evaluated via the model transport equation,

\[
\frac{\partial \tilde{\rho} \tilde{f}_v}{\partial t} + \frac{\partial \tilde{\rho}(\tilde{u}_j + \tilde{u}_{j}^{th})\tilde{f}_v}{\partial x_j} = \frac{\partial}{\partial x_j} \{ -\tilde{\rho} (\tilde{u}_j \tilde{f}_v - \tilde{u}_j \tilde{f}_v) \} - \frac{\partial \bar{q}_{f_{v,i}}}{\partial x_i} + \bar{\omega}_{f_v}. \quad (2.51)
\]

In the above equation, \( \tilde{u}_j^{th} \) is the filtered thermophoretic velocity. Here, a similar model as that of Kaplan et al. (1996) [113] is used,

\[
\tilde{u}_j^{th} = -0.54 \tilde{\mu} \frac{\partial \ln \tilde{T}}{\partial x_j}, \quad (2.52)
\]

where the non-filtered value of temperature is replaced by the filtered value [128]. The quantity \( \bar{q}_{f_{v,i}} \) in equation (2.51), is the filtered soot diffusion flux vector, modeled using the standard Fick’s law based on the filtered quantities as

\[
\bar{q}_{f_{v,i}} = -\frac{\tilde{\mu}}{\tilde{S}_c} \partial \tilde{f}_v \partial x_j, \quad (2.53)
\]

and the subgrid-scale flux of soot is modeled using gradient diffusion hypothesis as,

\[
\tilde{\rho} \left( \tilde{u}_j \tilde{f}_v - \tilde{u}_j \tilde{f}_v \right) = -\frac{\mu_t}{\tilde{S}_c} \frac{\partial \tilde{f}_v}{\partial x_j}. \quad (2.54)
\]

A semi-empirical model based on the work of Kaplan et al. (1996) [113], for the source term \( \bar{\omega}_{f_v} \), in which filtered quantities are used, is utilized. This model presumes that, soot is formed primarily through pyrolysis of the solid fuel and neglects soot
formation via combustion reactions occurring in the gas-phase, written as

\[
\bar{\omega}_{fv} = \frac{\bar{\rho}}{\rho_{\text{soot}}} \left( 0.01 \tilde{m}_{\text{pyr}} - \frac{6 \tilde{f}_v}{d_{\text{soot}}} W_{\text{NSC}} \right), \tag{2.55}
\]

where \( \rho_{\text{soot}} \) denotes the density of solid soot particles, which is taken to be 1800 kg/m\(^3\). A typical soot particle diameter value of \( d_{\text{soot}} = 10 \mu m \) is assumed. The sink term in equation (2.55) models soot oxidation via the Nagle and Strickland (NSC) oxidation mechanism, given by [129]:

\[
W_{\text{NSC}} = 120 \left[ \frac{k_A P_{O_2}}{1 + k_z P_{O_2}} \chi + P_{O_2} (1 - \chi) \right], \tag{2.56}
\]

where,

\[
\chi = \frac{1}{1 + \frac{k_T}{k_B P_{O_2}}}. \tag{2.57}
\]

In the above equations, \( P_{O_2} \) is the partial pressure of oxygen and various reaction rates \( k_A, k_B, k_T, k_z \) occurring in the expression of \( W_{\text{NSC}} \) depend on temperature in following way [129],

\[
k_A = 200 \exp(-30000/R\tilde{T}), \quad \text{kg/m}^2\text{s atm} \tag{2.58}
\]

\[
k_B = 4.46 \times 10^{-2} \exp(-15200/R\tilde{T}), \quad \text{kg/m}^2\text{s atm} \tag{2.59}
\]

\[
k_T = 1.51 \times 10^6 \exp(-97000/R\tilde{T}), \quad \text{kg/m}^2\text{s} \tag{2.60}
\]

\[
k_z = 21.3 \exp(4100/R\tilde{T}), \quad \text{atm}^{-1}. \tag{2.61}
\]
CHAPTER 3

NUMERICAL METHODS

3.1 Introduction

The governing equations described in Chapter 2 are discretized in a three dimensional Cartesian coordinate system on a uniform cubic mesh, using finite-volume formulation with a staggered grid arrangement for velocities and scalars. For the gas-phase equations, the quadratic upwind interpolation for convective kinematics with estimated streaming terms (QUICKEST) finite volume scheme proposed by Leonard (1979) [130], has been implemented. A detailed formulation of QUICKEST is provided in Section 3.2. The solid-phase equations are integrated in time using forward Euler method. Calculation of the time step is based on satisfying the stability criteria dictated by the Courant numbers, defined based on the cell face convective velocities. Also, in this chapter, discrete ordinates method (DOM) used to solve the radiation transport equation is explained in Section 3.3, the initial and the boundary conditions are described in Section 3.4 and Section 3.5, respectively, and, the pressure-velocity coupling and the solution algorithm are described in Section 3.6.
Figure 3.1: Variable storage arrangement for staggered mesh on a $xy$-plane, the scalars are stored at cell centers (indicated by $\bullet$), $x$-component of velocity at east-west cell faces (indicated by $\rightarrow$) and $y$-component of velocity at north-south cell faces (indicated by $\uparrow$).

3.2 QUICKEST Finite-Volume Scheme

A finite volume discretization of the governing equations, on staggered grids, is used. The typical staggered grid is shown in Figure 3.1, where, $i$, $j$ and $k$ are the indices used for $x$, $y$ and $z$ directions, respectively. Here the scalars are stored at cell centers $(i, j, k)$, the $x$-component of velocities at east-west cell faces $(i \pm 1/2, j, k)$, the $y$-component of velocities at north-south cell faces $(i, j \pm 1/2, k)$ and the $z$-component of velocities at up-down cell faces $(i, j, k \pm 1/2$, not shown in Figure 3.1), respectively.
The variable storage arrangement thus results into four sets of overlapping grids, for a three dimensional configuration. Since the cell face velocities, required to evaluate the scalar fluxes, do not have to be obtained through interpolation, the staggered grids provide a better coupling between scalar and velocity fields as compared to collocated grids [131]. A certain drawback associated with staggered grids is its implementation in unstructured grids, which does not concern the current study (for additional information refer [132, 133]).

When a finite volume based integration scheme is used, the volume integrals of convection and diffusion terms are converted to surface integrals using the Gauss-divergence theorem. The surface integrals represent the amount of flux, of the quantity under consideration, entering or leaving the control volume due to transport mechanisms such as convection and diffusion. In order to obtain the face fluxes the scalars need to be interpolated at the location of the face, using its value at the cell center. The basic type of interpolation schemes are upwind or upstream differencing and central differencing. In upstream differencing (i.e. the donor cell technique [134]), the value of the variable at the face is set equal to the value of the upstream cell center. This scheme is unconditionally stable but has first-order truncation error. The stability is achieved by the introduction of large amount of numerical diffusion which compromises the validity of the results. On the other hand, the central differencing approximation uses a linear interpolation based on the cell center values on either side of the face to approximate the face value [135]. This scheme maintains a second order accuracy on uniformly spaced grids but gives rise to unphysical oscillations in regions where the sharp gradients exist (i.e. where convection dominates the diffusion
The quadratic upwind interpolation for convective kinematics (QUICK) scheme, outlined by Leonard [130] for one dimensional scalar transport equation, possesses good accuracy as that offered by central differencing while simultaneously maintaining the directional feature of upwind differencing. The QUICK scheme uses a three-point upstream-weighted quadratic interpolation, consisting of two upstream and one downstream cells, to approximate the convection fluxes whereas central differencing is used for the diffusive flux calculation. Detailed description of QUICK scheme can be found in Ferziger and Perić (2002) [135]. When similar type of curvature terms are introduced in time differencing, the resulting formulation is called QUICK with estimated streaming terms (QUICKEST) [130].

The QUICKEST scheme uses a quadratic upwind procedure for approximating the fluxes at the cell faces along with an explicit Leith-type of temporal discretization [136] for the unsteady part. A detailed QUICKEST formulation is given for two-dimensional scalar transport equation by Pereira and Sousa (1993) [137]. Here the three dimensional version of the formulation is presented. Consider a generic scalar transport equation

$$\frac{\partial \phi}{\partial t} + \frac{\partial (u_i \phi)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \nu \frac{\partial \phi}{\partial x_i} \right) + S(x_i, t), \quad (3.1)$$

where, $\phi$ is a scalar, $u_i$ is the convective velocity field, $\nu$ is the diffusivity of the scalar and $S$ is the source term. It is noted that, while dealing with momentum conservation equation there will be an additional term on RHS accounting for the pressure force, which is dealt with as a volumetric source term in this scheme. We
start by integrating equation (3.1) over time interval $\Delta t$ and control volume $v$. The first term yields

$$
\int_t^{t+\Delta t} \int_v \phi_i d\mathbf{v} dt = \int_{-\Delta x_i/2}^{\Delta x_i/2} \int_{-\Delta y_i/2}^{\Delta y_i/2} \int_{-\Delta z_i/2}^{\Delta z_i/2} (\phi^{n+1} - \phi^n) d\xi_i = v (\tilde{\phi}^{n+1} - \tilde{\phi}^n), \tag{3.2}
$$

where $\tilde{\phi}$ represents the value of the scalar averaged over the control volume. Consider a uniformly spaced mesh in all co-ordinate directions. A local frame of reference $(\xi_i)$ is defined at the cell center under consideration and the dependent variable is assumed to have a quadratic distribution in this reference frame, given by

$$
\phi = \sum_{i,j=1}^{N} A_{i,j} \xi_i \xi_j + \sum_{i=1}^{N} B_i \xi_i + C, \tag{3.3}
$$

which, for $N = 3$ can be written as

$$
\phi = c_1 + c_2 \xi_1 + c_3 \xi_1^2 + c_4 \xi_2 + c_5 \xi_2^2 + c_6 \xi_3 + c_7 \xi_3^2 + c_8 \xi_1 \xi_2 + c_9 \xi_2 \xi_3 + c_{10} \xi_1 \xi_3. \tag{3.4}
$$

Note, in defined reference frame $\xi_1$ is oriented along $x$-direction, $\xi_2$ is oriented along $y$-direction and $\xi_3$ is oriented along $z$-direction. The average value within each cell can then be obtained by integrating this polynomial as

$$
\tilde{\phi} = \frac{1}{\Delta x \Delta y \Delta z} \int_{-\Delta x/2}^{\Delta x/2} \int_{-\Delta y/2}^{\Delta y/2} \int_{-\Delta z/2}^{\Delta z/2} \phi d\xi_1 d\xi_2 d\xi_3 = c_1 + \frac{c_3}{12} \Delta x^2 + \frac{c_5}{12} \Delta y^2 + \frac{c_7}{12} \Delta z^2. \tag{3.5}
$$
Thus, equation (3.2) can be written as

\[
\int_t^{t+\Delta t} \int_v \phi_t dv dt = \mathbf{v} \left[ (c_1^{n+1} - c_1^n) + \frac{\Delta x^2}{12} (c_3^{n+1} - c_3^n) + \frac{\Delta y^2}{12} (c_5^{n+1} - c_5^n) + \frac{\Delta z^2}{12} (c_7^{n+1} - c_7^n) \right].
\]  

(3.6)

The coefficients of the polynomial are, \( c_1 = \phi_t, c_3 = 0.5(\partial^2 \phi / \partial \xi_1^2), c_5 = 0.5(\partial^2 \phi / \partial \xi_2^2) \) and \( c_7 = 0.5(\partial^2 \phi / \partial \xi_3^2) \). Following the intermediate steps as described in [137], which involves taking second spatial derivative of equation (3.1) and neglecting fourth order derivatives, the final expression for integrated value of the time derivative can be written as

\[
\int_t^{t+\Delta t} \int_v \phi_t dv dt = \mathbf{v} \left[ (\phi_{i,j}^{n+1} - \phi_{i,j}^n) \right.
\]

\[
- \left[ \frac{\Delta x^2}{24} \left( C_{i+1/2,j,k}^{+} \text{CURVX}_{i+1/2,j,k}^+ - C_{i-1/2,j,k}^{+} \text{CURVX}_{i-1/2,j,k}^+ \right) \right.
\]

\[
+ \frac{\Delta y^2}{24} \left( C_{i,j+1/2,k}^{+} \text{CURVY}_{i,j+1/2,k}^+ - C_{i,j-1/2,k}^{+} \text{CURVY}_{i,j-1/2,k}^+ \right)
\]

\[
+ \frac{\Delta z^2}{24} \left( C_{i,j,k+1/2}^{+} \text{CURVZ}_{i,j,k+1/2}^+ - C_{i,j,k-1/2}^{+} \text{CURVZ}_{i,j,k-1/2}^+ \right) \bigg] \right].
\]  

(3.7)

where the curvature terms, denoting the finite difference approximation to second derivatives, are given in the formulation provided towards the end of this section for calculating flux at each specific face of the control volume. The cell face Courant numbers \( (C) \), for example at the east face, are calculated as \( C_{i+1/2,j,k} = u_{i+1/2,j,k} \Delta t / \Delta x \).
Moving our attention to the convection and diffusion terms, for simplicity consider the x-component only, which are evaluated as

$$\int_{t}^{t+\Delta t} \int_{v} \left[ \frac{\partial (u\phi)}{\partial \xi_1} - \frac{\partial}{\partial \xi_1} \left( \nu \frac{\partial \phi}{\partial \xi_1} \right) \right] dv dt = \int_{t}^{t+\Delta t} \left[ u\phi - \nu \frac{\partial \phi}{\partial \xi_1} \right]^{i+1/2,j,k}_{i-1/2,j,k} A dt, \quad (3.8)$$

where the area of the face $A = \Delta \xi_2 \Delta \xi_3$. The first term in equation (3.8) can be written as

$$\int_{t}^{t+\Delta t} [u\phi]^{i+1/2,j,k}_{i-1/2,j,k} A dt = \int_{t}^{t+\Delta t} [u\phi]^{i+1/2,j,k}_{i+1/2,j,k} A dt - \int_{t}^{t+\Delta t} [u\phi]^{i-1/2,j,k}_{i+1/2,j,k} A dt. \quad (3.9)$$

The convection flux at east face $(i+1/2, j, k)$, assuming $u_{i+1/2,j,k} \geq 0$, can be computed by converting the time integral to a Lagrangian integral as follows

$$\int_{t}^{t+\Delta t} [u\phi]^{i+1/2,j,k}_{i+1/2,j,k} A dt = \int_{t}^{t+\Delta t} \left[ \tilde{\phi} (\xi_1) \right] A d\xi_1, \quad (3.10)$$

where, $\Delta \xi_1$ is the distance traveled by the scalar field $\tilde{\phi}$ (averaged in $\xi_2$ and $\xi_3$ directions) due to local convection velocity $u_{i+1/2,j,k}$ in time interval $\Delta t$. Note, the convective velocities are assumed to be independent of space and time in the local
vicinity of the face under consideration [138]. Therefore

\[ \Delta \xi_1 = \int_t^{t+\Delta t} u_{i+1/2,j,k} dt = u_{i+1/2,j,k} \Delta t = C_{i+1/2,j,k} \Delta x, \quad (3.11) \]

with the average value of \( \phi \) at the east face given by

\[ \tilde{\phi} = \frac{1}{\Delta y \Delta z} \int_{-\Delta \xi_2/2}^{\Delta \xi_2/2} \int_{-\Delta \xi_3/2}^{\Delta \xi_3/2} \phi(\xi_1, \xi_2, \xi_3) d\xi_2 d\xi_3 = c_1 + c_2 \xi_1 + c_3 \xi_2 + \frac{c_5}{12} \Delta y^2 + \frac{c_7}{12} \Delta z^2. \quad (3.12) \]

The integral in equation (3.10) can therefore be evaluated as

\[ \int_0^{\Delta \xi_1} \left[ \tilde{\phi}(\xi_1) \right] A d\xi_1 = A \left[ c_1 \xi_1 + \frac{c_2}{2} \xi_1^2 + \frac{c_3}{3} \xi_3^3 + \frac{c_5}{12} \Delta y^2 \xi_1 + \frac{c_7}{12} \Delta z^2 \xi_1 \right]^{\Delta \xi_1/2}_{\Delta \xi_1/2-C_{i+1/2,j,k} \Delta x}, \quad (3.13) \]

where the coefficients \( c_1, c_2, c_3, c_5 \) and \( c_7 \) are evaluated from the quadratic function, equation (3.4), at time \( t \) in the \( (\xi_1, \xi_2, \xi_3) \) reference frame. In case of velocity reversal, i.e. \( u_{i+1/2,j,k} \leq 0 \), the origin of the reference frame \( (\xi_1, \xi_2, \xi_3) \), will be located at \( (i+1, j, k) \). Similar procedure can be followed to evaluate the integral of the second term in equation (3.8), to obtain the required diffusion flux at the cell face [137].
Putting it all together, the dependent variable at time \((n + 1)\), for each grid cell, can be obtained as

\[
\phi_{i,j,k}^{n+1} = \phi_{i,j,k}^n + \left[ F_{i-1/2,j,k} - F_{i+1/2,j,k} + F_{i,j-1/2,k} - F_{i,j+1/2,k} + R_{i,j,k} + S_{i,j,k} \right] \quad (3.14)
\]

where, \(F\) is the convective plus diffusive flux at the face, \(R\) is the pressure gradient term (nonzero only for the momentum transport equations) and \(S\) represents all source terms lumped together.

Starting with the east face, the equation for the flux can be written as follows,

\[
F_{i+1/2,j,k} = \psi_{1e} + \psi_{2e} + \psi_{3e}
\]

\[
\psi_{1e} = A \cdot C_{i+1/2,j,k} \Delta x \left[ \left( \frac{\phi_{i+1,j,k} + \phi_{i,j,k}}{2} \right) - C_{i+1/2,j,k} \left( \frac{\phi_{i+1,j,k} - \phi_{i,j,k}}{2} \right) \right]
\]

\[
\psi_{2e} = A \Delta x \left[ -\frac{\Delta x^2}{6} \left( 1 - C_{i+1/2,j,k}^2 \right) \left( \alpha_{i+1/2,j,k}^{+} \text{CURVX}_{i+1/2,j,k} + \beta_{i+1/2,j,k}^{-} \text{CURVZ}_{i+1/2,j,k} \right) \right.
\]

\[
+ \frac{\Delta y^2}{24} \left( \alpha_{i+1/2,j,k}^{+} \text{CURVY}_{i+1/2,j,k} + \beta_{i+1/2,j,k}^{-} \text{CURVZ}_{i+1/2,j,k} \right)
\]

\[
+ \frac{\Delta z^2}{24} \left( \alpha_{i+1/2,j,k}^{+} \text{CURVZ}_{i+1/2,j,k} + \beta_{i+1/2,j,k}^{-} \text{CURVZ}_{i+1/2,j,k} \right) \right]
\]

\[
\psi_{3e} = -A \gamma_{i+1,j,k} \Delta x \left[ (\phi_{i+1,j,k} - \phi_{i,j,k}) - \frac{\Delta x^2}{2} \left( \alpha_{i+1,j,k}^{+} \text{CURVX}_{i+1,j,k} + \beta_{i+1,j,k}^{-} \text{CURVZ}_{i+1,j,k} \right) \right]
\]
where the parameters are given as follows

\[
\alpha_e = \left( C_{i+1/2,j,k} + |C_{i+1/2,j,k}| \right) / 2
\]
\[
\beta_e = \left( C_{i+1/2,j,k} - |C_{i+1/2,j,k}| \right) / 2
\]
\[
\gamma_e = \nu_{i+1/2,j,k} \Delta t / \Delta x^2.
\]

The curvature terms appearing in the above formulation are given as

\[
\text{CURVX}^{+}_{i+1/2,j,k} = \left( \phi_{i+1,j,k} + \phi_{i-1,j,k} - 2\phi_{i,j,k} \right) / \Delta x^2
\]
\[
\text{CURVX}^{-}_{i+1/2,j,k} = \left( \phi_{i+2,j,k} + \phi_{i,j,k} - 2\phi_{i+1,j,k} \right) / \Delta x^2
\]
\[
\text{CURVY}^{+}_{i+1/2,j,k} = \left( \phi_{i,j+1,k} + \phi_{i,j-1,k} - 2\phi_{i,j,k} \right) / \Delta y^2
\]
\[
\text{CURVY}^{-}_{i+1/2,j,k} = \left( \phi_{i+1,j+1,k} + \phi_{i+1,j-1,k} - 2\phi_{i+1,j,k} \right) / \Delta y^2
\]
\[
\text{CURVZ}^{+}_{i+1/2,j,k} = \left( \phi_{i,j,k+1} + \phi_{i,j,k-1} - 2\phi_{i,j,k} \right) / \Delta z^2
\]
\[
\text{CURVZ}^{-}_{i+1/2,j,k} = \left( \phi_{i+1,j,k+1} + \phi_{i+1,j,k-1} - 2\phi_{i+1,j,k} \right) / \Delta z^2.
\]

The expressions for the fluxes at remaining faces are provided in the Appendix Section A.1.

### 3.3 Discrete Ordinates Method

The discrete ordinates method (DOM), proposed by Chandrasekhar (1960) [139], is used to compute intensities in \( M \) discrete directions, per octant. The value of \( M \) is given by \( N(N+2) \), where \( N \) is the index of \( S_N \)-method used. This method transforms...
the RTE, i.e., equation (2.46), into a set of simultaneous partial differential equations, given as

\[
\mu_i \frac{\partial \xi \tilde{I}_i}{\partial x} + \mu_i \frac{\partial \xi \tilde{I}_i}{\partial y} + \mu_i \frac{\partial \xi \tilde{I}_i}{\partial z} + \xi a_g \tilde{I}_i + \sum_{L=1}^{N_L} a_L \tilde{I}_i = \\
\xi a_g \left( \frac{\sigma T_i^d}{\pi} \right) + \sum_{L=1}^{N_L} \frac{\sigma T_L^d}{\pi}, \tag{3.15}
\]

where, \( i = 1 \ldots M \), each equation is associated with one discrete direction. The PDE’s are further integrated over each control volume, converting the volume integral into surface integrals as follows (shown only for the x-direction),

\[
\int_V \frac{\partial \xi \tilde{I}_i}{\partial x} dV = \int_A \xi \tilde{I}_i dA = \xi \left[ \tilde{I}_{ei} A_e - \tilde{I}_{wi} A_w \right], \tag{3.16}
\]

where \( \tilde{I}_{ei} \) and \( \tilde{I}_{wi} \) are the intensities in the \( i \)th discrete direction averaged over the east \((i + 1/2, j, k)\) and the west \((i - 1/2, j, k)\) cell faces, respectively. The procedure results into a set of algebraic equations which is then solved iteratively. A “weighted diamond differencing” scheme [140] with a weight of 0.5 is used to relate the cell face intensities to cell center intensities. Further details on this method can be found in Modest (2003) [119]. The integral appearing in equation (2.47) is evaluated using a rectangular quadrature approximation, given by

\[
G = \sum_{i=1}^{N} w_i I_i, \tag{3.17}
\]
where \( w_i \) is the discrete solid angle in the \( i^{th} \) direction over which radiative intensity is considered to be constant. The weights associated with the quadrature approximation in equation (3.17) and direction cosines used in equation (2.46) are those provided by Lathrop and Carlson (1965) [141] and reproduced in Modest (2003) [119].

### 3.4 Initial Conditions

All simulations are conducted in a quiescent environment, i.e., in the absence of externally imposed wind. Therefore, the flow field is initialized with zero velocities in all directions. The initial gas-phase temperature and pressure throughout the domain are assumed to be 300 K and 1 atm, respectively, equal to standard ambient conditions. The initial chemical composition throughout the domain is that of ambient air with relative humidity of 30\% [27]. The initial solid-phase temperature is equal to 300 K throughout the fuel matrix. In all cases to be discussed, the shape and initial dry mass of the shrub is same. To ignite the solid fuel a volumetric heating source is used, active only in the ignition zone. During ignition the heating of the solid fuel is modeled through the mechanism of convective heat transfer. After 80\% of the solid mass in the ignition zone is consumed, the igniter is turned off.

### 3.5 Boundary Conditions

A buoyancy driven flow field is generated by the shrub fires due to which the ambient air is entrained in the vertically rising plume. The lateral boundaries are thus modeled with a pressure based inlet boundary condition allowing the mass flux to enter and leave the domain. The outflow of mass is calculated by setting the
boundary normal gradients equal to zero. When the flow is entering the domain, the boundary normal component of inlet velocity is calculated based on the pressure inside the domain, using Bernoulli equation (applicable to inviscid, incompressible, steady flow) [142]. In doing so it is assumed that the fluid particle entering the domain is accelerated from the external stagnation condition, where the pressure is equal to one atmosphere, along a streamline to the point on the boundary. When the flow is entering the domain the values of scalars, such as temperature, species mass fraction, etc., at the boundary are set equal to the ambient conditions. These boundary conditions are thus essentially applicable to far-field open boundaries.

The bottom boundary of the domain is modeled as a wall with free-slip boundary condition, i.e., only the velocity component normal to the boundary is set equal to zero. The values of other two components of velocity, which are parallel to the wall, and the scalars are obtained by setting their respective wall normal gradients equal to zero. Using this boundary condition at bottom surface restricts any flow across the boundary.

For buoyancy driven flow simulations, two types of boundary conditions are popularly used for the top boundary. First is the convective outflow boundary condition [143–145] and second is the zero gradient boundary condition [146–148]. In the convective boundary condition all the flow structures are assumed to be convected out from the boundary at a certain specified velocity. The zero gradient boundary condition sets the boundary normal gradients, of all the transported variables, equal to zero, at the same time, all negative values of the normal component of velocity (flow entering the domain through this boundary) are also set equal to zero. Both
Figure 3.2: Time evolution of mass of shrub (kg), using convective boundary condition and zero gradient boundary condition for top surface of the computational domain.

these boundary conditions try to avoid flow reversal, which can be a potential source for numerical instabilities, at the top boundary. In current simulations both the boundary conditions were tried for the top surface of the domain. Results indicate negligible difference in global parameters (such as, time evolution of mass of a burning shrub shown in Figure 3.2) as well as local flow field generated (analyzed through snapshots of velocity vectors at various time instances; shown in Appendix B for one typical time instance), if the height of the computational domain is sufficiently large (the size of the computational domain is discussed in Results section as it changes from one case to another). Therefore, in simulations reported, the top boundary is modeled with convective outflow boundary condition where the convection velocity
is set equal to local boundary normal velocity calculated at an interior node adjacent to the boundary.

3.6 Pressure-Velocity Coupling and The Solution Procedure

For the sake of clarification of the solution procedure used to solve the governing equations, consider the following set of equations,

\[
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = S \tag{3.18}
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial u_i}{\partial x_j} \right) - \frac{\partial p}{\partial x_i} + E_i \tag{3.19}
\]

\[
\frac{\partial \rho \phi_k}{\partial t} + \frac{\partial \rho u_j \phi_k}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D_k \frac{\partial \phi_k}{\partial x_j} \right) + R_k \tag{3.20}
\]

\[
\rho = \frac{p_0}{(RT)} \tag{3.21}
\]

\[
\frac{\partial m_{solid}}{\partial t} = M_{solid} \tag{3.22}
\]

\[
\frac{\partial e_{solid}}{\partial t} = E_{solid}. \tag{3.23}
\]

Here, equations (3.18) to (3.20) are the gas-phase continuity, the \(i^{th}\) component of momentum, and the scalar transport equations, respectively. Equation (3.21) is the state equation and, equations (3.22) and (3.23) are the solid-phase mass balance and solid-phase energy balance equations, respectively. The scalar transport equation (3.20) for the \(k^{th}\) scalar, where \(k = 1 \ldots N_k\), represents the conservation of the \(N_k\) gas-phase species and \(k = N_k + 1\) is the gas-phase energy conservation equation. These equations are exactly the same as those discussed in Section 2.2 (for gas-phase) and Section 2.3 (for solid-phase) with the exception that all the source terms have been
lumped together. While numerically integrating these equations, all source terms are evaluated in a volumetric sense, therefore, combining the source terms makes it easy to distinguish between the flux quantities and the volume averaged quantities. The gas-phase equations are integrated using the QUICKEST algorithm (Section 3.2) and the solid-phase equations using forward Euler time scheme.

Let us use \( n \) to represent the time step and \( m \) to represent the inner iteration index. To obtain the variables at time step \( n + 1 \) we proceed as follows, using an explicit time integration procedure:

1. Evaluate the source terms appearing in above equations ((3.18) to (3.23)) at time step \( n \). The initial conditions corresponds to the time level \( n = 0 \).

2. Integrate the solid phase equations (3.22) and (3.23) using a forward Euler method.

3. Solve the scalar transport equations (3.20) as follows

\[
(\rho \phi_k)^{n+1} = (\rho \phi_k)^n + F^n_{\phi,k} + R^n_k, \tag{3.24}
\]

where \( F^n_{\phi,k} \) represents all the face fluxes, evaluated by QUICKEST algorithm (Section 3.2), and \( R^n_k \) the volumetric source terms appearing in the transport equation for \( k^{th} \) scalar, respectively.

4. Solve the momentum equations (3.19) neglecting the pressure gradient

\[
(\rho u_i)^* = (\rho u_i)^n + F^n_{\text{mom},i} + F^n_i, \tag{3.25}
\]

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where $F_{mom,i}^n$ represents the face fluxes, evaluated using QUICKEST algorithm (Section 3.2), and $E^n_i$ the volumetric source terms for the $i^{th}$ component of velocity, respectively. The velocity field obtained (indicated by superscript $*$) does not satisfy the continuity as the contribution of pressure is missing from it.

5. Start the inner iterations

5a. Obtain the scalar values using density from previous iteration, as

$$\phi_k^m = (\rho \phi_k)^{n+1} / \rho^{m-1}.$$  \hspace{1cm} (3.26)

If $m$ equals one then $(m - 1) = 0$, which corresponds to the $n^{th}$ time step. That is for $m = 1$, $\rho^{n-1} = \rho^n$.

5b. Since density is a function of thermodynamic properties and background pressure, it is evaluated using the equation of state (since all the scalars at $m^{th}$ inner iteration are known)

$$\rho^m = f(p_0, \phi_k^m)$$ \hspace{1cm} (3.27)

Due to the low Mach number (nearly incompressible) nature of the flow, the continuity equation (3.18) is used to ensure mass conservation at every time step.
5c. Pressure is obtained from the solution of the Poisson equation

\[
\frac{\delta}{\delta x_i} \left( \frac{\delta p^m}{\delta x_i} \right) = S^{n+1} - \left( \frac{\rho^m - \rho^n}{\Delta t} + \frac{\delta (\rho u_i)^*}{\delta x_i} \right). \tag{3.28}
\]

Here, \( \delta/\delta x_i \) represents a numerical discretization operator approximating the spatial differentiation [149]. The resulting system of equations is solved iteratively, using the strong implicit method described by Stone (1968) [150] to obtain \( p^m \).

5d. Update the velocities at the \( m^{th} \) inner iteration with pressure contribution

\[
(\rho u_i)^m = (\rho u_i)^* + \frac{\delta p^m}{\delta x_i}, \tag{3.29}
\]

where \( u_i^m = (\rho u_i)^m / \rho^m \).

5e. Calculate the residual (Res) from continuity equation using \( \rho^m \) and \( u_i^m \)

\[
\left( \frac{\rho^m - \rho^n}{\Delta t} \right) + \frac{\delta (\rho u_i)^m}{\delta x_i} - S^{n+1} = \text{Res}. \tag{3.30}
\]

5f. If the residual, Res, calculated from the continuity equation exceeds the specified error limit, go to step 5a and continue the inner iterations. If the residual is below the specified limit proceed to step 6.

6. The values of the variables calculated at the \( m^{th} \) inner iteration now represents the converged solution required at the \( (n + 1)^{th} \) time step. With the stage now set, the above steps from 1 to 6 are repeated till the end of simulation.
It is borne in mind that to obtain the Poisson equation for pressure, the numerical divergence ($\delta / \delta x_i$) is applied on equation (3.29) and then substituted in the discrete continuity equation. The time step size is determined based on satisfying the Courant number restriction of $C \leq 0.2$. 
CHAPTER 4

RESULTS - BURNING OF A SINGLE SHRUB

4.1 Introduction

Figure 4.1(b) shows the computational domain size and the fuel setup used for modeling the single shrub burn. The dimensions of the computational domain are 1.6 m, 3.2 m, and 1.6 m in $x$, $y$, and $z$ directions, respectively. Computations reveal that the results could be somewhat affected if the dimension of the domain in the vertical direction ($y$ direction) is too short. However, the results become insensitive to the domain height when this dimension is larger than 3.2 m. The rationale for simulation setup, surface and crown fuel dimensions etc., is guided by previous experimental conditions, to be discussed.

The grid resolution used here is $80 \times 160 \times 80$ in $x$, $y$, $z$ directions, respectively, resulting into a grid size of 2 cm in every direction. The computations in the code are performed through parallel processing based on the MPI (message passing interface) protocol. All computations reported in this chapter are done using 40 processors of a dense memory cluster (DMC, located at Alabama Supercomputing Center, Huntsville, Alabama) and 12 gigabytes of memory. The CPU time and the wall time for 100 seconds of fire spread simulation are about 5000 hours and 125 hours, respectively.
The LES model discussed in Chapter 2 is based on an implicit filtering approach, in which changing the grid resolution causes the LES results to change. This change of results continues as the resolution increases until the results converge to the DNS (Direct Numerical Simulation) results [151–153]. This means that LES converges to DNS when the grid size is at the order of Kolmogorov length scale, which for shrub fires is of the order of 0.1 to 0.5 mm [20]. Also, in chemically reacting flows, additional complications exist. For example, the smallest chemical length scales are of the order of $10^{-8}$ m for sooting turbulent fires, which are appreciably smaller than the smallest turbulence length scales [84]. In typical hydrocarbon flames the time scales associated with chemistry is of the order of $10^{-4}$ sec whereas that associated with turbulent transport is of the order of 1 sec, rendering the Damkohler number of $O(10^4)$ [20]. Resolving these time and length scales completely is computationally demanding. Because of this, the grid resolution study is not relevant to the LES modeling based on the implicit filtering. The approach in selecting this grid resolution was guided by the extensive grid independence study carried out in a closely related work (Zhou et al. (2005) [27], governing equations based on Unsteady-RANS and two dimensional computations); where, the solid phase combustion model, thermal radiation model and the computational parameters involved are exactly the same as those used here. Later, Zhou et al. (2007) [28] using the same LES model and grid resolution (discussed above), showed a good comparison between computational and experimental results. Therefore the grid resolution chosen represents a balance in obtaining results that are considered nearly independent of computational parameters and keeping the computational cost within reasonable limit.
While calculating the bulk density, defined as mass of dry solid fuel per unit volume, of fuel matrix, mass of all $N_L$ solid-phase species is taken into account. In all the results to be presented in this chapter, the surface fuel (aspen excelsior) has dimensions of 0.8 m, 0.1 m, 0.8 m in $x$, $y$, $z$ directions, respectively, and is modeled as a single solid phase species with a constant bulk density of 3.125 kg/m$^3$. Total wet mass of surface fuel is 250 gm, similar to that used in experiments. The shape of the crown-like elevated fuel is modeled as a conical frustum with its diameter changing as a function of its height. As a first approximation, the functional dependence of crown diameter on height ($y$) is modeled using a cubic polynomial. Figure 4.1(a) shows image of a typical chamise shrub, on which a computational shrub image has been superimposed. For the crown fuel used in this study, $N_L$ is equal to two, as the shrub contains branches and foliage. All simulations are performed with no-wind, zero slope condition.

4.2 Comparison with Experimental Data

In the experimental work of Li (2011) [46], used for the validation of modeling results, the ignition of the surface fuel is carried out by spraying 10 ml of isopropyl alcohol in the ignition region and then supplying external heat to this region (using a torch flame). Isopropyl alcohol is used to establish uniform burning of fuel in the ignition region. In computations the ignition is achieved by using a volumetric heating source, active only in the ignition zone, as described in Section 3.4. The external heat source is turned off when 80% of fuel in ignition zone is consumed. Since surface fuel in all of the simulations performed, reported in this chapter, was kept the same, the
Figure 4.1: (a) Computational shrub superimposed on the image of a real chamise shrub; (b) Three dimensional view of the modeling setup; (c) Bulk density distribution for chamise as a function of shrub height [46].
igniter gets turned off around 7 seconds. In the experiments, Li (2011) [46] observed the time history of gas-phase and solid-phase temperatures, at center of ignition zone, to match that obtained from computations; hence, we adopt the same ignition mechanism. The dimensions of the ignition zone (0.15 m×0.1 m×0.15 m in x, y and z directions respectively) used in experiments are kept the same while performing computations.

The experiments [46], were performed in an open wind tunnel at the University of California Riverside, Riverside, California. Chamise was used as the crown fuel with a medium bulk density (bulk density ranging from 3.17 to 4.2 kg/m$^3$, considered medium [154]), zero wind speed and a center ignition. Additional details on experimental setup, data acquisition and post processing can be found in Li (2011) [46]. The geometry and physical properties of the modeled crown, such as the total height, initial mass, bulk density, moisture content, etc, are set to match the properties of the actual chamise shrub, in a global sense. These properties are tabulated in Table 4.1. It is noted that there still exist local heterogeneities in the actual shrub that are neglected in the modeled shrub. Therefore, only the global features of fire behavior in experiments and simulations are compared against each other.

The bulk density of the crown fuel is spatially distributed along the vertical direction, with distribution modeled as a polynomial function of vertical space variable given as follows,

$$\rho_B = A + B\widehat{y} + C\widehat{y}^2 + D\widehat{y}^3,$$  \hspace{1cm} (4.1)
Table 4.1: Initial conditions of crown fuel during experiment and simulation.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Average Bulk density of crown fuel</td>
<td>3.8 kg/m³</td>
</tr>
<tr>
<td>Total height of crown fuel</td>
<td>1.0 m</td>
</tr>
<tr>
<td>Sample Diameter (crown fuel largest diameter)</td>
<td>0.7 m</td>
</tr>
<tr>
<td>Bottom surface diameter (crown fuel)</td>
<td>0.16 m</td>
</tr>
<tr>
<td>Top surface diameter (crown fuel)</td>
<td>0.56 m</td>
</tr>
<tr>
<td>Total initial mass of crown fuel</td>
<td>0.7 kg</td>
</tr>
<tr>
<td>Crown fuel moisture content</td>
<td>31.2 %</td>
</tr>
</tbody>
</table>

where \( \hat{y} = \frac{y}{H} \), with \( y \) and \( H \) as the vertical spatial variable and the height of the shrub, respectively. This polynomial, as shown in Figure 4.1(c), has been recently proposed and is based on experimental measurements with \( A = -0.025 \), \( B = 32.325 \), \( C = -58.746 \) and \( D = 29.239 \), for chamise [46].

The overall time evolution of the fire, i.e., the ignition at the surface fuel and the transition from the surface to crown fuel, can be seen in Figure 4.2, in which the contour plots of the gas-phase temperature (color contours) and the solid fuel bulk density (line contours) are displayed on an \( xy \)-slice passing through the domain at \( z=0.8 \) m, at various instants of time. It is observed that a low intensity flame is established in the ignition zone at earlier times during simulation when the igniter is on. The surface fuel is ignited at the center below the base of crown fuel. This type of ignition represents a basic example of spotting fire, commonly seen during wildland fires. As more amount of mass in the ignition zone begins to burn, the intensity of the fire increases, which enhances the amount of heat transferred to neighboring fuel elements. Since the igniter gets turned off at fairly earlier times (7 sec) in simulation, the effect of igniter on computational results can be considered negligible.
Figure 4.2: Gas-phase temperature in Kelvin (color contours) with solid fuel bulk density (line contours) at various times for Case 1 (see Table 4.3); Snapshots are from a $xy$-slice passing through $z = 0.8$ m.

The Figure 4.3, shows the relative importance of the convection and radiation heat transfer, in igniting fuel particles, at two different locations. Point 1 is located at the base of the crown fuel and point 2 is on the surface fuel just outside the ignition zone. In the initial stages of burning, fuel particles located at the base of crown fuel receives more heat through convection compared to that received in form of thermal radiation. In contrast, for fuel particles located on the surface fuel, outside the ignition zone, radiation plays a major role in starting the burning process. This difference in the heat transfer mechanism at two locations is due to the flow field resulting from the buoyancy effects, shown in Figure 4.4, where the color contour is for the gas-phase temperature and line contour for the stream lines. Cold air entering the ignition zone from outside leads to convective cooling of fuel particles at point 2, whereas the hot combustion gases, which tend to rise up from flames, heat the crown
Figure 4.3: Time history of radiation and convection heat fluxes (\(\bar{q}_{\text{rad},L}\) and \(\bar{q}_{\text{conv},L}\), from Equation 2.41) at two spatial locations for Case 1 (see Table 4.3). Loc. 1: \(x = 0.8\) m, \(y = 0.3\) m, \(z = 0.8\) m (a point on the base of crown fuel); Loc. 2: \(x = 1.0\) m, \(y = 0.05\) m, \(z = 0.8\) m (a point on surface fuel outside ignition zone); Positive heat flux means heat is transferred from gas-phase to solid fuel particle and negative heat flux means vice versa.

fuel base in a convective sense, including where point 1 is located. Ignition occurs in the crown fuel at around 8.4 sec when temperature of solid fuel at point 1 reaches 500 K, when pyrolysis and char oxidation processes commence. Crown fire initiation time, calculated based on solid fuel temperature averaged over the \(xz\)-surface located at \(y = 0.3\) m, for this case is 10.8 sec. The burn is completed when the mass loss rate, \(\dot{m} = -\frac{dm}{dt}\), for the crown fuel equals zero. The burn time for Case 1 is about 82 seconds.
Figure 4.4: Gas-phase temperature in Kelvin (color contours) with stream lines (line contours and arrows) at time equals 35.6 seconds (around peak mass loss rate); Snapshot is from Case 1 along a $xy$-slice passing through $z = 0.8$ m.
Table 4.2: Parameters concerned with global behavior of fire in experiments and simulations. Two values seen for experiments are based on two repetitions of the experiments [46] with crown fuel bulk density of $\rho_B = 3.17 \text{ kg/m}^3$ and $\rho_B = 4.42 \text{ kg/m}^3$ respectively. Average bulk density of the computational shrub is $3.8 \text{ kg/m}^3$.

<table>
<thead>
<tr>
<th>Results</th>
<th>Experimental</th>
<th>Computational</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fire spread rate along $y$, in crown fuel</td>
<td>25.3 - 23.2</td>
<td>27.0</td>
</tr>
<tr>
<td>(mm/sec)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Fire spread rate along $x$, in surface fuel</td>
<td>5.88 - 6.21</td>
<td>4.0</td>
</tr>
<tr>
<td>(mm/sec)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Maximum mass loss rate (g/sec)</td>
<td>30.0 - 31.0</td>
<td>44.0</td>
</tr>
<tr>
<td>Time required to reach maximum mass loss rate</td>
<td>32 - 45</td>
<td>34</td>
</tr>
<tr>
<td>Time (sec)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Burning time (sec)</td>
<td>73 - 112</td>
<td>82</td>
</tr>
<tr>
<td>Mass consumed, crown fuel (g)</td>
<td>402 - 553</td>
<td>493</td>
</tr>
</tbody>
</table>

Table 4.2 shows a comparison between experimentally obtained data and numerical simulation predictions. Parameters such as burning time, total mass consumed, spread rates and the time required to reach the maximum mass loss rate are in good agreement. The spread rate calculation from simulation data is based on average solid phase temperature, and is representative of an average rate of vertical spread. As the flow field generated is three dimensional and does not have homogeneity in any direction, averaging of the solid phase temperature is performed on horizontal surfaces ($xz$-plane) at various $y$ locations along crown fuel height. Vertical spread rate is calculated as follows,

$$\text{ROS}_y = \sum_{i=1}^{M} \left( \frac{y_{i+1} - y_{i}}{t_{500,i+1} - t_{500,i}} \right) / (M - 1).$$

(4.2)

Here, $\text{ROS}_y$ is the average spread rate in $y$ direction, $y_i$ is the location of $i^{th}$ horizontal ($xz$) surface of crown fuel along $y$ axis, $t_{500,i}$ is the time required by solid fuel in this
Figure 4.5: Solid-phase temperature equals 500 K (red), solid fuel bulk density (kg/m$^3$, line contour) and approximate location of pyrolysis front at two different time instances (tracked using solid-phase temperature of 500 K, white circles); on an xz-slice passing through surface fuel at $y = 0.05$ m.

horizontal surface to reach the average temperature equivalent to 500 K and $M$ is the total number of surfaces considered for spread rate calculation. For all simulations reported in this chapter, $M$ is set equal to 8, the horizontal surfaces separated by a distance of 0.1 m are used for averaging. The horizontal fire spread rate in surface fuel was measured by observing the solid-phase temperature contour of 500 K, along an xz-slice passing through $y = 0.05$ m at various times, as shown in Figure 4.5. In this figure the circles (white) are used to represent the approximate location of the
Figure 4.6: Time history of mass loss rate from experiments (Test 1 and Test 2) conducted by Li (2011) [46] and from simulation of Case 1 (from Table 4.3).

The time history of mass loss rate obtained from computation matches well with experiments in a global sense, which can be seen from Figure 4.6, but the predicted value of maximum mass loss rate differs considerably from experimental results (overestimated by a factor of 1.4). This difference may be attributed to the following reason: The crown fuel model accounts for the distribution of mass only in the vertical direction whereas in a real shrub, mass is non-uniformly distributed in all three directions. Distribution of mass also varies from shrub to shrub of the same species. Since the functional form of mass distribution in directions other than $y$ is
unknown, bulk density is kept constant along these directions in the current crown fuel model. Another source of error leading to discrepancies between computational and experimental results is the uncertainty involved in the experimental measurements. For example, FFT (fast Fourier transform) based smoothing was applied to the time history of mass that was obtained from experiments, before calculating the mass loss rate. This procedure, although necessary for removing high frequency white noise from the data, may also lower the peak values. Also, the horizontal fire spread rate, through the fuel bed, predicted by the model is slightly less than the experimental values. This discrepancy could be due to the shortcoming of the radiation model used, since fire spread in horizontal direction occurs mainly due to radiative heat transfer.

Next, we highlight the importance of two physical parameters, viz., distribution of solid fuel mass inside the crown fuel and the moisture content of crown fuel, involved in the current fire propagation problem with the aid of the simulation results. A total of 12 cases were modeled to study the effect of these two input parameters on shrub fires. The modeling setup has the same arrangement of the crown and ground fuel as discussed in Section 4.2. The conditions used for simulation of various cases,
are summarized in Table 4.3. Further in Section 4.5, effect of soot thermophoresis
(mechanism for soot particle transport) on shrub fires is highlighted using results
obtained from two cases consisting of same fuel arrangement.

4.3 Effects of Bulk Density Distribution

In this section we compare the performance of two models used to represent
the bulk density of the crown fuel. In the first model (Case 1 in Table 4.3), the
bulk density of the shrub is spatially distributed along vertical axis as described by
Equation 4.1 and shown in Figure 4.1(c). In the second model, used in simulation
of Case 2 from Table 4.3, the bulk density is kept constant and equal to 3.87 Kg/m$^3$
throughout the crown fuel volume. The fixed bulk density value represents the average
of the polynomial distribution given by Equation 4.1. The simulation setup, geometric
and the other physical properties of the solid fuel, boundary and initial conditions
are kept the same in simulation of Case 1 (to be referred as DBD: distributed bulk
density) and Case 2 (to be referred as FBD: fixed bulk density). Solid fuel parameters
to be presented, are mass averaged over $N_L$ solid phase species.

Figure 4.7(a) and (b) shows the time evolution of the gas-phase and solid-
phase temperatures, respectively, averaged on the bottom and top surfaces of the
crown fuel. Averaging is performed along the $xz$-planes as the bulk density remains
constant in this plane for both cases. As it can be seen in this figure, the time history
of the bottom surface temperature (gas- and solid-phase) for Case 1 is not significantly
different than that in Case 2. On the other hand, the time history of temperature (gas-
and solid-phase) for the top surface of crown fuel obtained from Case 1 is considerably
Figure 4.7: Time evolution of (a) gas-phase temperature; and (b) solid-phase temperature; $T_T$ and $T_B$ are obtained based on the averaging of temperatures on planes passing through the top and the bottom of the shrub; for crown fuel modeled with distributed bulk density (Case 1) and fixed bulk density (Case 2), respectively; Cases are from Table 4.3.
different than that for Case 2. This difference indicates that fire propagation rate inside the crown fuel matrix changes when bulk density distribution is accounted for. For both cases, the crown fire initiation time is about \( t = 11.0 \) seconds, i.e., when the average solid phase temperature at bottom surface of crown fuel reaches 500 K. In Figure 4.8(a), \( t_{500} \) is the time in seconds required by a horizontal surface in the crown fuel to reach a temperature equal to 500 K, which is plotted as a function of shrub height. Figure 4.8(b) shows the spread rate in mm/s as a function of the height of the crown fuel. The fire spread rate in the lower part of the crown for the DBD case is observed to be lower as compared to that in the FBD case, whereas, in the upper region fire spreads relatively faster for DBD than FBD. This difference in spread rates for these two models, can be explained based on bulk density values encountered for different regions of the crown fuel while moving along its vertical axis. The lower half of the crown with DBD has a higher bulk density compared to crown with FBD, which creates a higher resistance for the hot combustion gases to penetrate into the crown fuel matrix, resulting in lower spread rates.

Figure 4.9 shows the total energy, viz., \( \bar{q}_{\text{conv}} + \bar{q}_{\text{rad}} + \bar{q}_{\text{mass}} \) in Equation 2.41, of the solid fuel particles located at the crown fuel bottom \((x=0.8, y=0.4, z=0.8 \text{ m})\) as a function of time for Case 1 (DBD) and Case 2 (FBD). It can be seen that the amount of energy supplied to the fuel particles remains the same for both cases as this location is near the ignition zone. In Case 1 this energy is distributed among a larger number of solid particles as compared to that in Case 2; thus, the crown fuel ignition is seen to occur earlier in time for Case 2. Moreover, a higher value of bulk density means more amount of fuel is present in this region, for Case 1, resulting in
Figure 4.8: (a) Spatial variation of $t_{500}$ (time required by horizontal shrub surface to reach an average temperature of 500 K); (b) Spread rate versus shrub height (local spread rate at a generic location $y_2$ is calculated as $(y_2 - y_1)/(t_{500,2} - t_{500,1})$, therefore x-axis for starts from $y=0.4$); for crown fuel modeled with distributed bulk density (Case 1) and fixed bulk density (Case 2), respectively; Cases are from Table 4.3.
Figure 4.9: Time evolution of total energy \((\bar{q}_{\text{conv}} + \bar{q}_{\text{rad}} + \bar{q}_{\text{mass}})\), of solid fuel particles located at \(x = 0.8\) m, \(y = 0.4\) m, \(z = 0.8\) m, a point near bottom surface of crown fuel, for distributed bulk density (Case 1) and fixed bulk density (Case 2) crown fuel models, respectively; Cases are from Table 4.3.

A higher heat release. Therefore, once enough fuel starts to burn in this region, the spread rate increases dramatically for DBD in the range of \(y = 0.5\) m to \(y = 0.8\) m as seen from Figure 4.8(b). In the upper half of the crown, bulk density for FBD case is higher than that for the DBD case, and hence, the spread rate values for FBD in this region are observed to be lower than DBD.

Based on the results presented in this subsection it can be conclusively stated that fire spread rate through a single shrub depends strongly on the distribution of bulk density.
4.4 Effects of Moisture Content Variation

The fuel moisture content is defined as the amount of moisture per unit dry mass of solid fuel. In the models used in this study, the effect of fuel moisture on the ignition of the solid fuel is accounted via the term $\bar{q}_{\text{mass}}$ appearing in the solid-phase energy balance equation (2.41). In total, ten simulations have been performed to investigate the effects of fuel moisture content on fire behavior (refer Table 4.3). Cases 3a to 3e include a crown fuel with a distributed bulk density, where the distribution is modeled as given by equation (4.1) and shown in Figure 4.1(c), with moisture content of 20%, 40%, 60%, 80%, and 100%, respectively. Moisture content for Cases 4a to 4e varies in a similar manner as described above for Cases 3a to 3e, with an only difference that the crown fuel is modeled with a fixed bulk density of 3.8 kg/m$^3$, matching the average value of polynomial distribution (equation (4.1)). The initial dry mass of the crown fuel, simulation setup, boundary conditions, and initial flow field conditions for all 10 moisture cases are kept the same as discussed for Case 1.

Here, first we discuss the results obtained from the simulations of Cases 4a to 4e and then include the results of Cases 3a to 3e. Figure 4.10, shows the contour plots at various instances in time for a moisture content of 20% in the crown fuel (Case 4a). The snapshots show the gas-phase temperature (color contours) and the bulk density (line contours) on a $x-y$ plane located at $z = 0.8$ m. Similar contour plots are shown in Figure 4.11, for a moisture content of 100% in crown fuel (Case 4e). Since the surface fuel model, crown fuel bulk density and amount of external energy supplied
Figure 4.10: Gas-phase temperature in Kelvin (color contours) with solid fuel bulk density (line contours) at various times for burning of crown fuel with moisture content of 20% (Case 4a, see Table 4.3); Snapshots are from a \( xy \)-slice passing through \( z = 0.8 \) m.

Figure 4.11: Gas-phase temperature in Kelvin (color contours) with solid fuel bulk density (line contours) at various times for burning of crown fuel with moisture content of 100% (Case 4g, see Table 4.3); Snapshots are from a \( xy \)-slice passing through \( z = 0.8 \) m.
for ignition is the same for both cases, similar flow field patterns are generated at early times (before 10 sec) for both cases.

For the case with lower moisture content, i.e., Case 4a, the crown fire initiates earlier in time (around 9 seconds) as compared to Case 4e (around 17 seconds), because the amount of the heat required to evaporate the moisture and start the pyrolysis process is relatively low. This observation regarding crown fire initiation is in contrast to the earlier study of Cruz et al. (2006) [43], where a semi-empirical model was used to demonstrate that foliar moisture content has a negligible influence on the crowning phenomena. From the snapshot at time 25 seconds in Figure 4.10, it can be seen that a considerable portion of the crown fuel has started to burn for Case 4a, whereas for Case 4e, displayed in Figure 4.11 for time 25 seconds, burning has been initiated only in a small portion of the fuel at crown bottom. This behavior indicates that the ignition process is affected due to higher moisture content which in turn affects the fire spread rate. From snapshot at 45 seconds in Figure 4.10, it is seen that almost all the crown fuel is burned out for Case 4a and therefore the fire starts to extinguish due to unavailability of the fuel. On the other hand, in the snapshot at 45 seconds in Figure 4.11, it is seen that although considerable amount of the solid fuel is available, the fire intensity still reduces. The reason for this could be that, the amount of heat generated by flames is insufficient to heat unburnt fuel ahead of the flames, resulting in an imbalance between the amount of heat generated by the burning of fuel and the amount of heat required by the neighboring unburnt fuel particles to ignite. Thus, the fire extinction for high moisture content case (Case
4e) is not due to the unavailability of fuel but rather due to the lower intensity of generated fire.

To further investigate the effect of moisture content on distribution of gas- and solid-phase temperatures through the domain, instantaneous, local values of these variables are compared quantitatively. Figure 4.12(a) shows the gas-phase temperature for Case 4a and Case 4e at various time instances, along y-axis passing through the center of the domain (x=0.8, z=0.8 m). Similarly Figure 4.12(b) shows the plots of solid-phase temperature along the same probe line. From the plots at time 15, 25 and 35 seconds, in Figure 4.12, it is seen that both gas- and solid-phase temperatures, for Case 4a are higher when compared with gas- and solid-phase temperatures of Case 4e, respectively, indicating that intensity of fire is reduced by higher moisture content. In Figure 4.12(b), at times after 35 sec, the solid-phase temperature is considerably high throughout the entire height of shrub for Case 4a, whereas in Case 4e, higher solid-phase temperatures are encountered in only a small portion of shrub. This indicates that the time required by fire to consume the solid fuel increases with the rise in fuel moisture content. These observations, for cases where crown fuel is modeled with fixed bulk density, also apply to the simulations where the crown fuel is modeled with a distributed bulk density, which can be seen in Figure 4.13. Figure 4.13(a) shows gas-phase temperatures along y-axis passing through domain center, for Case 3a (DBD, 20% moisture) and Case 3e (DBD, 100% moisture), at various instances in time. Similarly Figure 4.13(b) shows solid-phase temperatures along the same probe line for Case 3a and 3e.
Figure 4.12: Spatial variation of (a) gas-phase temperature, and (b) solid-phase temperature along a line passing through the domain center, viz. $x = 0.8$ m, $z = 0.8$ m, in $y$ direction; For moisture contents of 20% (Case 4a) and 100% (Case 4e); Cases are from Table 4.3.
Figure 4.13: Spatial variation of (a) gas-phase temperature, and (b) solid-phase temperature along a line passing through the domain center, viz., $x = 0.8$ m, $z = 0.8$ m, in $y$ direction; For moisture contents of 20% (Case 3a) and 100% (Case 3e); Cases are from Table 4.3.
Figure 4.14(a) shows the time evolution of crown fuel dry mass obtained from simulation of Cases 4a, 4b, 4c, 4d and 4e respectively. This figure shows that, the rate at which fire consumes the fuel decreases with an increase in moisture content. It can also be seen that, amount of fuel left unburnt when fire extinction in crown fuel occurs, increases with increasing fuel moisture content. Similar observations are made from Figure 4.14(b), which shows time history of crown fuel dry mass for Cases 3a, 3b, 3c, 3d, and 3e.

Figure 4.15(a) plots the vertical fire spread rate through crown fuel as a function of fuel moisture content. Results obtained from all ten moisture cases are shown in Figure 4.15(a) along with the two experimental spread rate values obtained by Li (2011) [46]. The vertical rate of spread for all cases is calculated using equation (4.2), based on the $t_{500}$ criteria. It is seen that the fire spread rate decreases continuously as the moisture content increases from 20% to 100%, for both types of crown fuel models, i.e., crown fuel modeled with a fixed bulk density and with a distributed bulk density. A sharp decrease in spread rate is seen when moisture content increases from 20% to 40%. From moisture content 60% to 100%, the rate at which the fire spread rate decreases is almost steady, for cases using FBD crown fuel model (Cases 4a to 4e). For fuel moisture content below 80%, vertical spread rates obtained from cases with crown fuel model consisting DBD (Cases 3a to 3d), are almost equivalent to those obtained from FBD cases (Cases 4a to 4d) with similar moisture contents, as seen from Figure 4.15(a).

Finally, seen in Figure 4.15(b) is the mass of unburned fuel plotted against the initial fuel moisture content for all ten moisture cases. It can be seen that with the
Figure 4.14: Time evolution of crown fuel dry mass for (a) fixed bulk density (Cases 4a - e); and (b) distributed bulk density (Cases 3a - e); Cases are from Table 4.3.
Figure 4.15: (a) Average vertical fire spread rate, and (b) unburnt mass, as a function of fuel moisture content. Experimental data points in (a) are for two experimental tests [46] with the same moisture content of 31.2%; Cases are from Table 4.3.
increase of the moisture content, more amount of the crown fuel mass is left unburnt. The unburnt fuel mass increases dramatically within the range of moisture content between 80% and 100%, indicating that the fire spread in shrubs with higher moisture contents is slow or almost impossible. A similar observation was made for cases in which crown fuel was modeled with distributed bulk density, i.e., Cases 3a to 3e. For Case 3e as compared to Case 4e, fire spread rate decreases (Figure 4.15(a)) and unburnt mass increases (Figure 4.15(b)) drastically indicating that higher resistance is offered to fire propagation when crown fuel is modeled with spatially distributed bulk density, having functional form given by Equation 4.1. However, this observation is concerned with the spatial distribution of the bulk density rather than the moisture content effect.

4.5 Effects of Soot Thermophoresis

Thermal radiation is an important mode of heat transfer for fire propagation. As seen in Section 4.2, fire spread in horizontal direction, i.e. through the fuel bed, occurs mainly due to radiative heating of fuel particles in the vicinity of the flame. Equation (2.48) and equation (2.50) show that the propagation of radiation intensity through a multicomponent gas phase depends strongly on soot particle volume fractions, whereas other gas phase species have a considerable lower contribution. Thus it is reasonable to expect that to obtain proper predictions of fire behavior, soot particle evolution and radiative heat transfer needs to modeled with appropriate accuracy. Since soot exists as a particulate media, convection and thermophoresis are considered to be important transport mechanisms, whereas, diffusion is assumed to
play a negligible role. Here we highlight the relative importance of thermophoresis of soot as compared to its convective transport. Note, in all the results discussed so far the soot thermophoresis was accounted.

In order to understand the influence of thermophoretic displacement of soot particles on the behavior of fire, two additional cases are modeled. In the first case thermophoresis of soot is accounted, whereas, in the second case the term accounting for thermophoretic transport of soot has been neglected by setting $u^{th} = 0$, which appears in the transport equation for soot volume fraction (refer equation (2.51)). In both cases, the bulk density of the crown fuel is fixed with $\rho_B = 3.8 \text{ kg/m}^3$, average value of the polynomial distribution shown in equation (4.1). The setup for crown and ground fuel, initial and boundary conditions, size of ignition zone and the initial dry mass of shrub are kept exactly the same as that used in simulation of Case 1 (Table 4.3). The size of the computational domain is reduced in $y$-direction, to 1.6 m, in order to reduce the computational cost involved.

Figure 4.16 shows the time history of the crown fuel dry mass for cases accounting for and neglecting the soot thermophoresis. It can be seen that inclusion of thermophoresis of soot particles has almost a negligible global impact on how the fire consumes the solid fuel and the time required to burn the crown fuel, consistent with expectation. By analyzing the simulation results it is observed that, thermophoretic velocity magnitude is always at least one order of magnitude lower than the convective velocity magnitudes, throughout the domain for the type of flow field generated in these simulations. Our simulations reveal that the crown fire initiation time (calculated based on the $t_{500}$ criteria) and the calculated fire spread rate (using equa-
Figure 4.16: Time evolution of crown fuel dry mass; with thermophoretic forces of soot included (——) and thermophoretic forces of soot neglected (- - -).

tion (4.2)) in y direction are not influenced with the inclusion of the thermophoresis forces.

Figure 4.17 shows the instantaneous values of soot particle volume fraction, gas-phase temperature and solid-phase temperature, obtained from simulations of cases accounting for and neglecting the soot thermophoresis. Results are shown along a vertical line (along y-axis) passing through the center of domain ($x=0.8$ m, $z=0.8$ m), at time approximately equals 40 seconds. Thermophoretic forces are dependent on the gradient of temperature and higher temperature gradients are generated as fire propagates. For this reason, relatively weak thermophoresis forces exist at the initiation of fire, they grow stronger as the intensity of fire increases, and drop again
Figure 4.17: Spatial variation of (a) soot volume fraction, (b) gas-phase temperature, and (c) solid-phase temperature along a line passing through the domain center, viz. $x = 0.8$ m, $z = 0.8$ m, in $y$ direction; at time approximately equal to 37.0 seconds; with thermophoretic forces of soot included (——) and thermophoretic forces of soot neglected (- - -).

as the fire intensity reduces towards the end of simulation. Therefore, the snapshots shown in Figure 4.17 are from time approximately equals maximum mass loss rate, i.e., when the intensity of fire is maximum. Results in this figure indicates that the local flow field is slightly affected when thermophoretic forces are included in the calculations. As far as the solid fuel temperature distribution is concerned, there is no change observed at all (Figure 4.17(c)). This also confirms the reason, why global parameters such as, crown fire initiation time and rate of spread are unaffected as both are primarily functions of solid fuel temperature.
CHAPTER 5

RESULTS - BURNING OF MULTIPLE SHRUBS

5.1 Introduction

In this chapter, the focus is on analyzing the interactions between multiple shrub fires. As discussed in the introduction Section 1.3.4, flame merging is an important phenomenon which can considerably alter the behavior of fire and the nature of the resulting flow field. To study the flame merging phenomena, two types of shrub arrangements were considered. The first arrangement consists of two shrubs placed next to each other and the second arrangement consists of three shrubs placed at the vertices of an equilateral triangle. An additional case consisting of a single shrub is also modeled here for comparison purposes. In all three arrangements, the modeled shrubs are identical to each other with thermophysical properties of chamise (Adenostoma fasciculatum, as discussed in Section 2.3 and Section 4.2). Each shrub has a fixed bulk density of 3.8 kg/m$^3$, which is the average value of the polynomial distribution shown in equation (4.1), throughout the canopy volume. The shape of the shrub is the same described in Figure 4.1(a) (Section 4.2). It is noted that the presence of external wind, depending upon its direction and velocity, can substantially change the thermo-fluid behavior of the flame [155]. Some of the effects due to
external wind include flame tilting, increase in the fire spread rate [156], generation of fire whirls [157], etc., which can complicate the analysis of flame merging. Dealing with this complication is beyond the scope of the current study. The focus here is on analyzing the shrub fire merging in quiescent environment, i.e., with zero external wind speed.

Figure 5.1(a) shows the computational domain size, the setup of shrub and the ignition zone adopted for the modeling of a single-shrub case. The snapshot shows line contour of the solid fuel bulk density on an \( xy \)-slice passing through \( z = 2.0 \) m. The length of the computational domain in \( x \), \( y \) and \( z \) directions is 4.0 m, 6.0 m and 4.0 m, respectively, with the ignition zone and crown fuel placed at the center. The dimensions of the ignition zone are 0.2 m, 0.1 m and 0.2 m in \( x \), \( y \) and \( z \) directions, respectively. The ground fuel used for the simulations discussed in Chapter 4 is replaced with a small ignition zone to minimize its influence on the evolution of shrub fires. The two- and the three-shrub arrangements that are chosen to study the interactions of shrub fires are shown in Figure 5.1(b) and Figure 5.1(c), respectively. In Figure 5.1(b,c), the line contour represents the solid fuel bulk density on a \( xz \)-slice passing through \( y = 1.0 \) m (top view of the computational domain), where \( d \) is the distance between edges of the shrubs and \( D \) is the largest diameter of a shrub encountered along its vertical axis. Each shrub has an individual ignition zone located below the crown fuel, similar to the one shown in Figure 5.1(a).

Two different kinds of solid phases are considered in the crown: foliage and branches, which are assumed to have identical moisture content. It is recalled that the effect of moisture content on the burning of a single isolated shrub, as discussed
Figure 5.1: (a) A front view of the computational domain in the single-shrub case; Top view of the computational domain showing generic arrangement for (b) the two-shrub cases and (c) the three-shrub cases.
in Section 4.4, is that flame size decreases with an increase in moisture content. For this reason, moisture content of the shrubs used in this chapter is set to a small value of 10% to lead to a larger flame size and appreciable flame interactions. The ignition mechanism replicates ignition by spotting phenomena, which is commonly seen during the wildfires [46]. Since excelsior is typically used as ground fuel during burn experiments, the ignition zone is modeled with properties of excelsior and a typical moisture content of 7% [45]. Fire initiation modeling is similar to that explained in Section 3.4. The external heat source is turned off when 80% of the fuel in the ignition zone is consumed. From this point on the fire evolution occurs as described by the governing equations explained in Chapter 2. The effect of external ignition mechanism on the simulation results is considered negligible since the igniter is switched off fairly early (around 10 sec) for all simulations to be discussed in this chapter.

The grid resolution adopted here is $200 \times 300 \times 200$ in $x$, $y$ and $z$ directions, respectively, rendering a grid size of 2 cm in each direction. Since two or more shrubs are burned simultaneously, the size of computational domain is chosen to be larger in all directions, as compared to that used in Chapter 4 for single shrub cases, to avoid any interference from the boundaries. The simulations reported in this chapter were performed using message passing interface (MPI) protocol on 40 processors of High Performance Technical Computing (HPTC) cluster located at the College of Engineering of The University of Alabama in Huntsville. A typical simulation of 70 seconds required a wall time of about 340 hours and 28 GB of memory.

Overall nine cases with different crown separation distances were modeled for the two-shrub (Figure 5.1(b)) and the three-shrub (Figure 5.1(c)) configurations.
The crown separation distance is defined as the distance between the inner edges of the crowns normalized by the maximum shrub diameter encountered along its height. For the two-shrub configuration, four different values of 0.0, 0.1, 0.3 and 0.5, and for the three-shrub configuration, five different values of 0.0, 0.1, 0.3, 0.5 and 1.0 are considered for \( d/D \). An additional case with a single shrub configuration (Figure 5.1(a)) is also modeled to serve as a base case. Results obtained from the burning of two and three shrubs are compared against those obtained from the burning of a single shrub to explore the effects of neighboring fires on the burning of individual shrubs.

### 5.2 Zero Separation Distance

The time evolution of shrub fires and the resulting flow field obtained for single-shrub, two-shrub and three-shrub cases with \( d/D = 0 \), respectively, are shown in Figure 5.2 and Figure 5.3. The times of the snapshots shown in these figures, i.e., \( t \approx 16, 23, \) and 45 sec, correspond to instances when the mass lost rate \((-\frac{dm}{dt}, \text{where } m \text{ is the mass of one shrub})\) is equal to 50%, 100%, and 50% of its peak value, respectively.

Figure 5.2 shows the flames in the gas phase using pyrolysis gas mass fraction iso-surface of 0.025 (\( \approx 5\% \) of maximum, orange) and the solid fuel using a bulk density iso-surface of 3.8 kg/m\(^3\) (green). It can be seen that a low intensity flame has been established inside the shrubs at \( t \approx 16 \) seconds, approximately 6 seconds after the igniter is turned off. Until this point, no interactions between the flames are seen for the two-shrub case while some flame merging phenomena can be seen for the
Figure 5.2: Pyrolysis gas mass fraction iso-surface of 0.025 (≈5% of maximum, orange) and solid fuel bulk density iso-surface of 3.8 kg/m$^3$ (green) at $t \approx 16.0$ sec (first column), $t \approx 23.0$ sec (second column) and $t \approx 45.0$ sec (third column) in single-shrub (a-c), two-shrub (d-f), and three-shrub (g-i) cases; $d/D = 0.0$ in all cases.
Figure 5.3: Vorticity magnitude iso-surface (∼25% of the maximum) colored with second invariant of the velocity gradient tensor ($Q = 0.5(\| \Omega \|^2 - \| S \|^2)$) at $t \approx 16.0$ sec (first column), $t \approx 23.0$ sec (second column) and $t \approx 45.0$ sec (third column) in single-shrub (a-c), two-shrub (d-f), and three-shrub (g-i) cases; $d/D = 0.0$ in all cases.
three-shrub case. At the time when the peak mass loss rate \((t \approx 23 \text{ sec})\) is reached, the multiple shrubs appear to be a single source of fire, as seen is Figure 5.2(e) and Figure 5.2(h). Towards the end of the simulation \((t \approx 45 \text{ sec})\), the individual flames are again separated in the two-shrub case (Figure 5.2(f)) whereas the individual flames still seem to be merged in the three-shrub case (Figure 5.2(i)).

The buoyancy driven flow field generated by the shrub fires is shown in Figure 5.3, using a vorticity magnitude iso-surface of \(35 \text{ s}^{-1} \approx 25\% \text{ of maximum}\). Superimposed on this iso-surface is the color contour of second invariant of the velocity gradient tensor \((Q)\), often used as a criterion for the vortex identification [158]. The vorticity vector is obtained by taking the curl of the velocity field whereas \(Q\) can be written as \[ Q = \frac{\|\Omega\|^2 - \|S\|^2}{2} \] [159]. Here, \(\Omega\) (defined as \(\Omega_{ij} = (\partial u_i / \partial x_j - \partial u_j / \partial x_i)/2\)) is the rotation rate tensor and \(S\) (defined as \(S_{ij} = (\partial u_i / \partial x_j + \partial u_j / \partial x_i)/2\)) is the strain rate tensor. Thus positive values of \(Q\) identifies regions in the flow field where rotation dominates strain and negative values indicate vice versa. The plumes generated by the three-shrub case shows higher magnitudes of both vorticity and strain as compared to those generated by the two-shrub and single-shrub cases, which can be seen by comparing the snapshots from Figure 5.3 at corresponding time instances. The cause and effect of higher vorticity magnitudes seen in the three-shrub case are discussed later in this section.

The time evolution of the mass of a shrub and its rate of change are shown in Figure 5.4(a) and Figure 5.4(b), respectively, for the single-shrub, two-shrub and three-shrub cases. As seen in Figure 5.4(a), the difference between the three curves is negligible until 20 sec, indicating minimal flame interactions for the two- and three-
Figure 5.4: Time evolution of (a) mass of shrub in Kg and (b) mass loss rate of shrub in gm/sec for single-, two- \((d/D = 0.0)\), and three-shrub \((d/D = 0.0)\) cases. For the two- and three-shrub curves, only one of the shrubs is used to obtain the required data (refer Figure 5.1).
shrub cases. From 20 seconds until the end of simulations (70 sec), the curve for the three-shrub case falls much more rapidly as compared to the other two curves, indicating rapid consumption of the solid mass. The rapid burning of the solid fuel translates into higher mass loss rates for the three-shrub configuration, which is readily observed in Figure 5.4(b). The peak value of the mass loss rate is seen to be the largest for the three-shrub case and lowest for the single-shrub case. Due to the rapid decomposition of the solid fuel, higher amounts of pyrolysis gases are generated, resulting in bigger flames in the gas phase, as seen in Figure 5.2(h) for the three-shrub configuration (at peak mass loss rate, $t \approx 23$) as compared to two- and single-shrub cases seen in Figure 5.2(e) and Figure 5.2(b), respectively. The resulting plumes generated by the buoyancy effects appear to be stronger and drawn towards the center of the domain for the three-shrub configuration (Figure 5.3(h)), indicating the presence of much stronger indrafts of ambient air.

Figure 5.5 shows the time history of the heat release rate (the source term appearing in the gas-phase energy balance equation (2.6) due to the chemical reactions, KW) divided by the number of shrubs in the computational domain, for the single-shrub, two-shrub and three-shrub cases, respectively. The heat release rate is obtained by summing up $(\sum_{K=1}^{N_K} \dot{\omega}_K \Delta h_{f,K}^0) \Delta V$ over the entire computational domain. Here, $\dot{\omega}_K$ is the production rate for the $K^{th}$ gas-phase species, $\Delta h_{f,K}^0$ is the formation enthalpy for the $K^{th}$ gas-phase species, $N_K$ is the total number of gas-phase species and $\Delta V$ is the volume of the computational grid cell. Since for the two-shrub and three-shrub cases more amount of fuel is burned, the total heat released is expected to be larger as compared to that in the single-shrub case. For this reason, the total
heat release rate is divided by the number of shrubs in the two-shrub and three-shrub cases. It is recalled that all the shrubs are identical to each other and are ignited by the same mechanism at the same time. In the time interval between 20 to 30 sec, seen in Figure 5.5, the heat release per shrub in the three-shrub case is observed to be much higher than that in the two-shrub and single-shrub cases. Within the same time interval, the heat release per shrub for the two-shrub case is higher than the single-shrub case. This effect highlights the occurrence of the flame merging phenomena where the heat released from the merged flame is higher than the heat released from the individual flames combined. A similar observation was made by Morvan et al. (2013) [79] who studied fires that propagate through grasslands, where appearance
Figure 5.6: Gas-phase temperature in Kelvin (color contours) along an $xy$-slice at $z = 2.0$ m at $t \approx 23.0 \pm 0.5$ sec (around the time of peak mass loss rate); (a) single-, (b) two- ($d/D = 0.0$), and (c) three-shrub ($d/D = 0.0$) cases, respectively.

of a spike in the heat release rate was reported during the time instance of flame merging between a head and a back fire.

Figure 5.6 shows the gas-phase temperature (color contour) on an $xy$-slice passing through the center of the computational domain ($z=2.0$ m) at the time of peak mass loss rate ($t \approx 23.0$ sec). The flame height, based on gas-phase temperature iso-contour of 500 K, for the three-shrub case (Figure 5.6(c)) is observed to be considerably larger than those seen for the single- (Figure 5.6(a)) and the two-shrub (Figure 5.6(b)) cases. By analyzing snapshots at different time instances of shrub burning, gas-phase temperatures in the three-shrub case were found to be higher than those in the single- and the two-shrub cases.

The strength of the generated plumes is analyzed by comparing the total kinetic energy of the flow field, shown in Figure 5.7 (color contours), on an $xy$-
Figure 5.7: Kinetic energy in \((m/s)^2\) (color contours) along an \(xy\)-slice at \(z = 2.0\) m at \(t \approx 23.0 \pm 0.5\) sec (around the time of peak mass loss rate); (a) single-, (b) two- \((d/D = 0.0)\), and (c) three-shrub \((d/D = 0.0)\) cases, respectively.

slice passing through the center of the computational domain \((z=2.0\) m\), for the single- (Figure 5.7(a)), two- (Figure 5.7(b)) and three-shrub (Figure 5.7(c)) cases. The snapshots shown are at the time of peak mass loss rate \((t \approx 23.0\) sec\). The kinetic energy of the plume for the three-shrub case is observed to be much higher as compared to that in the single- and two-shrub cases. This observation indicates that the ambient air is displaced at higher velocity magnitudes generating a stronger plume for the three-shrub case. To quantitatively see how the flow in the interaction zone, i.e., the region between the shrubs for multiple crown fuels, changes from the two-shrub case to the three-shrub case, gas-phase variables are plotted as a function of \(y\) along the centerline of the domain in Figure 5.8. The panels (a), (b) and (c) are for the gas-phase temperature, total kinetic energy and pressure, respectively, at the time of peak mass loss rate \((t \approx 23.0\) sec\). It is noted that the pressure
Figure 5.8: Spatial variation of (a) gas-phase temperature in Kelvin; (b) kinetic energy in (m/s)^2; and (c) pressure in Pa, along a line passing through the center of the domain (x=2.0 m, z=2.0 m) in y-direction at t ≈ 23.0 ± 0.5 sec (around the time of the peak mass loss rate).

shown in Figure 5.8(c) is the gauge pressure. It is seen that the maximum value of the kinetic energy in the three-shrub case is almost 2.5 times higher than that in the two-shrub case. Also higher temperatures and lower pressures, with minimum pressure being approximately 2 times lower, are seen in the three-shrub configuration compared to those in the two-shrub case. By comparing the velocity components along the centerline of the domain, it is found that the velocity component along the vertical direction (y) for the three-shrub case is much higher than that for the single- and two-shrub cases. Presence of a strong updraft in the three-shrub case, driven by conservation of mass, results in larger cross-stream velocities (in x and z directions) in regions near to the shrubs, which is the base of the plume. These strong indrafts are seen to further enhance the burning of the solid fuel and generate high vorticity in the central region surrounded by the three shrubs for the three-shrub case.
The vorticity transport equation (5.1), obtained by applying the curl operator on the momentum transport equation (2.5), contains terms such as baroclinic torque, gravitational torque, vorticity modification by volumetric expansion, vortex stretching, etc., [160].

\[
\frac{D\omega}{Dt} = \underbrace{(\omega \cdot \nabla)\mathbf{V}}_{\text{vortex stretching}} - \underbrace{\omega(\nabla \cdot \mathbf{V})}_{\text{dilatation}} + \frac{1}{\rho^2}(\nabla \rho \times \nabla p)_{\text{baroclinic torque}} + \frac{\rho_\infty}{\rho^2}(\nabla \rho \times g)_{\text{gravitational torque}} + \nabla \times \left(\frac{\nabla \cdot \tau}{\rho}\right)_{\text{viscous torque}} + \cdots \quad (5.1)
\]

Of these terms, the baroclinic torque, which represents the interaction between density gradient and pressure gradient, and the gravitational torque, which represents the interaction between density gradient and gravitational acceleration, contributes to the generation of vorticity [161]. Recent studies on buoyancy driven plumes have shown that the gravitational torque is the dominant factor for vorticity generation at the plume source [160], arising due to misalignment between the density gradient vector and the gravitational acceleration vector. Figure 5.9 shows the magnitude of gravitational torque (color contours), vorticity (vector field) and the solid fuel bulk density (line contour) on a \(xz\)-plane passing through the top surface of the shrubs \((y=1.0 \text{ m})\) at the time of the peak mass loss rate \((t \approx 23.0 \text{ sec})\). The zone between the shrubs in the three-shrub case has high magnitudes of the gravitational torque as seen in Figure 5.9(c), compared to that in the single- and two-shrub cases seen in Figure 5.9(a) and (b), respectively. A similar observation is made by examining the snapshots of the baroclinic torque (Appendix Figure B.8). It is seen that baroclinic
Figure 5.9: Gravitational torque magnitude $\rho_\infty \| \vec{\nabla} \rho \times \vec{g} \| / \rho^2$ in s$^{-2}$ (color contours), vorticity in s$^{-1}$ (vector field), and solid fuel bulk density of 3.8 kg/m$^3$ (line contour) on an $xz$-slice at $z = 1.0$ m, at $t \approx 23.0 \pm 0.5$ sec (around the time of the peak mass loss rate); (a) single-, (b) two- ($d/D = 0.0$), and (c) three-shrub ($d/D = 0.0$) cases, respectively.
torque has the same order of magnitude as that of the gravitational torque. The higher magnitudes of these two source terms in the vorticity transport equation contribute to the generation of higher vorticity for the three-shrub case. This highly rotational flow enhances the process of mixing between the pyrolysis gases and the ambient air for the three-shrub case and to some extent for the two-shrub case, resulting in vigorous combustion as well as amplification of interactions between the individual plumes.

To investigate the effect of the flame merging phenomena on solid fuel combustion, various terms present in the solid-phase energy balance equation (2.41) (refer Section 2.3) are considered. Figure 5.10 shows the instantaneous snapshots at the time of the peak mass loss rate for the solid-phase temperature (first row), convective heat transfer between solid- and gas-phase (second row), and radiative heat transfer between solid- and gas-phase (third row). Results are shown along an $xz$ slice passing through $y=0.71$ m. This $y$-location approximately matches with the location of the pyrolysis front, which is defined based on a solid-phase temperature equal to 500 K criteria (refer equation (4.2)), at the time of peak mass loss rate. Higher solid-phase temperatures are seen in regions close to the interaction zone, i.e. center of the domain, for the three-shrub case as compared to the single- and two-shrub cases. This observation indicates a stronger feedback mechanism of energy from the combustion of pyrolysis gases, in the gas-phase, to the solid phase. Two important modes of heat transfer between the gas and solid phases, which are responsible for the fire spread, are convection and radiation heat transfer [48]. In Figure 5.10(e) for the two-shrub case, values of the convective heat transfer in the solid fuel near the interaction zone, where the two shrubs touch each other, are larger than those for the single-shrub case.
Figure 5.10: Solid-phase temperature in Kelvin (a-c), convective heat transfer between the solid and gas phases in KW/m$^3$ (d-f), and radiative heat transfer between the solid and gas phases in KW/m$^3$ (g-i) along an $xz$-slice at $y = 0.71$ m at the time of the peak mass loss rate ($t \approx 23.0 \pm 0.5$ sec) for single- (first column), two- (second column), and three-shrub (third column) cases, respectively; $d/D = 0.0$ for all cases.
The convective heat transfer between the gas- and solid-phase is further enhanced for the three-shrub case (Figure 5.10(f)), especially in regions close to the interaction zone. Negative values of convective heat transfer are seen in the three-shrub case due to the heat being transferred from the solid- to gas-phase, indicating that the solid-phase temperature is higher than the gas-phase temperature. Mostly negative values of radiative heating are seen in Figure 5.10 (last row), indicating that heating of solid-phase is mainly convection dominant. This observation agrees well with the findings from the previous study on single isolated shrub fires (Section 4.2) where convective heating was seen to be responsible for the vertical fire spread through the shrub.

Time evolution of solid fuel variables at various point locations has been analyzed to identify the effect of the convective and the radiative heating mechanisms on the solid fuel temperature. Figure 5.11 shows the time history of the solid-phase temperature (Figure 5.11(a)), convective heat transfer (Figure 5.11(b)) and radiative heat transfer (Figure 5.11(c)) for the two- and three-shrub cases at one typical point located near the interaction zone. Since the crown fuels are ignited at the bottom surface, the fire typically spreads vertically along $y$ direction inside the shrub. For this reason, the two point locations used in Figure 5.11 for two-shrub and three-shrub cases, have the same height from the ground. The solid fuel for the three-shrub case shows faster heating as compared to the two-shrub case (Figure 5.11(b)). Because of this, in the three-shrub case, temperature rises earlier in time (Figure 5.11(a)). This indicates that the fire spread inside the shrub is faster for the three-shrub case as compared to the two-shrub case. Also, much higher solid-phase temperatures are
Figure 5.11: Time evolution of (a) solid-phase temperature in Kelvin, (b) convective heat transfer between the gas and solid phases in KW/m$^3$, and (c) radiative heat transfer between the gas and solid phases in KW/m$^3$. Data extracted from a single point located at $x = 1.93$ m, $y = 0.71$ m, $z = 1.99$ m for the two-shrub case ($d/D = 0.0$) and $x = 1.97$ m, $y = 0.71$ m, $z = 2.01$ m for the three-shrub case ($d/D = 0.0$).
encountered in the three-shrub arrangement. As seen in Figure 5.11(c), the radiative heat is mainly transferred from the solid to gas phase while its magnitudes are seen to be much higher for the three-shrub arrangement.

Figure 5.12(a) shows the time required by the horizontal shrub surfaces, i.e., \( x-y \) planes to reach an average temperature of 500 K. This time is denoted by \( t_{500} \). As the statistical homogeneity is lacking in any spatial directions for the generated flow field, averaging of the solid-phase temperature is performed on horizontal surfaces \( (xz\text{-plane}) \) at various \( y \) locations along the height of the shrub. As mentioned in Section 4.2, in wildfire modeling, a solid-phase temperature equal 500 K is often used as the criteria to track the location of the pyrolysis front [23,162]. The fire spread rate calculated based on this criteria, is shown in Figure 5.12(b) as a function of the shrub height. It is seen that \( t_{500} \) is almost the same for the single-, two- and the three-shrub cases for the shrub heights below 0.5 m (Figure 5.12(a)), which leads to almost similar spread rates to this height as seen in Figure 5.12(b). From the shrub height of 0.5 m to 0.7 m, the pyrolysis front is seen to move faster in the three-shrub case, the corresponding time interval being approximately between 20 sec to 30 sec. During this time interval, a strong flame merging phenomena is seen for the three-shrub case (Figure 5.2(h)). The maximum spread rate for the three-shrub case is seen at \( y = 0.7 \) m where the corresponding \( t_{500} \) this \( xz \) plane matches with its peak mass loss rate time. This observation indicates that the maximum fire spread rate occurs in the same time interval when the maximum mass loss rate and maximum heat release rate take place. The spread rates for the two-shrub case are seen to be
Figure 5.12: (a) $t_{500}$ in seconds (time required by the horizontal shrub surface to reach an average temperature of 500 K), and (b) spread rate in mm/sec as a function of shrub height for single-, two- ($d/D = 0.0$), and three-shrub ($d/D = 0.0$) cases, respectively. For the two- and three-shrub cases, only one of the shrubs is used to obtain the required data (refer Figure 5.1).
lower than the three-shrub case but higher than the single-shrub case, indicating an existence of a weak flame merging phenomena in the two shrub-arrangement.

5.3 Nonzero Separation Distance

In the preceding discussion (Section 5.2) we saw that the mass loss rate of a shrub, the heat release rate per shrub and the fire spread rate within the shrub increases when another shrub is placed next to a single isolated shrub (two-shrub configuration). These quantities increase much more when a third shrub is added (three-shrub configuration). Up to this point, only the two-shrub and three-shrub cases with zero separation distance ($d/D = 0.0$) were considered. We now explore the effects of increasing the separation distance on the burning of multiple shrubs. Shown in Figure 5.13 is the time history of the mass loss rate of a shrub obtained for the two-shrub (Figure 5.13(a)) and the three-shrub (Figure 5.13(b)) cases with various separation distances. The time evolution of the mass loss rate for the single-shrub case is also included in Figure 5.13 for comparison purposes. In a global sense, the time evolution of the mass loss rate in various cases follows a similar trend but some deviations can be seen mainly in the vicinity of the time of the peak mass loss rate which corresponds to the time interval between 20 and 30 sec. In both two- and three-shrub arrangements, as the separation distance increases, the trends of the mass loss rate become more similar to those in the single-shrub case, indicating a decrease in fire-fire interactions.

A similar observation can be made for the time variation of the heat release rate per shrub, as shown in Figure 5.14. The sub-figures (a) and (b) are for the two-
Figure 5.13: Time evolution of the mass loss rate of a shrub in gm/sec for (a) two- and (b) three-shrub cases, respectively, with various separation distances \((d/D)\). Mass loss rate obtained from the single-shrub case is shown with dots.
Figure 5.14: Time evolution of the heat release rate divided by number shrubs in KW for (a) two- and (b) three-shrub cases, respectively, with various separation distances (d/D). Heat release rate obtained from the single-shrub case is shown with dots.
and the three-shrub cases, respectively, where the heat release rate obtained from the single-shrub case is also included. The interactions between the individual fires cease to exist at a separation distance of 0.5 \((d/D = 0.5)\) for the two-shrub case. Due to the presence of stronger interactions in the three-shrub arrangement, a separation distance with at least \(d/D = 1.0\) is required to avoid the flame merging between the individual shrub fires. Some plume interactions are still seen for the two-shrub case with \(d/D = 0.5\) and the three-shrub case with \(d/D = 1.0\) in the far field region above the shrubs, but these interactions do not affect the burning of the shrubs in any way.

Figure 5.15(a) shows the change in the peak mass loss rate for the two-shrub and the three-shrub cases normalized by the peak mass loss rate for the single-shrub case, as a function of shrub separation distance \((d/D)\). Similarly, Figure 5.15(b) shows the change in the peak heat release rate per shrub for the two-shrub and the three-shrub cases normalized by the peak heat release rate obtained from the single-shrub case. The peak mass loss rate (Figure 5.15(a)) is seen to continuously drop as the separation distance between the shrubs is increased, becoming equal to that for the single-shrub case at \(d/D = 0.5\) and 1 for two- and three-shrub cases, respectively. The peak heat release rate per shrub, as seen in Figure 5.15(b), also follows the same trend as the peak mass loss rate for the two-shrub arrangement. However, for the three-shrub arrangement, it increases for the case with \(d/D = 0.1\) as compared to the case with \(d/D = 0\).

By analyzing the velocity field, it is seen that due to a small gap between the shrubs, the ambient air is able to enter the region surrounded by shrubs for the three-shrub case with \(d/D = 0.1\). Velocity magnitude and \(O_2\) mass fraction along the
Figure 5.15: (a) Peak mass loss rate for the two- and three-shrub cases normalized by the peak mass loss rate for the single-shrub case, and (b) peak heat release rate per shrub for the two- and three-shrub cases normalized by the peak heat release rate for the single-shrub case, as a function of crown separation distance ($d/D$).
Figure 5.16: Spatial variation of (a) velocity magnitude in m/sec and (b) oxygen mass fraction, along a line passing through the center of the domain \((x = 2.0 \, \text{m}, \, z = 2.0 \, \text{m})\) in \(y\)-direction at \(t \approx 23.0 \pm 0.5 \, \text{sec}\) (around the time of the peak mass loss rate), for the three-shrub cases with \(d/D = 0.0, 0.1\) and 1.0, respectively.

centerline of the domain at the time of the peak mass loss rate \((t \approx 23.0 \, \text{sec})\) is shown in Figure 5.16(a) and Figure 5.16(b), respectively, for the three-shrub cases with \(d/D\) equal to 0.0, 0.1 and 1.0. Due to the flow of ambient air into the interaction zone, i.e. the region surrounded by three shrubs, higher magnitudes of velocity and oxygen concentration is seen for the three-shrub arrangement with a separation distance of 0.1 as compared to the three-shrub case with \(d/D = 0\) (Figure 5.16). A region with almost negligible oxygen concentration is seen to exist for the three-shrub case with \(d/D = 0\), near the top surface of the shrub \((y = 1.0 \, \text{m})\), as seen in Figure 5.16(b), at the time of the peak mass loss rate \((t \approx 23.0 \, \text{sec})\). By comparing similar snapshots (shown in Appendix Figure B.12) at other time instances, the oxygen depletion region
was seen to prevail throughout the time interval between 20 sec and 30 sec for the three-shrub case with $d/D = 0$. Thus, the reduction of the heat release rate seen for the three-shrub case with $d/D = 0$ as compared to the three-shrub case with $d/D = 0.1$, could be attributed to the unavailability of oxygen. Also, the cross-stream velocities generated by the gap between the shrubs in the three-shrub case with $d/D = 0.1$, are seen to increase the vorticity magnitudes through the gravitational torque generation mechanism, as explained earlier for the three-shrub case with $d/D = 0$ Figure 5.9. This increase leads to an enhanced mixing between pyrolysis gases and oxidizer. Faster combustion could be another cause for higher heat release rates in the three-shrub case with $d/D = 0.1$ as compared to the three-shrub case with $d/D = 0$. Due to a lack of interactions between neighboring fires for the three-shrub case with $d/D = 1$, the velocity magnitude and the $O_2$ mass fraction along the centerline of domain remains equivalent to the ambient conditions (seen in Figure 5.16).

Finally, we investigate the effect of the shrub separation distance on the fire spread rate and the amount of fuel consumed, two parameters which are considered important from the prescribed burning standpoint [163]. Figure 5.17(a) shows the variation of average fire spread rate inside the shrub along $y$ direction for the two- and the three-shrub cases normalized by the average fire spread rate obtained for the single-shrub case, as a function $d/D$. The average spread rate is calculated by averaging the spread rates over various horizontal $xz$ shrub planes based on $t_{500}$ criteria, given in equation (4.2), ranging from 0.3 m (base of the shrub) to 0.8 m (approximate height to which the shrub is burned in 60 sec). Similarly, Figure 5.17(b) shows the variation of the amount of fuel consumed in 60 seconds for the two- and
Figure 5.17: (a) Average fire spread rate along $y$ direction for the two- and three-shrub cases normalized by the average fire spread rate along $y$ direction for the single-shrub case, and (b) the amount of shrub mass consumed in first 60 seconds for the two- and three-shrub cases normalized by the amount of mass consumed for the single-shrub case in first 60 seconds, as a function of separation distance ($d/D$).
the three-shrub cases, normalized by the amount of the fuel consumed for the single-shrub case in the first 60 seconds, as a function of separation distance \((d/D)\). Both parameters, the spread rate and the amount of solid mass consumed, decrease with the increase of the separation distance. As seen earlier, the three-shrub configuration with \(d/D = 0\) generates stronger interactions between individual fires, leading to higher fire spread rates (approximately 1.24 times higher) with an increased amount of mass consumed (approximately 1.16 times higher) as compared to the two-shrub configuration with \(d/D = 0\). For the three-shrub case with \(d/D = 1.0\) and the two-shrub case with \(d/D = 0.5\), the average spread rate and the mass consumed are equal to that for the single-shrub case, indicating that the neighboring fires no longer affect the burning of individual shrubs.
CHAPTER 6

CONCLUSIONS AND FUTURE WORK

6.1 Summary and Conclusions

A physics based model used to simulate laboratory-scale shrub fires was described in detail. The model was used to study the fire behavior of a single isolated shrub as well as the fire-fire interactions generated due to the burning of multiple shrubs.

The considered basic configuration for the single isolated shrub involved a 0.1 m deep surface fuel and an elevated crown-like fuel matrix (chamise shrub) situated 0.2 m above the surface fuel. Global characteristics of an isolated shrub fire predicted by the model were found to be in fairly good agreement with the available experimental results. However, the model overestimated the maximum mass loss rate by a factor of 1.4. The main reasons behind this discrepancy could be the random distribution of mass in the shrub canopy volume which is not accounted for in the model, the uncertainties involved in the experimental procedure, the lack of enough experimental samples, and the uncertainties involved with the physical models used in the computations.
From the modeling studies, it was found that the spatial variation of crown fuel bulk density and the fuel moisture content have a significant impact on the burning of isolated shrubs in still air. Both the crown fire initiation time and local vertical fire spread rate were influenced by variations in local fuel bulk density and the fuel moisture content. The variation in bulk density in the vertical direction was modeled via a cubic polynomial with no variation assumed in the horizontal planes. This bulk density distribution model resulted in an increase in the time required to initiate the combustion process in lower parts of the shrub. A similar effect was seen when solid fuel contains higher amount of moisture, though the mechanism causing the delay in ignition was found to be completely different. When a region has higher bulk density, the heat received is distributed among a larger number of solid particles; thus, reducing the amount of heat gained by an individual fuel particle, which in turn delays the combustion process. On the other hand, fuel particles with a higher moisture fraction delayed the ignition as drying process took longer time to be completed.

For a shrub with a bulk density distributed along its height, uneven fire spread rates were observed inside the shrub in the vertical direction. In the lower region, fire propagation speed remains lower and then increases as it moves into the upper portion of the crown. This behavior was not observed when a constant bulk density was used throughout the shrub. The time required to complete the burning of a shrub is thus not significantly affected when its bulk density is distributed. When moisture content is high, e.g., 80% or 100%, fire spread rates drop by almost 80%, compared to the fire spread rate of a shrub with 20% moisture content. It was
also found that, flames begin to extinguish at higher moisture contents even though a considerable amount of unburnt solid fuel was present in the shrub. A two-fold increase in the moisture content, from 40% to 80% for instance, results in a 250% increase in the amount of unburnt mass. This increase is attributed to that the fuel particles undergoing combustion did not generate sufficient energy required to initiate ignition in neighboring fuel particles, resulting in an increase in the amount of unburnt mass.

Soot particles primarily influence the heat transfer by affecting thermal radiation since the gas-phase absorptivity is directly proportional to the soot volume fraction. Thermophoresis of soot particles is considered an important transport mechanism of soot in the presence of high temperature gradients. Neglecting the thermophoretic forces on soot affected the flow field locally; however, this effect, due to its low magnitude, was found not to be influential on the global fire parameters such as the mass loss and fire spread rates. The thermophoretic velocities of soot particles were found to be at least an order of magnitude less than their convective velocities generated by the buoyancy. It was seen that the instantaneous values of soot volume fraction and the gas-phase temperature were somewhat influenced if the thermophoretic velocity of soot was neglected. However, this neglect had no effect on the temperature of the solid fuel.

Computational modeling of multiple shrubs fires was performed to study the flame merging phenomena and its effects on fire behavior. Considered shrub arrangements were two shrubs placed next to each other (two-shrub cases) and three shrubs placed at the vertices of an equilateral triangle (three-shrub cases). In both
arrangements, all shrubs were ignited simultaneously with the aid of small ignition zones placed at the bottom of shrubs. For comparison purposes, an additional setup consisting of a single isolated shrub (single-shrub case) was also modeled.

When the shrubs were placed at zero separation distance \((d/D = 0)\), flames from individual shrub fires interacted strongly, displaying an almost unified flame for the three-shrub arrangement. Fire-fire interactions, though present, were seen to be much weaker for the two-shrub arrangement with \(d/D = 0\). Larger flame height, as compared to the single-shrub case, was seen for the two-shrub arrangement with \(d/D = 0\) which increases further for the three-shrub case with \(d/D = 0\). The buoyancy driven flow field for the three-shrub arrangement with \(d/D \leq 0.5\) appeared to be drawn towards the center of the domain.

The region surrounded by three shrubs for the three-shrub cases with \(d/D \leq 0.1\) was characterized by high magnitudes of vorticity. Analyzing the source terms from vorticity transport equation indicated that vorticity was mainly generated through the gravitational torque mechanism, which essentially represents the misalignment between the density gradient vector and the gravitational acceleration vector. This mechanism for the vorticity generation was found much weaker for the two-shrub and single-shrub cases. Higher vorticity seen for the three-shrub cases with \(d/D \leq 0.1\) led to a faster mixing of pyrolysis gases and surrounding air which resulted in vigorous gas-phase combustion. The effect of this phenomena was confirmed by analyzing the time history of heat release rate per shrub, i.e., the total heat release in the gas phase divided by the number of shrubs in the domain. The peak value of this parameter was found to be 15% higher for the three-shrub case with \(d/D = 0\) as compared to
that for the single-shrub case. Similarly, the peak value of heat release rate per shrub for the two-shrub case with \( d/D = 0 \) was 5% higher than the single-shrub case. Due to the higher heat feedback from gas- to solid-phase, the average fire spread rate for three-shrub case with \( d/D = 0 \) increased by almost 35% and for the two-shrub case with \( d/D = 0 \) by 10%, as compared to that of the single-shrub case. An approximately 20% increase was seen in the peak mass loss rate value for the three-shrub case with \( d/D = 0 \) over the single-shrub case. This increase for the two-shrub case with \( d/D = 0 \) was 5%.

It was found that fire-fire interactions and the corresponding flame merging reduced as the separation distance between the shrubs was increased. For the two-shrub arrangement with \( d/D = 0.5 \), the behavior of fire was seen to be similar to that of a single isolated shrub, which indicated the absence of interactions between the two fires. For the three-shrub arrangement, a separation distance of 1.0 (\( d/D = 1.0 \)) was required to cease the fire-fire interactions. The peak value of heat release rate per shrub for the three-shrub arrangement with \( d/D = 0 \) was found to be approximately 6% lower than the corresponding value observed in the three-shrub case with \( d/D = 0.1 \). The reason was the inability of ambient air to enter the combustion zone, which created an oxygen deficient region near the top surface of the shrubs for the three-shrub case with \( d/D = 0 \). The peak mass loss rate, the vertical fire spread rate within the shrub and the amount of mass consumed in the first 60 seconds decreased with an increase in separation distance for both two- and three-shrub cases until the respective values were equal to those seen in the single-shrub case.
6.2 Future Work

When a model accounting for solid-fuel mass distribution in one spatial direction was used for the shrub, fire behavior predictions such as crown ignition time and fire spread rate changed. For a real chamise shrub, the mass is distributed in all three spatial directions. For this reason, only the global parameters predicted by the model were compared against experiments. A better model, which can be developed by systematic measurements of the shrubs with different physical characteristics, is required to account for the random distribution of mass inside the shrub canopy. An approach for conducting these measurements could be scanning the shrub using a 3D scanner, and then importing the geometrical structure of the shrub in the physics-based model. A rigorous validation of the model through experimentation should be one of the focuses of the future works.

It was shown in this work that the burning of individual shrubs is affected by the presence of neighboring fires, which is due to the fire-fire interactions and the resulting flame merging. Only two types of shrub arrangements, consisting of two shrubs and three shrubs, were used here as a preliminary setup to investigate the phenomena of simultaneous burning of multiple shrubs. The flame merging phenomena strongly depends on both the size and the number of individual fires contributing to this effect, as reported in the literature. Therefore, a more comprehensive investigation of the interactions between multiple shrub fires can be performed through the inclusion of a larger number of shrubs. Using different patterns for the arrangement of the shrubs would also be interesting. Studying the merging of shrub fires in presence
of external wind with various velocities could also be an important focus of the future work.
APPENDIX A

ADDITIONAL FORMULATION

A.1 Face Fluxes Evaluated using QUICKEST

The fluxes at the west face are given by

\[ F_{i-1/2,j,k} = \psi_{1w} + \psi_{2w} + \psi_{3w} \]

\[
\psi_{1w} = A \left(C_{i-1/2,j,k} \Delta x \left[ \left( \phi_{i,j,k} + \phi_{i-1,j,k} \right) - C_{i-1/2,j,k} \left( \frac{\phi_{i,j,k} - \phi_{i-1,j,k}}{2} \right) \right] \right)
\]

\[
\psi_{2w} = A \Delta x \left[ -\frac{\Delta x^2}{6} \left( 1 - C_{i-1/2,j,k}^2 - 3\gamma_w \right) \left( \alpha_w \text{CURVX}^+_{i-1/2,j,k} + \beta_w \text{CURVX}^-_{i-1/2,j,k} \right) + \frac{\Delta y^2}{24} \left( \alpha_w \text{CURVY}^+_{i-1/2,j,k} + \beta_w \text{CURVY}^-_{i-1/2,j,k} \right) + \frac{\Delta z^2}{24} \left( \alpha_w \text{CURVZ}^+_{i-1/2,j,k} + \beta_w \text{CURVZ}^-_{i-1/2,j,k} \right) \right]
\]

\[
\psi_{3e} = -A \gamma_w \Delta x \left[ \left( \phi_{i,j,k} - \phi_{i-1,j,k} \right) - \frac{\Delta x^2}{2} \left( \alpha_w \text{CURVX}^+_{i-1/2,j,k} + \beta_w \text{CURVX}^-_{i-1/2,j,k} \right) \right]
\]
where the parameters are given as follows

\[ \alpha_w = \left( C_{i-1/2,j,k} + |C_{i-1/2,j,k}| \right) / 2 \]

\[ \beta_w = \left( C_{i-1/2,j,k} - |C_{i-1/2,j,k}| \right) / 2 \]

\[ \gamma_w = \nu_{i-1/2,j,k} \frac{\Delta t}{\Delta x^2}. \]

The curvature terms appearing in the above formulation are given as

\[ \text{CURVX}^+_{i-1/2,j,k} = \left( \phi_{i,j,k} + \phi_{i-2,j,k} - 2\phi_{i-1,j,k} \right) / \Delta x^2 \]

\[ \text{CURVX}^-_{i-1/2,j,k} = \left( \phi_{i+1,j,k} + \phi_{i-1,j,k} - 2\phi_{i,j,k} \right) / \Delta x^2 \]

\[ \text{CURVY}^+_{i-1/2,j,k} = \left( \phi_{i-1,j+1,k} + \phi_{i-1,j-1,k} - 2\phi_{i-1,j,k} \right) / \Delta y^2 \]

\[ \text{CURVY}^-_{i-1/2,j,k} = \left( \phi_{i,j+1,k} + \phi_{i,j-1,k} - 2\phi_{i,j,k} \right) / \Delta y^2 \]

\[ \text{CURVZ}^+_{i-1/2,j,k} = \left( \phi_{i-1,j,k+1} + \phi_{i-1,j,k-1} - 2\phi_{i-1,j,k} \right) / \Delta z^2 \]

\[ \text{CURVZ}^-_{i-1/2,j,k} = \left( \phi_{i,j,k+1} + \phi_{i,j,k-1} - 2\phi_{i,j,k} \right) / \Delta z^2. \]

The flux at the north face is

\[ F_{i,j+1/2,k} = \psi_{1n} + \psi_{2n} + \psi_{3n} \]
\[ \psi_{1n} = A C_{i,j+1/2,k} \Delta y \left[ \frac{1}{2} \left( \phi_{i,j+1,k} + \phi_{i,j,k} \right) - C_{i,j+1/2,k} \left( \frac{\phi_{i,j+1,k} - \phi_{i,j,k}}{2} \right) \right] \]

\[ \psi_{2n} = A \Delta y \left[ \Delta y^2 \left( 1 - C_{i,j+1/2,k}^2 - 3 \gamma_n \right) \left( \alpha_n \text{CURVY}_{i,j+1/2,k}^+ + \beta_n \text{CURVY}_{i,j+1/2,k}^- \right) \right. 
\left. + \frac{\Delta x^2}{24} \left( \alpha_n \text{CURVX}_{i,j+1/2,k}^+ + \beta_n \text{CURVX}_{i,j+1/2,k}^- \right) \right. 
\left. + \frac{\Delta z^2}{24} \left( \alpha_n \text{CURVZ}_{i,j+1/2,k}^+ + \beta_n \text{CURVZ}_{i,j+1/2,k}^- \right) \right] \]

\[ \psi_{3n} = -A \gamma_n \Delta y \left[ (\phi_{i,j+1,k} - \phi_{i,j,k}) - \frac{\Delta y^2}{2} \left( \alpha_n \text{CURVY}_{i,j+1/2,k}^+ + \beta_n \text{CURVY}_{i,j+1/2,k}^- \right) \right] \]

where the parameters are given as follows

\[ \alpha_n = \left( C_{i,j+1/2,k} + |C_{i,j+1/2,k}| \right) / 2 \]
\[ \beta_n = \left( C_{i,j+1/2,k} - |C_{i,j+1/2,k}| \right) / 2 \]
\[ \gamma_n = \nu_{i,j+1/2,k} \frac{\Delta t}{\Delta y^2} \]

The curvature terms appearing in the above formulation are given as

\[ \text{CURVY}_{i,j+1/2,k}^+ = \left( \phi_{i,j+1,k} + \phi_{i,j-1,k} - 2\phi_{i,j,k} \right) / \Delta y^2 \]
\[ \text{CURVY}_{i,j+1/2,k}^- = \left( \phi_{i,j,k} + \phi_{i,j+2,k} - 2\phi_{i,j+1,k} \right) / \Delta y^2 \]
\[ \text{CURVX}_{i,j+1/2,k}^+ = \left( \phi_{i+1,j,k} + \phi_{i-1,j,k} - 2\phi_{i,j,k} \right) / \Delta x^2 \]
\[ \text{CURVX}_{i,j+1/2,k}^- = \left( \phi_{i+1,j+1,k} + \phi_{i-1,j+1,k} - 2\phi_{i,j+1,k} \right) / \Delta x^2 \]
\[ \text{CURVZ}_{i,j+1/2,k}^+ = \left( \phi_{i,j,k+1} + \phi_{i,j,k-1} - 2\phi_{i,j,k} \right) / \Delta z^2 \]
\[ \text{CURVZ}_{i,j+1/2,k}^- = \left( \phi_{i,j+1,k+1} + \phi_{i,j+1,k-1} - 2\phi_{i,j+1,k} \right) / \Delta z^2. \]
Flux at the south face

\[ F_{i,j-1/2,k} = \psi_{1s} + \psi_{2s} + \psi_{3s} \]

\[ \psi_{1s} = A \, C_{i,j-1/2,k} \, \Delta y \left[ \left( \frac{\phi_{i,j,k} + \phi_{i,j-1,k}}{2} \right) - C_{i,j-1/2,k} \left( \frac{\phi_{i,j,k} - \phi_{i,j-1,k}}{2} \right) \right] \]

\[ \psi_{2s} = A \, \Delta y \left[ -\frac{\Delta y^2}{6} \left( 1 - C_{i,j-1/2,k}^2 - 3\gamma_s \right) \left( \alpha_s \text{CURVY}^+_{i,j-1/2,k} + \beta_s \text{CURVY}^-_{i,j-1/2,k} \right) \right. \]
\[ \left. + \frac{\Delta x^2}{24} \left( \alpha_s \text{CURVX}^+_{i,j-1/2,k} + \beta_s \text{CURVX}^-_{i,j-1/2,k} \right) \right] \]
\[ + \frac{\Delta z^2}{24} \left( \alpha_s \text{CURVZ}^+_{i,j-1/2,k} + \beta_s \text{CURVZ}^-_{i,j-1/2,k} \right) \]

\[ \psi_{3s} = -A \, \gamma_s \Delta y \left[ (\phi_{i,j,k} - \phi_{i,j-1,k}) - \frac{\Delta y^2}{2} \left( \alpha_s \text{CURVY}^+_{i,j-1/2,k} + \beta_s \text{CURVY}^-_{i,j-1/2,k} \right) \right] \]

where the parameters are given as follows

\[ \alpha_s = \left( C_{i,j-1/2,k} + |C_{i,j-1/2,k}| \right) / 2 \]
\[ \beta_s = \left( C_{i,j-1/2,k} - |C_{i,j-1/2,k}| \right) / 2 \]
\[ \gamma_s = \nu_{i,j-1/2,k} \frac{\Delta t}{\Delta y^2}. \]
The curvature terms appearing in the above formulation are given as

\[
\begin{align*}
\text{CURVY}^+_{i,j-1/2,k} &= \left( \phi_{i,j,k} + \phi_{i,j-1,k} - 2\phi_{i,j-2,k} \right) / \Delta y^2 \\
\text{CURVY}^-_{i,j-1/2,k} &= \left( \phi_{i,j+1,k} + \phi_{i,j-1,k} - 2\phi_{i,j,k} \right) / \Delta y^2 \\
\text{CURVX}^+_{i,j-1/2,k} &= \left( \phi_{i+1,j-1,k} + \phi_{i-1,j-1,k} - 2\phi_{i,j-1,k} \right) / \Delta x^2 \\
\text{CURVX}^-_{i,j-1/2,k} &= \left( \phi_{i+1,j,k} + \phi_{i-1,j,k} - 2\phi_{i,j,k} \right) / \Delta x^2 \\
\text{CURVZ}^+_{i,j-1/2,k} &= \left( \phi_{i,j+1,k+1} + \phi_{i,j-1,k-1} - 2\phi_{i,j,k} \right) / \Delta z^2 \\
\text{CURVZ}^-_{i,j-1/2,k} &= \left( \phi_{i,j,k+1} + \phi_{i,j,k-1} - 2\phi_{i,j,k} \right) / \Delta z^2.
\end{align*}
\]

The flux at the down face is

\[
F_{i,j,k+1/2} = \psi_{1d} + \psi_{2d} + \psi_{3d}
\]

\[
\begin{align*}
\psi_{1d} &= A \, C_{i,j,k+1/2} \, \Delta z \left[ \left( \frac{\phi_{i,j,k+1} + \phi_{i,j,k}}{2} \right) - C_{i,j,k+1/2} \left( \frac{\phi_{i,j,k+1} - \phi_{i,j,k}}{2} \right) \right] \\
\psi_{2d} &= A \, \Delta z \left[ -\frac{\Delta z^2}{6} \left( 1 - C^2_{i,j,k+1/2} - 3\gamma_d \right) \left( \alpha_d \text{CURVZ}^+_{i,j,k+1/2} + \beta_d \text{CURVZ}^-_{i,j,k+1/2} \right) \right. \\
&\quad + \frac{\Delta y^2}{24} \left( \alpha_d \text{CURVX}^+_{i,j,k+1/2} + \beta_d \text{CURVX}^-_{i,j,k+1/2} \right) \\
&\quad + \frac{\Delta y^2}{24} \left( \alpha_d \text{CURVY}^+_{i,j,k+1/2} + \beta_d \text{CURVY}^-_{i,j,k+1/2} \right) \bigg] \\
\psi_{3d} &= -A \, \gamma_d \, \Delta z \left[ \phi_{i,j,k+1} - \phi_{i,j,k} - \frac{\Delta z^2}{2} \left( \alpha_d \text{CURVZ}^+_{i,j,k+1/2} + \beta_d \text{CURVZ}^-_{i,j,k+1/2} \right) \right]
\end{align*}
\]
where the parameters are given as follows

\[\alpha_d = \frac{(C_{i,j,k+1/2} + |C_{i,j,k+1/2}|)}{2}\]

\[\beta_d = \frac{(C_{i,j,k+1/2} - |C_{i,j,k+1/2}|)}{2}\]

\[\gamma_d = \nu_{i,j,k+1/2} \frac{\Delta t}{\Delta z^2}.\]

The curvature terms appearing in the above formulation are given as

\[\text{CURVZ}^+_{i,j,k+1/2} = \frac{(\phi_{i,j,k+1} + \phi_{i,j,k-1} - 2\phi_{i,j,k})}{\Delta z^2}\]

\[\text{CURVZ}^-_{i,j,k+1/2} = \frac{(\phi_{i,j,k} + \phi_{i,j,k+2} - 2\phi_{i,j,k+1})}{\Delta z^2}\]

\[\text{CURVX}^+_{i,j,k+1/2} = \frac{(\phi_{i+1,j,k} + \phi_{i-1,j,k} - 2\phi_{i,j,k})}{\Delta x^2}\]

\[\text{CURVX}^-_{i,j,k+1/2} = \frac{(\phi_{i+1,j,k+1} + \phi_{i-1,j,k+1} - 2\phi_{i,j,k+1})}{\Delta x^2}\]

\[\text{CURVY}^+_{i,j,k+1/2} = \frac{(\phi_{i,j+1,k} + \phi_{i,j-1,k} - 2\phi_{i,j,k})}{\Delta y^2}\]

\[\text{CURVY}^-_{i,j,k+1/2} = \frac{(\phi_{i,j+1,k+1} + \phi_{i,j-1,k+1} - 2\phi_{i,j,k+1})}{\Delta y^2}.\]

The flux at the up face is

\[F_{i,j,k-1/2} = \psi_{1u} + \psi_{2u} + \psi_{3u}.\]
\[ \psi_{1u} = A C_{i,j,k-1/2} \Delta z \left[ \left( \frac{\phi_{i,j,k} + \phi_{i,j,k-1}}{2} \right) - C_{i,j,k-1/2} \left( \frac{\phi_{i,j,k} - \phi_{i,j,k-1}}{2} \right) \right] \]

\[ \psi_{2u} = A \Delta z \left[ -\frac{\Delta z^2}{6} \left( 1 - C_{i,j,k-1/2}^2 - 3 \gamma_u \right) \left( \alpha_u \text{CURVZ}_{i,j,k-1/2}^+ + \beta_u \text{CURVZ}_{i,j,k-1/2}^- \right) \right. \]
\[ + \frac{\Delta x^2}{24} \left( \alpha_u \text{CURVX}_{i,j,k-1/2}^+ + \beta_u \text{CURVX}_{i,j,k-1/2}^- \right) \]
\[ + \frac{\Delta y^2}{24} \left( \alpha_u \text{CURVY}_{i,j,k-1/2}^+ + \beta_u \text{CURVY}_{i,j,k-1/2}^- \right) \right] \]

\[ \psi_{3u} = -A \gamma_u \Delta z \left[ (\phi_{i,j,k} - \phi_{i,j,k-1}) - \frac{\Delta z^2}{2} \left( \alpha_u \text{CURVZ}_{i,j,k-1/2}^+ + \beta_u \text{CURVZ}_{i,j,k-1/2}^- \right) \right] \]

where the parameters are given as follows

\[ \alpha_u = \frac{(C_{i,j,k-1/2} + |C_{i,j,k-1/2}|)}{2} \]

\[ \beta_u = \frac{(C_{i,j,k-1/2} - |C_{i,j,k-1/2}|)}{2} \]

\[ \gamma_u = \nu_{i,j,k-1/2} \frac{\Delta t}{\Delta z^2} \]

The curvature terms appearing in the above formulation are given as

\[ \text{CURVZ}_{i,j,k-1/2}^+ = \frac{(\phi_{i,j,k} + \phi_{i,j,k-2} - 2\phi_{i,j,k-1})}{\Delta z^2} \]

\[ \text{CURVZ}_{i,j,k-1/2}^- = \frac{(\phi_{i,j,k-1} + \phi_{i,j,k+1} - 2\phi_{i,j,k})}{\Delta z^2} \]

\[ \text{CURVX}_{i,j,k-1/2}^+ = \frac{(\phi_{i+1,j,k-1} + \phi_{i-1,j,k-1} - 2\phi_{i,j,k-1})}{\Delta x^2} \]

\[ \text{CURVX}_{i,j,k-1/2}^- = \frac{(\phi_{i+1,j,k} + \phi_{i-1,j,k} - 2\phi_{i,j,k})}{\Delta x^2} \]

\[ \text{CURVY}_{i,j,k-1/2}^+ = \frac{(\phi_{i,j+1,k-1} + \phi_{i,j-1,k-1} - 2\phi_{i,j,k-1})}{\Delta y^2} \]

\[ \text{CURVY}_{i,j,k-1/2}^- = \frac{(\phi_{i,j+1,k} + \phi_{i,j-1,k} - 2\phi_{i,j,k})}{\Delta y^2} \].
APPENDIX B

ADDITIONAL FIGURES

B.1 Burning of Single Shrub
Figure B.1: Gas-phase temperature iso-surface of 500 K (orange) with solid fuel bulk density iso-surface of 1 kg/m³ (green) at various times in simulation, shrub modeled with distributed bulk density (DBD) and a moisture content of 31.2%.
Figure B.2: Gas-phase temperature in Kelvin (color contours), solid fuel bulk density (line contours) and velocity field (vectors) at time approximately equals peak mass loss rate ($\approx 43.0$ sec); Snapshots are from a $xy$-slice passing through $z = 0.8$ m for case with convective boundary condition and outflow boundary condition, respectively, for top surface.
Figure B.3: Gas-phase temperature in Kelvin (color contours) with solid fuel bulk density (line contours) on a $xy$-slice passing through $z = 0.8$ m at various time instances, for a distributed bulk density (DBD) shrub (first row) and a fixed bulk density (FBD) shrub (second row), with moisture content of 31.2%, respectively.
Figure B.4: Gas-phase temperature in Kelvin (color contours) with solid fuel bulk density (line contours) at time equals 27.0 seconds, on a $xy$-slice passing through $z = 0.8$ m, for a fixed bulk density (FBD) shrub; sub-figures (a), (b), (c), (d) and (e) are for 20%, 40%, 60%, 80% and 100% moisture content in shrub, respectively.
Figure B.5: Gas-phase temperature in Kelvin (color contours) with solid fuel bulk density (line contours) at time equals 27.0 seconds, on a $xy$-slice passing through $z = 0.8$ m, for a distributed bulk density (DBD) shrub; sub-figures (a), (b), (c), (d) and (e) are for 20%, 40%, 60%, 80% and 100% moisture content in shrub, respectively.
B.2 Burning of Multiple Shrubs

Figure B.6: Snapshots for vorticity magnitude in $s^{-1}$ (color contours) along a $xy$-slice at $z = 2.0$ m, at peak mass loss rate (i.e., $t \approx 23.0 \pm 0.5$ sec); (a) single-shrub case, (b) two-shrub case with $d/D = 0.0$, (c) three-shrub case with $d/D = 0.0$, respectively.
Figure B.7: Snapshots for the second invariant of the velocity gradient tensor ($Q = 0.5(\| \Omega \|^2 - \| S \|^2)$) (color contours) and pyrolysis gas mass fraction of 0.025 (≈5% of maximum, line contour) along a $xy$-slice at $z = 2.0$ m, at peak mass loss rate (i.e., $t \approx 23.0 \pm 0.5$ sec); (a) single-shrub case, (b) two-shrub case with $d/D = 0.0$ and (c) three-shrub case with $d/D = 0.0$, respectively.
Figure B.8: Snapshots for baroclinic torque magnitude (vorticity transport equation source term, $|\nabla \rho \times \nabla p|/\rho^2$, color contours) and solid fuel bulk density of 3.8 kg/m$^3$ (line contour) along a $xz$-slice at $z = 1.0$ m at peak mass loss rate (i.e., $t \approx 23.0 \pm 0.5$ sec); (a) single-shrub case, (b) two-shrub case with $d/D = 0.0$ and (c) three-shrub case with $d/D = 0.0$, respectively.
Figure B.9: Snapshots for pressure (N/m², color contour), solid fuel bulk density of 3.8 kg/m³ (line contour) and velocity field (m/sec, vector field) along a xz-slice at y = 0.71 m, at peak mass loss rate (i.e., t ≈ 23.0 ± 0.5 sec); (a) single-shrub case, (b) two-shrub case with d/D = 0.0 and (c) three-shrub case with d/D = 0.0, respectively.
Figure B.10: Pyrolysis gas mass fraction iso-surface of 0.025 (≈5% of maximum, orange) and solid fuel bulk density iso-surface of 3.8 kg/m$^3$ (green) at peak mass loss rate (i.e., $t \approx 23.0$ sec); (a), (b) and (c) for the two-shrub cases with separation distance $(d/D)$ equals 0.1, 0.3 and 0.5, respectively; (d), (e), (f) and (g) for the three-shrub cases with separation distance $(d/D)$ equals 0.1, 0.3, 0.5 and 1.0, respectively.
Figure B.11: Vorticity magnitude iso-surface ($\approx 25\%$ of the maximum) colored with second invariant of the velocity gradient tensor ($Q = 0.5(\| \Omega \|^2 - \| S \|^2)$) at peak mass loss rate ($t \approx 23.0$ sec); (a), (b) and (c) for the two-shrub case with separation distance ($d/D$) equals 0.1, 0.3 and 0.5, respectively; (d), (e), (f) and (g) for the three-shrub case with separation distance ($d/D$) equals 0.1, 0.3, 0.5 and 1.0, respectively.
Figure B.12: Spatial variation of oxygen mass fraction along a line passing through the center of the domain (x=2.0 m, z=2.0 m) in y-direction at various time instances; highlighting the region of oxygen deficiency seen in the three-shrub case with $d/D = 0$. 
REFERENCES


ERRATA

Equation (3.28) on page 64 is missing a $1/(\Delta t)$ term on the RHS, as follows

$$\frac{\delta}{\delta x_i} \left( \frac{\delta p^m}{\delta x_i} \right) = \frac{1}{\Delta t} \left[ S^{n+1} - \left( \frac{\rho^m - \rho^n}{\Delta t} + \frac{\delta(\rho u_i)^*}{\delta x_i} \right) \right]. \quad (F.1)$$

Equation (3.29) on page 64 is missing a $-\Delta t$ term on the RHS, as follows

$$(\rho u_i)^m = (\rho u_i)^* - \Delta t \left( \frac{\delta p^m}{\delta x_i} \right). \quad (F.2)$$