THE SMOULDERING OF PEAT

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A model examining underground smouldering peat combustion is presented. A one-step chemical reaction is considered where the gas and solid are assumed to be in thermal equilibrium. The full model allows porosity, permeability and gas density to vary and considers a buoyant velocity field determined by Darcy’s law. Due to the low bulk thermal conductivity of peat, the diffusion of oxygen through it is characterised by a Lewis number much less than one. This results in thermal-diffusive instabilities. These instabilities can cause flame balls to arise in gaseous combustion and a fingering regime to arise in solid combustion.

Analytical solutions to simplified spherically symmetrical equations are derived. These equations assume diffusion to be the dominant transport mechanism as well as taking that the porosity, gas molecular weight and gas density all remain constant. The underlying structure of the combustion region is found to be analogous to that of a flame ball.

When studied in cylindrical symmetry a single, stable finger can be modelled propagating against an imposed air flow. The effects of heat losses, velocity magnitude and the Lewis number can be studied and results are compared to existing experimental smouldering combustion data. Although no detailed experiments have studied this phenomenon in peat, predicted results capture key qualitative trends found in both filtration combustion of polyurethane foam and in the fingering combustion of paper. In addition to this, when the imposed air flow is reduced to zero a propagating combustion front is predicted, analogous to a self-travelling flame ball.

When the velocity field is determined by Darcy’s law the dimensionless permeability of the peat plays a key role in determining the range of values over which fingering combustion can occur. Whilst there is little impact of taking the gas molecular weight to be constant, when porosity is allowed to vary and a relationship between porosity and permeability is included an over-blowing extinction limit is identified. This limit is not found in the constant-porosity model where a low-fuel extinction limit is predicted. Peats of differing ages and locations can possess significantly different characteristics. However, the fingering regime is predicted to occur within the range of parameters in which peat soils lie.

Experiments suggest that fingering combustion can take the form of both sparse fingers and a complex fingering regime. The cylindrically symmetrical model can not capture tip-splitting. Hence the model does not explicitly account for the distance between two neighbouring fingers. However, an estimate for this value can be made if peat smouldering were to occur in a regime of multiple fingering.

An averaged continuum model describing the spread of an ember storm is also presented. The dominant mechanism determining the spread-rate of the fire is the lofting and landing of embers and individual fires are taken to grow in an elliptical manner under the influence of the wind. When an ember storm is spreading at a steady speed, its spread rate is found to be described by a single similarity solution.
Declaration

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# Nomenclature

- $A$: pre-exponential factor
- $c$: specific heat
- $d$: distance between neighbouring fingers
- $D$: diffusivity
- $g$: gravity
- $F$: dimensionless heat loss constant
- $K$: permeability of solid with respect to air
- $K'$: dimensionless permeability
- $Le$: Lewis number
- $m$: mass
- $p$: variation from ambient pressure
- $P$: pressure
- $Q$: heat of reaction per mass of char
- $R$: universal gas constant
- $S$: propagation speed
- $t$: time
- $T$: temperature
- $T_A$: activation temperature
- $u$: gas velocity
- $V$: volume
- $W$: molecular weight
- $y$: mass fraction
- $Y$: dimensionless mass fraction
- $\alpha$: heat release factor
- $\beta$: Zeldovich number
\( \delta \) ratio of characteristic gas density to characteristic peat density
\( \epsilon \) ratio of gas specific heat to peat specific heat
\( \gamma \) ratio of characteristic temperature to initial temperature
\( \lambda \) thermal conductivity
\( \rho_s \) solid bulk density
\( \bar{\rho} \) non-dimensional burnt peat bulk density
\( \rho \) bulk density of all gas species
\( \mu \) stoichiometric coefficient
\( \bar{\mu} \) dynamic viscosity
\( \phi \) porosity
\( \omega \) reaction rate
\( \Omega \) dimensionless reaction rate
\( \nu \) ratio of gas thermal conductivity to peat thermal conductivity

**Subscripts**

0 absolute
g gas
s solid
in intrinsic
A air
C char
N nitrogen
P reaction product gas
X oxygen
CO carbon monoxide producing combustion
CO\(_2\) carbon dioxide producing combustion
\( \infty \) value in unburnt region
Chapter 1

Introduction and Background

1.1 Overview of Wildfires

Wildfires occur all over the world, in many different climates and types of vegetation. Press coverage of wildfires often focuses on the large scale forest fires in developed countries such as Australia and America. However, as shown in Figure 1.1, almost every country in the world suffers from wildfire to some degree. Although wildfires in the UK usually occur on a relatively small scale they can still have devastating effects. Animals and plants are killed, soil integrity is lost and homes and livelihoods are destroyed.

Figure 1.1: Map showing fires between 20th and 29th May 2012 produced by NASA-FIRMS [1]. Fire locations are detected by satellite. Each coloured dot indicates a location where at least one fire was detected during the ten day period. Red dots represent a small number of fires, yellow dots a high number of fires.
Despite the negative consequences of wildfires, they do in fact play an important role in decomposing biomass and recycling nutrients. Fallen trees, large branches and pine needles lying on a forest floor decay at a very slow rate. Large logs can take over 100 years to decompose and it takes more than one year for just 10% of pine needles on a forest floor to decay [2]. Fires help to significantly speed up decomposition, allowing nutrients vital for growth to leach back into the soil. Given the rapid build up of flammable materials on the forest floor, preventing fires in forest areas can in fact lead to an increasingly hazardous environment. Once started, a surplus of fuel would make a fire very difficult to control. In addition to this plants and animals living in fire prone areas have not only developed adaptations making survival possible, but some in fact thrive in such environments [3].

Wildfires can occur naturally, ignited by lightening strikes, volcanoes and spontaneously ignited coal seams. It is in fact thought that natural wildfires would be self sustaining if humans did not intervene. Burnt areas would create buffers, minimising the effects of subsequent fires. This theory is supported by fire control practices used at Yellowstone National Park where lightening caused fires in remote areas were allowed to burn without interference. Of over 200 fires between 1972 and 1988 83% went out before half a hectacre had burnt [4]. However, wildfires can also be ignited by human activities. Land clearing, cooking fires, discarded cigarettes and arson can all lead to wildfires, resulting in a far greater number than would occur naturally [3].

Controlling wildfires can be a difficult task, with fires often taking place in areas where access by large fire-fighting machinery is limited. One of the most effective methods to fight wildfires is to create firebreaks. These are gaps in the vegetation which slow down the progression of the combustion front. Whilst some firebreaks will already exist, such as roads and rivers, they can also be created by cutting down and removing vegetation or by burning it. Not only can fire be used indirectly in this manner to help slow the spread of a wildfire, fire can also be used as a tool to directly fight a wildfire. Controlled fires can be ignited under conditions as to ensure the combustion front moves slowly towards a wildfire. When the two fires meet the surrounding area will all be burnt. This either significantly slows the propagation rate of the fire or completely extinguishes the fire in this area [5]. Use of both of these techniques requires accurate predictions of how a combustion front will develop,
making predictive models a very useful tool.

Wildfire models consist of a collection of equations. The solution of these equations provides the evolution of the fire over space and time allowing a detailed description of the behaviour of the fire to be built up. Used alone these models aid the understanding of a number of wildfire variables such as spread-rates, ignition probabilities and fuel consumption. Several models can also be used together and in conjunction with computer software to allow very detailed predictions of wildfire behaviour to be made. Whilst the use of mathematical models to predict wildfire spread is still not standard in Mediterranean Europe, they are expected to become an indispensable tool in the medium term [6].

There are four broad categories into which wildfire models can be separated: ground fires, surface fires, crown fires and spotting fires. The first three categories are defined by the strata of the fuel in which the combustion occurs. These fires occur in fuels at ground level and below, fuels which are within 2 metres of ground level and aerial fuels located high in the air respectively. In all of these fires the transport mechanisms of oxygen and heat are seen as key parameters in establishing how a front would propagate. In spotting fires it is spotting, the lofting and landing of embers, which is taken to dominate the spread rate of the fire.

This thesis presents a ground fire model for the smouldering combustion of peat. A spotting fire model considering the spread of an ember storm is also presented in Appendix B.

### 1.2 Peat Characteristics and Peat fires

**Peat and Peatland Characteristics**

Peat is a dark organic soil, geologically regarded as an intermediate stage between plant substance and coal. It is formed under waterlogged conditions by an accumulation of partly decomposed or undecomposed remains of plant materials [7]. When the water content of peat is high anaerobic conditions slow decomposition. Much of the original plant structure is retained resulting in the formation of a highly porous, fibrous peat. Lower water contents lead to increased aeration and hence a higher level of decomposition. Peat formed under these conditions is denser and has a lower
CHAPTER 1. INTRODUCTION AND BACKGROUND

permeability and porosity [8].

Peatlands exist in over 175 countries around the world, in many different climates. The highest proportion of peatland cover is found in Canada, Northern America, Indonesia, Russia and Northern Europe as highlighted in Figure 1.2. Despite being a small country, the UK is in fact in the top ten countries in the world in terms of its total peatland, containing approximately 10% of Europe’s peatland area [9]. Peat bogs can reach great depths. Peat depths of 5-10 metres accumulated over thousands of years are not uncommon, although the average depth is usually closer to 2-3 metres [10].

![Figure 1.2: Worldwide peatlands cover. Produced by Joosten [11].](image)

Dry peat has a number of characteristics which make it susceptible to smouldering. The porosity of peat can be as high as 0.97 [12]. This allows oxygen to travel through the peat towards a combustion site, even when combustion is occurring deep underground. Fluid flow through peat is also aided by naturally occurring pipe networks. These channels are found in both deep peat layers and close to the surface of the peat. Mean diameters of these pipes range from 3cm to 70cm with some pipes being over 150 metres long [13]. Dry peat is also characterised by a very low thermal conductivity. In fact in the summer it can be almost as good an insulator as fibreglass [14]. This allows heat losses to be minimised and aids deep peat combustion.

The Lewis number of a substance is defined as the ratio of its thermal diffusivity to molecular diffusivity. Due to the low bulk thermal conductivity of peat, the diffusion of oxygen through it is characterised by a Lewis number much less than one (see Appendix A). This is of particular significance as low Lewis number combustion has
1.2. **PEAT CHARACTERISTICS AND PEAT FIRES**

a number of interesting features. These features are discussed in Section 1.5.

Peatlands also play important ecological roles. Many plant and animal species are adapted to living in and around waterlogged acidic areas. In fact peatlands in the UK have been found to support an exceptionally high proportion of bird species with protection under UK and European law. In addition to this peatlands can help to reduce the costs of drinking water. In the UK most drinking water is taken from areas fed by peat dominated soils. Healthy peatlands provide high quality water which can be treated at a relatively low cost. Damaged peatlands produce water containing higher concentrations of carbon, the treatment of which costs significantly more [9].

**Overview of Peat Fires**

Whilst large peat fires do not occur regularly on a local level, they do occur regularly on a global level [15]. Peat fires have been reported in South-East Asia, Northern America, Siberia, Southern Africa, Finland and the UK amongst other places [16]. As peat fires spread at a far slower rate than other forms of wildfires, they can often be seen as less of a threat. However, peat fires can have a detrimental effect on both the local economy and surrounding ecosystems.

Peat has been known to smoulder for several months [17]. Whilst peatlands only cover approximately 3% of the surface of the world, the quantity of carbon they hold is comparable to that in the atmosphere [10]. As a result of this, when peat smothers on a large scale and for prolonged periods of time, vast amounts of carbon are released into the atmosphere. This has become of increasing concern over the last few decades due to the impact of carbon emissions on global warming. Many governments have policies in place with the aim of reducing carbon emissions from homes and businesses. However, a large scale peat fire can result in carbon emissions estimated to equal 10% of the annual global emissions from fossil fuel consumption [18].

Peat fires have the ability to spread deep underground which can make extinguishing the fire extremely difficult. It is also difficult to predict when and where the fire may resurface as fires have the ability to appear long after flames were extinguished [16]. Peat fires have been known to burn under roads and often there is little sign that the combustion is occurring except for smoke rising from the ground. Whereas firebreaks are a useful tool in fighting ground-level fires, they are less effective in fighting
peat fires. Here firebreaks need to consist of trenches all the way down to the mineral soil. For relatively shallow peat this can be effective, but when the peat is several metres deep this is no longer a practical tool. Bulldozers can be used to turn and compress the soil in order to suffocate the combustion, but again this is only found to have limited success. The best results are found when the peat is completely flooded, requiring thousands of gallons of water [19, 20].

Peat bogs have been drained for centuries in response to agricultural demand, forestry and for the horticultural and energy properties of peat [21]. This results in dryer and significantly more flammable peat. Due to both global warming and the continued draining of peat bogs there is concern that large scale peat fires may begin to occur on an increasingly regular basis [22, 23]. For this reason peat fires, and the mechanisms by which they spread, have become an important area of study over the last few decades.

One of the largest peat fires on record occurred in Indonesia between mid 1997 and April 1998. These fires smouldered for long periods of time and regularly transformed into flaming fires. The final report of the National Development Planning Agency on the Indonesia peat fires of 1997 and 1998 [22] shows what a devastating effect these fires can have on both the ecosystem and the economy.

The study found that not only was plant and animal life above ground disrupted or destroyed, but there were significant biodiversity losses from the soil ecosystems due to the peat fire. Microorganisms, roots and seeds were killed and the damage to the peat was expected to drastically alter the capacity of the peat to store water. This caused problems for the forests, agriculture and aquatic ecosystems the peatlands usually helped to maintain. It was also estimated that 60% of the resulting haze from the fires was due to the burning of the peat. The haze contained toxic chemicals affecting the health of many of those that came into contact with it. The resulting health impact of the fires was estimated to cost 145 million USD. In addition to this the firefighting costs were estimated to be in the order of 12 million USD. Whilst this is an extreme example of the consequences that peat fires can have, these events do help to highlight the importance of studying this form of combustion.
1.3 The Physics and Chemistry of Combustion

Combustion is the sequence of exothermic chemical reactions between an oxidiser and a fuel, creating heat and new chemical species. The full scheme for an oxidation reaction will often involve several hundred individual reaction steps and hundreds of intermediary species. These species include radicals, short-lived intermediate species which are produced by some reactions but consumed by others, so that they do not appear at any significant concentration in the final products. Combustion can also occur in conjunction with pyrolysis: the thermal decomposition of materials at high temperatures. Pyrolysis reactions do not require oxygen and, in contrast to oxidative reactions, they are typically endothermic. In solid fuels pyrolysis results in the production of char, tar and gases. Although these reactions are endothermic, they can play an important role in aiding combustion. It is the oxidation of chars which often provides the majority of the heat required to sustain both pyrolysis and oxidation in smouldering combustion [24].

Whilst research has been conducted to investigate the exact pathways by which fuels combust, the accuracy of the data currently available is questionable, and few fuels have been studied [25]. For this reason, and for simplicity, when modeling combustion the full reaction scheme is usually replaced by a few overall reactions. Whilst simplifying the reactions in this way will not capture the exact processes by which combustion occurs, when chosen correctly, they can be used to capture the main features of a system.

In order to mathematically study the process of combustion conservation laws are normally considered. These take the form

\[
\frac{\partial}{\partial t} \text{(property per unit volume)} + \text{div} \text{(flow-rate, or flux, of the property)} = \text{(nett rate of production per unit volume)}.
\]

These equations can be applied to each individual chemical species, along with the overall mass, energy and momentum of the system producing a set of coupled partial differential equations. The solution of these equations describes the evolution of the system over space and time.

In combustion the nett rate of production is due to chemical reactions using or creating mass, energy or momentum. Reactions occur when molecules collide with
enough kinetic energy to overcome short-hand repulsive forces and to break apart the existing molecular structures. This results in a threshold of activation energy, a value below which the molecules have too little energy for reactions to occur. The Arrhenius law uses this idea to relate the dependence of the reaction-rate constant, $\kappa$, on temperature, $T$, and activation energy, $E_A$.

$$\kappa = A \exp \left( \frac{-E_A}{RT} \right)$$

Here $A$ is the pre-exponential factor, which takes into account how often molecules collide, and $R$ is the gas constant. The equation is simply stating that the reaction-rate constant ($\kappa$) is equal to the total number of collisions per second ($A$), multiplied by the probability that any given collision will result in a reaction ($\exp(-E_A/RT)$).

Whilst this is not the only equation describing the relationship between the reaction rate and temperature, this equation is found to hold well for most reactions [26].

The flow-rates of heat and oxidiser play very important roles in determining how a combustion front propagates. Heat is transported away from the reaction zone by conduction, convection and radiation. These processes raise the temperature of the surrounding fuel until it reaches a temperature where combustion can occur. The significance of the role that each of these mechanisms plays on the propagation of the front depends on the type of combustion being studied. The oxidiser is transported to the reaction zone through diffusion and advection, with the same processes moving reaction products away.

The adiabatic temperature of combustion is the temperature obtained during a complete combustion process that occurs without any heat losses due to mechanisms such as work or heat transfer. In many combustion regimes heat transfer mechanisms such as radiation and conduction result in lower peak temperatures than the adiabatic temperature. However, flame curvature and certain smouldering regimes can result in thermal energy being concentrated in one area resulting in superadiabatic combustion temperatures [27, 28].

Whilst combustion often conjures the image of a flame, this is but one of many forms that combustion can take. Homogeneous reactions between a gaseous fuel and oxidiser can lead to modes of combustion such as stationary, spherically symmetrical flame balls and explosive, rapidly propagating aerosol fuel combustion. Combustion can also be flameless, in the form of smouldering combustion, when heterogeneous
1.4 Characteristics of Smouldering Combustion

Smouldering is a slow, relatively low-temperature (approximately 500-700°C), flameless form of combustion, sustained by the heat evolved when oxygen directly attacks the surface of a condensed-phase fuel [29, 30]. Examples of smouldering combustion can be found in many commonplace situations such as coal fires, smoking cigarettes and burning incense. The principal difference between smouldering combustion and flaming combustion is the fuel involved. Flaming combustion takes place when homogeneous reactions occur between a gaseous fuel and a gaseous oxidiser. Smouldering combustion occurs when heterogeneous reactions occur between a gaseous oxidiser and a solid fuel.

Porous materials which form a solid carbonaceous char when heated can undergo self-sustained smouldering combustion [30]. The structure of porous media ensures a high surface area to volume ratio, allowing oxygen to diffuse to the combustion zone and combustion products to diffuse away. Due to the high air content of these fuels they are also often characterised by a high level of thermal insulation. This ensures heat losses are minimised and allows combustion to be sustained despite low heat release rates. Both porous fuels and their carbonaceous chars are capable of oxidation. The chars, however, react in a significantly more exothermic manner. Thus it is the coupled process of fuel pyrolysis and char oxidation which is often seen as driving smouldering combustion [24].

The differences between the homogeneous reactions of flaming combustion and the heterogeneous reactions of smouldering combustion lead to a number of significantly diverse characteristics. Less heat is lost to the environment in smouldering combustion and so it can be sustained at significantly lower temperatures than flaming combustion. Typical temperatures found in flaming combustion are of the order of 1000-1500°C, compared to 500-700°C in smouldering combustion. The low temperature of smouldering is also accompanied by a reduced spread rate. Typical spread rates for smouldering combustion are of the order 0.1 mm/s which is approximately 10 times lower than flame spread over solid fuel [31]. Finally, the emissions from the
two forms of combustion also differ significantly. Smouldering combustion is typically incomplete, resulting in the production of partially oxidised toxic compounds. This is due to both insufficient heat in the gas phase and a lack of oxygen in the combustion region [32]. In flaming combustion a ratio of CO to CO$_2$ is usually expected to be around 1:10 whereas in smouldering combustion a ratio of around 1:1 is more likely [17].

Smouldering combustion occurring inside a fuel-bed is a form of filtration combustion. Filtration combustion is the propagation of an exothermic reaction wave in a porous medium, involving fluid oxidiser filtration [33]. This term encompasses both the cases where a gaseous reactant is present within the pores of a medium and where the porous medium itself is the reactant. The latter case is a form of smouldering combustion. Unlike most forms of smouldering combustion where free air outside the medium provides the oxidiser for the reaction, in filtration combustion it is the air flowing through the pores which provides oxygen to the reaction site. Thus this form of combustion has particular applications to deep-peat fires. In addition to this filtration combustion has a number of other practical uses including the treatment of ores, regeneration of coked catalysts, gasification of coal and extraction of oil [33].

Filtration combustion is often studied in one dimension and usually takes into account the existence of a gaseous velocity. This flow can either be imposed, such as forced flow of the oxidising gas, or can occur naturally due to buoyancy. In this system the modes of combustion can be separated into two schemes: forward smoulder and opposed (or reverse) smoulder. The combustion wave moves with the imposed airflow in forward smoulder and against the flow in opposed smoulder (Figure 1.3). One of the best examples of forward smoulder is inhaling through a cigarette. Here both the oxidiser and the combustion front move towards the smoker. Conversely, exhaling through a cigarette is an example, albeit less often seen, of opposed smoulder [25]. It is worth noting that these forms of combustion are analogous to two forms of flaming combustion: premixed flames and diffusion flames [34]. In premixed flames the fuel and oxidiser are present on the same side of the flame sheet, in diffusion flames they are present on opposite sides of the flame sheet. Considering this, Figure 1.3 highlights that forward smouldering is analogous to a diffusion flame and opposed smouldering is analogous to a premixed flame.
In forward smoulder all three heat transport mechanisms (conduction, convection and radiation) move the heat in the same direction; towards the fresh fuel. Thus pre-heating of fresh fuel is aided by forward smouldering allowing the combustion to reach superadiabatic temperatures. In opposed smouldering, whilst convection transports heat downstream, conduction and radiation transport the heat upstream. As these mechanisms are working in opposing directions they act to balance each other out. For this reason, whilst opposed propagation is usually steady, forward propagation is usually unsteady and accelerates as it propagates [35, 28, 36]. In fact it has been suggested that it is the self-accelerating nature of forward smouldering which triggers a transition to flaming combustion which is not observed in opposed smouldering [37]. When problems are extended to two or three dimensions a number of other schemes describing the direction in which the combustion front propagates become possible. In general, however, the idea of forward or opposed smouldering still holds when the dominant directions of the oxidiser flow and the front propagation are considered.

1.5 Combustion Instabilities

One dimensional studies of smouldering combustion are common. Not only are these models much simpler than their multi-dimensional counterparts, which aids when seeking analytical solutions, but a number of experiments into smouldering combustion
have been conducted and found to produce a planar combustion front [38, 36]. However, the existence of a planar combustion wave does not necessarily imply that this front is stable [39]. Experiments are often conducted in samples where the reaction wave thickness (preheat zone and reaction zone) is comparable to the sample width. Thus the production of a planar propagation front may just imply that the channel width used in the experiment is sufficiently small to preclude any instabilities.

In smouldering combustion there are two main types of instability which may cause a propagating planar front to fragment: thermal-diffusion instabilities and hydrodynamical instabilities. The former is due to a disparity between molecular and thermal diffusivity, found when the Lewis number is less than one. This instability can be understood by considering a protrusion from a planar front. When the Lewis number is less than one curvature enhances the incoming oxygen flux more strongly than it enhances the outgoing heat flux, causing the temperature to rise; this promotes combustion. Thus curvature is promoted and a planar front fragments [40]. Hydrodynamical instabilities in smouldering combustion on the other hand can be caused by factors such as permeability jumps between burnt and unburnt zones and the production of gaseous reaction products. These instabilities are comparable to the Saffman-Taylor instabilities found when a fluid is injected into a porous medium filled with a second fluid with higher viscosity.

An interesting result of the thermal-diffusive instability in premixed gaseous combustion is the production of flame balls. Under low gravity conditions, when the Lewis number of a lean fuel in a gaseous mixture is small, combustion fronts are found to break into cellular structures. The curvature of these structures makes them robust and gives them the ability to survive under heat losses which would extinguish a planar flame. Under the correct conditions these cellular structures form stationary, stable flames balls which can reach superadiabatic temperatures [27, 41].

Numerical studies of this phenomenon suggest that there exists a class of flame ball which, rather than being stationary and spherically symmetrical, are travelling and exhibit a “logarithmic tail”. The travelling nature of these flame balls is not brought on by external stimuli such as a velocity field, but rather found to occur naturally as a bifurcation of the stationary flame ball solution above a critical heat loss threshold [42, 41]. Thus this class of flame ball has been referred to as “self travelling” [42].
In solid combustion low Lewis number instabilities can also lead to the fragmentation of planar fronts into cellular, or cap-like combustion regions [43]. As the solid fuel cannot diffuse the burnt area can be used to map the progression of combustion front. The combustion regime can consist of steady fingers propagating against an opposing air flow (either alone or with a regime of other fingers) or as a complex structure consisting of tip splitting and extinction of certain fingers (see Figure 2.1 on page 31).

1.6 Other forms of Smouldering Combustion

Whilst this thesis will focus on the smouldering combustion of peat, biomass combustion is not the only area of smouldering combustion to receive significant interest in recent years. One of the most common fuels to be investigated is polyurethane foam. Polyurethane foam is found in a number of household items such as bedding and upholstery. Thus the study of this material is of particular relevance to fires in the home. Ignition of the foam by discarded cigarettes can lead to prolonged smouldering or even transition to flaming combustion. This is particularly concerning due to the fact that fuels which are resistant to flaming combustion are not necessarily resistant to smouldering combustion and vice versa [44]. The gaseous products released from smouldering combustion often comprise of a number of highly toxic components. As the mass of toxic gas produced is low, there are usually few fatalities when people come in to contact with smouldering fires. In enclosed spaces, however, these gases can build up. In fact the toxic products emitted from smouldering barbecues have been known to kill when left in sealed rooms or tents for prolonged periods of time [45, 46].

The effects of microgravity on smouldering combustion have also become increasingly studied in recent years. Due to the establishment of the International Space Station, and as incidents of charred cables and electrical components on space shuttle flights have been reported, understanding how smouldering spreads under microgravity has become increasingly important [47]. Studying smouldering combustion in space not only has important safety applications, but it also acts as a useful comparison for standard gravity based tests. This allows the effects of buoyancy on smouldering combustion to be assessed. It was in fact in a microgravity environment where stable
flame balls were first successfully ignited [27].

Another smouldering fuel commonly studied is coal. There are a number of similarities between coal mine fires and peat fires. Like peat, coal is highly susceptible to smouldering combustion with prolonged smouldering having significant environmental and economical impacts. Coal burning underground can lead to huge financial losses if the coal was intended to be sold on the international market. In fact, coal fires in the Rujigou coal basin in China result in an estimated yearly loss of 300,000 tons of coal at a cost of 15 million USD [48]. Whilst piping aids underground combustion in peat fires, coal fires are aided by mine shafts and naturally occurring fractures. Both fuels also have the ability to self ignite [49]. In fact, there are over 40 coal mines in England alone with a history of self ignition which are currently considered to be high risk [50]. Due to the fact that peat is a precursor form of coal, similarities between the two fuels would be expected. The main difference between the fuels is the structure. Peat is highly porous and highly deformable. Coal is rigid and has a much lower porosity (0.13-0.25). As a result of this diffusion through fractures is the dominating oxygen transport mechanism in coal [51]. Whilst pipes naturally occur in peat and aid with gaseous transport systems, the high porosity of peat makes these structures of less importance than fractures are in coal diffusive systems.

Although many of the forms of smouldering combustion discussed up to this point have negative effects on the environment, smouldering combustion is utilised as a tool by a number industries. Opposed smouldering is used in underground coal gasification. This is an *in situ* process by which coal is turned into a gas and extracted from the ground to be used as a fuel. In order to prepare a mine, two deep wells are dug. For the process to work effectively the permeability of the coal between the two wells needs to be enhanced. This is done using a combination of drilling and controlled smouldering combustion [52]. In addition to coal gasification, there are novel environmental and energy technologies currently in development using smouldering combustion as an industrial tool. These include the remediation of contaminated soils and the production of biochar for long-term carbon storage [31].
1.7 The Current Contributions

The objective of this thesis is to develop a model capturing the key features and mechanisms involved in an underground smouldering peat fire. Due to low Lewis number instabilities a planar combustion front is found to fragment and develops a complex fingering pattern. Experimental results previously obtained suggest that, under the same conditions, the characteristics of a single finger would match those found in a system of fingers [43]. Thus a single finger can be studied independently of any other finger as a travelling wave. Effects of parametric changes on this travelling wave can then be studied numerically along with a buoyancy induced profile. The resulting model takes into account one chemical reaction which drives the combustion process and predicts that, for a certain range of parameters, downwards propagation can be sustained by buoyancy alone.

The contributions of this thesis are summarised by,

- Chapter 1. Description of the characteristics and processes involved in smouldering combustion. Discussion of the forms of instabilities that may arise, and the economical and environmental impact of smouldering peat fires.
- Chapter 2. Literature review of experimental studies and mathematical models of smouldering combustion. Both planar combustion fronts and fingering instabilities are discussed.
- Chapter 3. Introduction of the mathematical model.
- Chapter 4. Analytical solutions to the one-dimensional spherically symmetrical problem are presented and compared to numerical simulations. Fingering instabilities, suppressed by one-dimensional simulations, are found to arise when the problem is solved numerically in cylindrical symmetry.
- Chapter 5. Cylindrically symmetrical numerical solutions for a smouldering combustion finger propagating against an imposed velocity are presented. The effects of heat losses, velocity magnitude and Lewis number on the solution are presented. Constant and non-constant density models for the gaseous phase are compared and contrasted with each other and with existing experimental data. An equation estimating the distance between two neighbouring fingers is derived.
• Chapter 6. A smouldering combustion finger propagating against a buoyancy driven velocity field determined by Darcy’s law is considered. Cylindrically symmetrical numerical solutions are presented. The effects of permeability and the constant molecular weight assumption are assessed and both carbon monoxide and carbon dioxide producing combustion are examined. The constant porosity assumption is assessed over a range of permeabilities and initial porosities. The non-constant porosity model takes into account that burnt peat is more permeable than fresh peat by use of the Kozeny-Carman equation.

• Chapter 7. Conclusions of this thesis

In addition to the smouldering peat model, a model describing the spread of an ember storm is presented in Appendix B.
Chapter 2

Literature Review

This chapter reviews some of the most relevant experiments and models of smouldering combustion. In Section 2.1 experimental studies of smouldering combustion in peat and other fuels are discussed. These results are used to review appropriate kinetic schemes in Section 2.2. An alternative reaction rate law to the Arrhenius law is discussed in Section 2.3 and a range of models of smouldering combustion are presented in Section 2.4. Finally instabilities found to arise in smouldering combustion fronts are discussed in Section 2.5

2.1 Experimental Studies of Peat Combustion

Both oxidation and pyrolysis reactions play important roles in smouldering combustion. A review of the latter process in peat is given in Roy et al [7]. The three main products of peat pyrolysis are: char, tar and gas. The char is an almost isotropic carbonaceous residue obtained by heating the peat to approximately 550°C. Peat tar is a semi-solid or a viscous liquid at room temperature. The majority of peat tar distills within the range 180-350°C. Thus if the combustion occurs in a large fuel bed the tar can condense on fresh fuel away from the combustion front. This gives the tar further opportunity to pyrolyse. Finally, a non-condensible pyrolysis gas is produced. The ratio of the three pyrolysis products is found to vary with temperature. Low temperature pyrolysis (up to 600°C) yields up to 30% tar. However at higher temperatures a significantly lower tar yield is found due to the increased occurrence of cracking reactions.
CHAPTER 2. LITERATURE REVIEW

Experimental studies of peat combustion conducted by Rein et al [17, 16] identified three distinct combustion zones. Firstly there is a preheating and evaporation zone. Heat from the reacting front is transported to this zone increasing the temperature and causing water within the peat to evaporate. Next is the combustion zone. Pyrolysis reactions use heat to convert the peat into volatile gases, water vapour and char. Oxidation reactions involve the exothermic reactions of oxygen with both peat and peat char. Peak temperatures of approximately 600°C are found in this region and it is where the majority of the fuel mass is lost. Finally there is a char and ash region where the smouldering has ceased and the matter cools down to ambient temperatures.

Frandsen also conducted a series of experiments on the combustion properties of peat [53, 54]. These studies involved heating samples of peat moss of base 50mm × 50mm and of 40mm depth. The samples were surrounded with ceramic board with a similar thermal property to peat. Rows of heated coils were held closely to the surface of the peat for 2 minutes to ignite the peat. The experiments found that the heat produced by the combustion of the peat increased with organic mass (once living material) and decreased with moisture content. Later work found a critical moisture content of 110% in dry base \(^1\) above which ignition did not occur [55].

A series of experiments have more recently been carried out by Grishin et al in order to verify mathematical models for the smouldering of peat [56, 57, 58]. Peat was placed on a concrete base and surrounded by bricks, leaving the top uncovered. A thinly wound spiral of wire was used to replicate a cigarette, or match, as an ignition source. Results showed the rate of combustion depended on the density and moisture content of the peat. The presence of water initially increased the combustion rate by 30% due to the rise in effective thermal conductivity. However further increases to the water content resulted in a sharp decrease in combustion rate. The minimum energy of ignition was determined as a function of botanical composition, moisture content, density and ash content [56]. In addition to this the specific heat and thermal conductivity of peat were found to be nonmonotonic functions of temperature and moisture content [57]. Finally, wind speeds of between 2.5 and 3.0 m/s were found to lead to flaming combustion of the peat [58].

\(^{1}\)Moisture content is calculated by dividing the mass of water in a sample by the oven-dried mass of the sample. Hence moisture contents above 100% are possible.
2.1. EXPERIMENTAL STUDIES OF PEAT COMBUSTION

The effect of moisture content on the combustion of peat has also been studied by Rein et al [16]. Samples of a 100mm × 100mm square base with a height of 50mm were ignited by a coil and the evolution of the combustion fronts were compared at different moisture contents. Above moisture contents of 135% combustion did not occur. Between 115% and 135% ignition occurred but was not sustained and below 115% the fuel ignited and combustion was sustained. This led to the suggestion that peat moisture content could be used to determine a danger rating system for fire risk in peat.

It has been pointed out that whilst there has been a huge increase in the understanding of the mechanisms involved in peat combustion over the last few decades, more work is still needed to obtain a complete picture [15]. One particular mode of peat combustion in which experimental data is lacking is the smouldering combustion of deep peat fires. For practical reasons studies of deep peat fires are difficult. Laboratory experiments have been limited to using small samples as obtaining large samples and transporting them to a laboratory whilst maintaining the structural integrity of the peat is difficult. Whilst studies in the field would be possible, these not only have to take into account the additional variables that changing weather conditions give, they may also be a practical fire risk should the smouldering not be contained.

Smouldering combustion experiments with features comparable to deep peat fires have, however, been conducted. One worth noting is a study of reverse combustion linking used in coal gasification [59]. When reverse smouldering is initiated in a coal seam the combustion front is found to break down and form finger-like channels. In the case of coal this appears to be due to a hydrodynamical instability brought on by the significantly differing characteristics of the coal in burnt and unburnt zones. Unlike peat, coal has a relatively low permeability and porosity, thus differences between characteristics in burnt and unburnt zones in coal are significantly more pronounced than they are in peat combustion. Thermal results were limited due to the remoteness of the combustion, however, a combustion channel diameter of between 2.5 and 3.5 feet was found, with the front widening as the oxidiser flow increased.

Experiments into the effects of the thermal-diffusive instability on smouldering combustion have also been conducted. When a thin cellulosic fuel smoulders horizontally under normal gravitational conditions, and in the presence of an external laminar
airflow, a uniform smoulder front is seen. However, when the same experiment is conducted under microgravity conditions a complex and unexpected finger-shaped char growth pattern can be observed [60]. This behaviour can also be induced under normal gravitational conditions when buoyant oxidiser flow is limited by using a thin horizontal channel with forced flow [61, 43]; combustion of a thin fuel (such as paper) is initiated between two plates to minimise buoyancy driven flows. For large forced velocities an even combustion front is found (Figure 2.1(a)). As the velocity is reduced the front moves through periods of unevenness (Figure 2.1(b)), a periodic phase (Figure 2.1(c)), fingering with tip splitting (Figure 2.1(d)) and finally fingering without tip splitting (Figure 2.1(e)). Due to the narrow, fixed gap between the two plates the instability causing this behaviour has been determined to be thermal-diffusive, not hydrodynamical [39].

Both the distance between neighbouring fingers and the propagation speed are found to depend on the Péclet number, the ratio of molecular advection to the coefficient of molecular diffusion. Above a critical value fingering is not observed. Below this value lies a small range of Péclet numbers which mark the onset of fingering combustion. Below a second critical value, where combustion is oxygen limited, a developed fingering state is found. In this developed state a reduction in the Péclet number increases the distance between neighbouring fingers and decreases the propagation rate.

The finger width was determined to be a decreasing function of the ability of the front to release heat. As heat losses due to the advection of reaction products are more effective in a narrow channel, as the distance between the two plates decreases, the finger width also decreases. Similarly adding a cooling non-reactive gas to the flow (whilst maintaining the oxygen flux) increases heat losses and results in a narrower finger. However, it was also found that replacing the bottom plate with a thin steel foil in fact increased the finger width.

In regimes where tip-splitting does occur, average finger width and spacing are maintained. In addition to this, when the system is forced to produce single fingers by reducing the fuel width, these fingers are found to have the same characteristics as those found in the multi-fingered tip-splitting regime. The authors conclude that the tip-splitting instability is not a collective effect but a local feature involving a single
2.1. EXPERIMENTAL STUDIES OF PEAT COMBUSTION

Figure 2.1: Experimental results showing fingering patterns of opposed smoulder with varying oxidiser velocities. For (a)-(e) the velocity of the oxidising gas is given by 11.4, 10.2, 9.2, 1.3 and 0.1 cm/s respectively. Produced by Zik and Moses [43].
CHAPTER 2. LITERATURE REVIEW

Figure 2.2: Infrared images of opposed smouldering in peat, taken at 5 minutes after ignition, for a range of oxygen concentrations. Produced by Hadden et al [64].

A similar study was also conducted by Olson et al where the spread of flaming combustion over a thin solid fuel in microgravity was considered [62]. Experiments were conducted under both microgravity conditions and using a regime similar to that presented by Zik and Moses. Both experiments found uniform flaming fronts became corrugated before breaking into separate “flamelets”. These flamelets were steady in terms of persistence, spread rate and the fraction of fuel consumed. The move from a planar to a cellular combustion front was attributed to be a flame adaptation to the limited oxygen environment. Systems of flamelets such as these have previously been found to form a dynamic population, stable in an aggregate sense, interacting competitively for oxygen. This system is analogous with biological models of populations [63].

Both the work of Olson and Zik and Moses consider thin sheets of fuel, so that the problem can be considered as essentially two-dimensional. Little work has been done to extend this work into three dimensions by conducting experiments on a block of fuel. Hadden et al have, however, investigated peat combustion in deep fronts [64]. Deep peat combustion is well insulated from heat losses, but there is a limited oxygen supply. In order to investigate this form of combustion small samples of dry peat (30mm deep with a diameter of 125mm) were ignited from above using a uniform radiant heat flux. A gas comprising of both oxygen and nitrogen was imposed from below, leading to opposed smouldering combustion. It was noted that the effects of an oxidiser flux on combustion have been investigated by both varying the velocity of the air flow and by varying the oxygen concentration at a fixed gas velocity. The former method was used by Zik and Moses when studying fingering combustion in paper [43], and the latter is used by Hadden et al. Infrared images of the surface of
the peat, 5 minutes after ignition, are shown at oxygen concentrations of 17, 21, 25 and 35% in Figure 2.2. As the oxygen concentration reduces the infrared images suggest a movement from a planar combustion front to more localised hot-spots. Whilst this finding was not discussed by the author, the results appear to by analogous to those presented by Zik and Moses [43], shown in Figure 2.1. An oxygen concentration of 17% would thus correspond to fingering combustion with a small amount of tip splitting, whilst an oxygen concentration of 35% corresponds to a planar, or cellular, combustion front.

A number of experiments into filtration combustion have also taken place. Torero et al [65] studied opposed smouldering against an imposed air flow in polyurethane foam. At low gas velocities the reaction temperature and spread rate were low due to weak reaction rates. Initially an increase in velocity led to an increase in the propagation speed and temperature. Further increases however caused both values to peak and then decrease before reaching the over-blowing extinction limit. Initial increases to the temperature and propagation rate were attributed to the oxygen supply enhancing the reaction and releasing more heat. As the gas velocity continued to increase the rise in heat produced by the reaction compensated for the higher heat losses to convection. Eventually the heat generated and heat lost balance and the temperature and propagation rate peak. Further increases to the gas velocity cause heat losses to dominate, resulting in a decrease to the temperature and propagation rate. Whilst higher temperatures were found to imply a higher smoulder velocity, a small temperature variation led to a large variation in velocity. It was also found that when no forced airflow was imposed, and buoyancy forces alone created the velocity field, combustion could be sustained. However the propagation speed and temperature were both low. In addition to this the over-blowing extinction limit was reached before all the fuel had been consumed. Thus it was not a lack of fuel or oxygen which quenched the combustion, but rather the high inlet velocities resulted in excessive convective heat losses.
One of the main difficulties with modelling smouldering combustion is the present limitation in our ability to characterise fuels in terms of their thermal and oxidative degeneration [25]. Cellulose is currently one of the most studied materials and the mechanisms by which this combusts are still not fully understood. Thus significantly simplified kinetic schemes are inevitable and kinetic parameters are often based on empirical estimation [24].

A number of studies have focused on studying pyrolysis of a porous medium in an inert atmosphere. Kravtsova and Smolyaninov [66] studied the pyrolysis of peat assuming tar to be an intermediary species.

\[
\text{Peat} \rightarrow \text{Tar} \\
\text{Tar} \rightarrow \text{Gases} \\
\text{Tar} \rightarrow \text{Coke}
\]  

(2.1)

This scheme is supported by experimental data of the pyrolysis of peat, showing the three products to be char, peat and gases [7]. However, it assumes that peat must go through a tar phase before producing either gases or char. Experiments performed by Ohlemiller et al have suggested that the tar pathway could be promoted at the expense of a char reaction in polyurethane foams [67]. This implies that, rather than being consecutive, the char and tar reactions were competing.

A similar model has been used for the pyrolysis of cellulose [68, 69]. Here the cellulose was taken to go through an activated stage, as opposed to a tar phase, before the final combustion products are obtained.

\[
\text{Cellulose} \rightarrow \text{Active Cellulose} \\
\text{Active Cellulose} \rightarrow \text{Char} + \text{Gas} \\
\text{Active Cellulose} \rightarrow \text{Tar}
\]  

(2.2)

Whilst this model does show a higher level of agreement with Ohlemiller’s experiments it assumes that the ratio of gas to char yield is constant. It has been shown experimentally however that at higher temperatures cracking reactions to gases arefavoured, whilst at lower temperatures char forming reactions are favoured [70].
Due to these weaknesses Di Blasi [71] proposed a model of wood pyrolysis to take into account the varying proportions of char and gas yields. This model also included both primary wood pyrolysis reactions and secondary tar cracking reactions.

\[
\begin{align*}
\text{Wood} & \rightarrow \text{Gas} \\
\text{Wood} & \rightarrow \text{Tar} \\
\text{Wood} & \rightarrow \text{Char} \\
\text{Tar} & \rightarrow \text{Gas} \\
\text{Tar} & \rightarrow \text{Char}
\end{align*}
\] (2.3)

Di Blasi notes that gaseous products could migrate through the unreacted wood where they may condense; subsequently as the pyrolysis front progressed they would evaporate which would lead to changes in the apparent kinetics of degradation. However, in applying this model tar was assumed to only be a gaseous species and condensation of the tar was not accounted for.

One of the most commonly used kinetic mechanisms for smouldering combustion in air is Ohlemiller’s 3-step scheme [24].

\[
\begin{align*}
\text{Fuel} & \rightarrow \text{Char} + \text{Gas} \\
\text{Fuel} + \text{O}_2 & \rightarrow \text{Char} + \text{Gas} \\
\text{Char} + \text{O}_2 & \rightarrow \text{Ash} + \text{Gas}
\end{align*}
\] (2.4)

This model is supported by studies showing that during the heating of wood, tobacco, polyurethane and peat there are two global reaction peaks in the presence of oxygen [24, 72]. This suggests that two consecutive oxidation reactions are taking place. Ohlemiller notes that whilst this scheme does not take into account oxidation of a gas-phase fuel as a heat source, if the peak temperature is below 600°C this role is likely to only play a supplementary role, if any. Many other authors have used this 3-step model [73, 74, 75] and the model has gone on to produce good qualitative agreement with experiments. It does, however, have a tendency to over-predict mass loss due to the consideration of a single, one step pyrolysis reaction. In order to overcome the weaknesses of the three step model, Rein [25] extended the model to include 5 chemical reactions. The extended scheme took into account two fuel oxidation reactions, two fuel pyrolysis reactions and a char oxidation reaction. Four solid species and two gas
species were accounted for. Experimental studies of polyurethane foam combustion have shown that a minimum of 5 steps are needed to accurately describe thermal decomposition. Thus this model results in a higher level of quantitative agreement with experimental data.

Although increasing the number of chemical reactions does lead to a higher level of quantitative accuracy, it is worth noting that simple one-step reactions can have good qualitative agreement with experiments [76]. A one-step global reaction of the form,

$$\text{Fuel} + \text{O}_2 \rightarrow \text{Char} + \text{Gas},$$

is found to be sufficient to model the key features of opposed smouldering. This model assumes that pyrolysis is not necessary to capture the key features of smouldering combustion. It also utilises experimental evidence suggesting that whilst char oxidation reactions are more exothermic than fresh fuel oxidation reactions it is the former which have been found to, perhaps exclusively, drive opposed smouldering [36].

Whist the previous model assumes fuel oxidation to be dominant, a one-step mechanism of this form has also been used assuming char oxidation to be the mechanism driving combustion. Fatehi et al [38] considered smouldering combustion of a packed bed of wood particles. They suggest that fuel oxidation is less significant than char oxidation for large particles, although it can become more significant, and even dominant for small particles. In addition to this, they utilise the fact that pyrolysis kinetics are much slower than char oxidation kinetics and that the heat released from char oxidation is much greater than the heat consumed by pyrolysis. Thus if char oxidation is taken to drive combustion, the influence of the char forming pyrolysis reaction can be taken as being negligible. Hence consideration of a char oxidation reaction was assumed sufficient to capture the key features of smouldering combustion of large wood particles.

Although both char oxidation and fresh fuel oxidation have been considered to be the mechanism driving smouldering combustion, in mathematical models the problem is often non-dimensionalised. This removes characteristic values such as heat release rates and kinetic values from the problem. Thus, when results are displayed in dimensionless form, there is no impact of choosing one reaction over the other.

A final kinetic scheme worth noting is that used by a number of Russian authors
in recent years [77, 78, 79, 80]. This scheme is far more complex than the schemes discussed previously, and takes into account 6 gas species (CO, H$_2$O, O$_2$, CO$_2$, CH$_4$ and N$_2$) along with four solid species (peat, bound water, char and ashes). Evaporation of bound water, pyrolysis of peat, oxidation of peat char and oxidation of both carbon monoxide and methane are taken into account. The model assumes gas-phase oxidation and char oxidation to be the dominant sources of heat production. Ohlemiller’s review on smouldering combustion, however, suggests that an attack of oxygen on the fresh fuel would be likely to play a larger role in producing the heat required for pyrolysis than an attack of oxygen on a gas phase species [24]. This idea is echoed by the work of Rein et al [16, 17] who only note the presence of peat and char oxidation reactions during peat combustion. Despite this shortcoming, smouldering peat research is limited and this model has been shown to have a good level of agreement with experiments [78].

2.3 Reaction Rate Laws

The way in which the reaction rate is approximated is an important factor in all combustion models. The most common approximation for the reaction rate uses the Arrhenius equation detailed in Section 1.3. This equation has become the customary way to model both heterogeneous and homogeneous combustion.

An alternative reaction rate equation for heterogeneous combustion has been introduced by Frank-Kamenetskii [81]. This rate takes into account the fact that the observed reaction rate is determined partly by the chemical kinetics at the surface of the solid and partly by the rate of transport of reactants to the surface through diffusion. If it can be assumed that all areas of the surface are uniformly accessible the reaction rate can be given by,

$$q = \left( \frac{1}{1/k + 1/D_v} \right) C,$$

where $k$ is given by the Arrhenius law, $C$ is the reactant concentration and $D_v$ is the diffusion velocity constant.

If $k \gg D_v$ the overall process is determined entirely by the rate of diffusion and this reaction is said to lie within the diffusional range. Here the diffusion velocity constant plays the role of the reaction rate constant. If $k \ll D_v$ the process lies within the
kinetic range. The reaction rate is determined entirely by the true chemical kinetics of the reaction at the surface and the concentration of the reactant at the surface is approximately the same value as its concentration in space.

However, when both \( k \) and \( D_v \) are of the same order they both play an important role in the reaction rate. Norbury and Stuart [82, 83] developed a model for the combustion of a porous medium which could take into account this two-stage reaction rate by way of a Heaviside function.

\[
q = H(C_c)H(T - T_{cr})D_vC_X
\]

Here \( C_X \) is the oxygen concentration and \( C_c \) the fuel concentration. The Heaviside function is not artificially imposed, but rather is found to arise naturally when the large-activation energy analysis is performed. For temperatures below a critical temperature, \( T_{cr} \), the reaction rate is found to be negligible. Above \( T_{cr} \) the rate is found to be controlled by the ability of the gaseous components to diffuse to, or away from the reactant site.

This technique for modelling the reaction rate of a porous medium has only been utilised by a small number of authors. These studies tend to focus on investigating the underlying mathematics of the problem in more detail, such as existence and uniqueness of solutions [84] and the bifurcation of positive solutions [85].

The Heaviside model presented by Norbury has very useful applications when both diffusion and kinetics determine the reaction rate. However, in situations where only one of these factors plays a crucial role this model may be overly complex. Whilst combustion of carbon above 1100-1300°C is known to lie in the diffusional range, temperatures below 1100°C comprise of an intermediate range and the kinetic range [81]. It has also been noted that Frank-Kamenetskii’s model has been applied to coal, where the particle sizes are taken to be of the order cm [86]. However for pulverised particles diffusional rates may be higher than chemical rates in the 1000-2000°C range [26]. In fact pulverised coal combustion below 760K has been found to have a reaction rate controlled by chemical kinetics alone [87]. Hence low temperature combustion of small particles would be expected to lie within the kinetic range. In this range a reaction rate based on the Arrhenius reaction rate would be applicable, as has been used by a number of authors when studying smouldering combustion of porous fuels [71, 70, 24, 25].
2.4 Models of Smouldering Combustion

A number of types of smouldering fires found in nature occur on the surface of a solid fuel in the presence of free air. This results in a two or three-dimensional combustion front. However few studies have been conducted into investigating the structure of a multi-dimensional combustion wave and identifying the mechanisms controlling its propagation [75, 88]. One such model has, however, been presented by Di Blasi [75]. Here the two-dimensional spread of a combustion front through a cellulosic bed in still air was modelled. One pyrolysis reaction and two oxidation reactions were considered in a bed 40cm long and 30cm deep. Di Blasi’s results showed that except for a 1cm thick superficial layer where both oxidation and pyrolysis took place, decomposition in the rest of the bed was only due to pyrolysis. A good level of qualitative agreement was found between a number of features of the model and experiments. However, quantitative comparisons were difficult due to the accuracy of kinetic data used and differing scales of the model and the experiment. Di Blasi also found that the structure of the front significantly depended on the ratio of the cellulose oxidation rate to the char oxidation rate. When the char oxidation rate was higher than the fuel oxidation rate it was the former reaction which dominated the combustion process. This form of combustion was found to be comparable to that of 1-dimensional forward smoulder. When the fuel oxidation rate was higher fuel oxidation dominated and the process was found to resemble 1-dimensional reverse smouldering.

There are significant differences between combustion occurring in free air and combustion in which an oxidiser must diffuse through a porous medium to a reaction zone. A study by Aldushin et al [89] investigated how the form of oxygen supply to the smouldering front changed the speed at which a front spread. Waves propagating with a constant velocity were found when combustion was fed solely by the oxygen stored in the pores of a porous media. However, when oxygen diffused to the combustion front from the external environment the movement of the front was found to decrease with time, showing $\sqrt{t}$ behaviour.

A large proportion of the models studying filtration combustion have involved considering the problem as one-dimensional, focusing on the idea of either forward or opposed smoulder. Whilst two-dimensional filtration combustion studies have been
conducted, these often focus on investigating instabilities of the problem. Ohlemiller et al [67] presented a model for forward smouldering in a polyurethane foam. The airflow was calculated to be comparable to that created by buoyancy effects in an upholstery fire. Two oxidation reactions were included, the oxidation of foam and of foam char. Most of the qualitative characteristics of smouldering were captured by this two-step reaction model. The model considered a very open porous medium, so that the dominating heat transfer mechanisms were conduction and radiation. The intensity of the smoulder was found to be almost entirely controlled by the oxygen supply to the combustion zone, with combustion continuing to be sustained at remarkably low oxygen levels.

Leach et al [90] studied a 1-dimensional, transient, reverse smoulder wave taking into account both an oxidation and a pyrolysis reaction. A char oxidation reaction was not used due to the fact that oxidation of fresh fuel has experimentally been shown to drive reverse smouldering [36]. The model found that radiation was a weak mechanism for heat transfer in fuels with narrow pores. However it would be likely to play a more important role as the pore diameter increased. The model also predicted that as the gas velocity increased the temperature and smoulder velocity initially increased, before plateauing. Further increases caused the smouldering combustion to be extinguished due to convective cooling. This model was found to capture the main qualitative trends found by Torero et al [65]. In addition to this the assumption of a thermal equilibrium existing between the gas and solid species was tested. The results suggested that for sufficiently low velocities this assumption was valid, but as the gas velocity increased discrepancies were found. The model correctly predicted the existence of an over-blowing extinction limit due to heat losses from the reaction zone. One-step reaction schemes have previously been found to predict extinction only when all fuel has been consumed. This extinction limit has also been correctly predicted by both inclusion of a second oxidation reaction [91] and inclusion of a pyrolysis reaction when thermal equilibrium is assumed [92].

Whilst most studies consider a forced flow of oxidiser, the case of gravity induced buoyant flow has also been considered by Aldushin et al for both opposed [93] and forward combustion [28]. These papers considered a container, open on both ends,
filled with a porous fuel. The fuel was ignited on the top (bottom) for opposed (forward) smoulder and the combustion front spread as a planar wave. The problem was modelled as 1-dimensional, taking into account one oxidation reaction. Although there were a number of similarities between buoyant flow and forced flow models, in both buoyant flow models the buoyancy acted as a feedback mechanism. The filtration strength determined the burning temperature, which in turn determined the buoyant filtration strength. Steady-state wave solutions were not predicted to exist for forward smoulder, where the combustion was expected to accelerate as it progressed. However, for sufficiently long samples where heat losses were sufficiently high to localise the high temperature region, steady-state wave solutions were expected to exist for opposed combustion. For both forward and opposed smouldering buoyancy was predicted to support filtration combustion in sufficiently long porous samples with high permeability, but only in forward smouldering were superadiabatic temperatures predicted to be attainable. Both forward and opposed smouldering models were also found to compare favourably with experiments.

Although opposed smouldering combustion is often assumed not to reach superadiabatic temperatures, this is not necessarily the case. In forward smoulder it is usually the fact that all heat transport mechanisms are working in the same direction which causes superadiabatic temperature to be attained. However this is not the only way in which the combustion temperature can be raised. Zhang et al found that for thermally thin porous media (where heat transport only occurred in the gaseous phase) that opposed smouldering temperature and spread rates were both dependent on the Lewis number [94]. The reason for Lewis number effects often being overlooked was attributed to the fact that many experiments employ O$_2$-N$_2$ atmospheres for which the Lewis number is approximately one. Zhang et al found that mixtures with a low Lewis number would experience higher combustion temperatures and higher spread rates than unit Lewis number models would predict. In fact this finding is not limited to thermally thin porous media. Herbert et al asymptotically investigated diffusion-controlled smouldering of a steady travelling wave through a two dimensional bed [95]. This study also led to the conclusion that the combustion temperature depended on both the Lewis number and the exothermicity of the reaction. Temperatures were found to increase as the Lewis number decreased and the exothermicity increased.
One-dimensional models of smouldering combustion have also been put forward in peat. Golovanov et al [77] considered the development of a smouldering peat fire propagating vertically downwards. A one-temperature, one-dimensional, unsteady problem was considered. The study found that increasing moisture content, decreasing porosity and decreasing oxygen all reduced the peat fire spread-rate. A similar situation was considered by Grishin and Yakimov [78], whose model showed that smouldering propagation was limited by the intensity of the ignition source, the initial oxygen content of the pores along with the processes of drying, pyrolysis and oxidation. The authors also studied a particular case of the model, heating in the absence of reactions, and found results coincided with a well known analytical solution. It was also confirmed that results from the model agreed with experimental studies.

2.5 Instabilities and Low Lewis Number Combustion

As discussed in the previous chapter, a number of characteristics are shared by forward filtration combustion and diffusion flames (where oxidiser and reactant are found on opposite sides of a flame sheet) and opposed filtration combustion and premixed flames (where oxidiser and reactant are found on the same side of a flame sheet). Due to the similarities between certain modes of flaming and smouldering combustion, it would seem reasonable to expect similar instability phenomena to appear in both modes of combustion [34]. For this reason instabilities found in the far more researched area of flaming combustion can also be of significance to smouldering combustion studies.

Aldushin and Matkovsky [39] identified two causes of hydrodynamical destabilisation in smouldering combustion waves. The first was a reduction in resistance of flow due to the consumption of the solid fuel and the second was the production of gaseous products. Whilst the first cause was destabilising in both forward and reverse smoulder, the latter was only destabilising in forward smoulder. In reverse smoulder the gaseous products in fact served to stabilise the problem. It was also found that when the front is only weakly hydrodynamically stable or unstable, diffusion effects may be decisive. In fact in opposed filtration combustion the instability may be caused entirely by diffusion whilst hydrodynamical forces play a stabilising role. Brailovsky
et al also investigated hydrodynamical instabilities of a porous combustion front [96]. They found that to observe fingering in forward smouldering the aspect ratio of the system needs to be large enough, which could explain the lack of experimental evidence of this phenomena.

Fingering caused by low Lewis number instabilities has also been studied. Lu et al studied this phenomenon in both forward [34] and opposed [97] smouldering. In forward smoulder, in the absence of heat losses, combustion was found to be linearly stable. However when convection was included fingering emerged near to the 1-dimensional extinction limit. It was found that whilst similarities between flaming and smouldering combustion instabilities could be drawn there were significant differences. Cellular instabilities in diffusion flames occur near the low Damköhler number (dimensionless reaction time) limit, whereas in smouldering combustion they occur near the large Damköhler number limit. It was concluded that these differences could lead to different extinction mechanisms influencing instabilities in different ways. This would explain why fast time instabilities seen in flaming combustion are not observed in smouldering combustion. In opposed smouldering, when the problem was oxygen limited, a planar front was found to fragment into a steady cellular structure. A more surprising result was found when the combustion was fuel limited. Here the instabilities gave rise to tribrachial structures which eventually extinguished.

Due to the low Lewis number associated with peat combustion it is likely that thermal-diffusive instabilities will have a significantly greater impact than hydrodynamical instabilities. Flame balls, which are a result of thermal-diffusive instabilities in low Lewis number gaseous combustion, have a number of interesting features which have analogies with smouldering combustion phenomena. A great deal of analytical research has been conducted into flame balls. Studies have considered the structure of non adiabatic flame balls [98], stationary spherical flames with either a source or sink at the origin [99], flame balls traveling along an axis at a constant speed [42, 41], and flame balls stabilised by a porous medium [100]. It is the latter two which have most application to smouldering combustion phenomenon. Travelling flame balls have particular applications to fingering instabilities due to their propagating nature and the superadiabtic temperatures they attain. Whist little research has been conducted in this area, the similarities between flamelets and self-drifting flame balls, and flamelets
and reverse filtration combustion have been noted by Kagan and Sivashinsky [101].

The growth of flame balls at different ignition energies has also been studied [102]. Radially propagating spherical premixed flames were studied for mixtures characterised by a Lewis number less than unity. Below a certain value ignition was not initiated. For an intermediary class of self-extinguishing flames the radius was found to grow with $\sqrt{t}$ behaviour before extinguishing. Finally a class of sustained balls were identified where $\sqrt{t}$ behaviour could be displayed at early times, but with later behaviour becoming linear. As these flames expanded the temperature was found to drop from the superadiabatic temperature found in flame balls ($T_{ad}/Le$) to the adiabatic temperature ($T_{ad}$). However, this study was restricted to one-dimension and instabilities were not investigated.
Chapter 3

The Mathematical Model

3.1 The Problem

The model will be represented by a set of partial differential equations expressing the conservation laws for mass, momentum and energy. In the natural world the moisture content of peat, and the role it would play in combustion, would be an important feature of combustion. However the present study focuses only on the most essential parts of the process, with suitable simplifications invoked. Accordingly, as with other refinements of the most basic models, only the combustion of dry peat is considered.

A full model for the combustion of dry peat could be taken to have the form

\[
\begin{align*}
\text{peat} & \rightarrow \text{char} + \text{gases} \\
\text{peat} & \rightarrow \text{tar (gas)} \\
\text{char} + \text{oxygen} & \rightarrow \text{ash} + \text{gases} \\
\text{peat} + \text{oxygen} & \rightarrow \text{char} + \text{gases} \\
\text{tar (gas)} & \rightleftharpoons \text{tar (solid)}. \quad (3.1)
\end{align*}
\]

These equations take into account two pyrolysis reactions, two oxidation reactions and a condensation reaction. However, a simplified model with only one reaction for the oxidisation of peat is enough to drive the combustion process.

\[
\text{peat} + \text{oxygen} \rightarrow \text{gases} \quad (3.2)
\]

Use of a single reaction of this form has been found to lead to a good level of qualitative agreement with opposed smouldering experiments [36, 76, 103]. One-step reaction
models have been used for both fresh fuel oxidation and char oxidation. Whilst here the former is considered, both reactions lead to the same non-dimensional solutions and lead to only quantitative changes to the dimensional solutions. Although only a single solid species is taken into account, a change in the porosity and permeability of the burnt peat is considered. An equation for the latter is not included here, but is derived in Chapter 6.

3.2 The Model

The reaction presented in (3.2) and the various transport processes are modelled by the set of partial differential equations

\[ \rho_t + \nabla \cdot (\rho \mathbf{u}) = \omega \]  
\[ \rho_{st} = -\omega \]  
\[ \rho (y_{Pt} + \mathbf{u} \cdot \nabla y_P) = \nabla \cdot (\rho D \nabla y_P) + \omega \frac{\mu_p W_p}{\mu_c W_c} \]  
\[ \rho (y_{Xt} + \mathbf{u} \cdot \nabla y_X) = \nabla \cdot (\rho D \nabla y_X) - \omega \frac{\mu_s W_x}{\mu_c W_c} \]  
\[ \left( \rho_s c_s + \rho c_g \right) T_t + \rho c_g \mathbf{u} \cdot \nabla T = \nabla \cdot \left( \left( \phi \lambda_g + (1 - \phi) \lambda_s \right) \nabla T \right) + Q \omega \]  
\[ u = \frac{K}{\mu} \left( \frac{\rho}{\phi} g - \nabla p \right) \]  
\[ \frac{R}{W} \frac{T}{\phi} = P_0 + p \]  
\[ \phi = 1 - \frac{\rho_s}{\rho_{s0}} (1 - \phi_0) \]  
\[ \omega = A \rho_s g y_X \exp \left( \frac{-T_A}{T} \right) \],

with the relations

\[ y_P + y_X + y_N = 1 \]  
\[ \mu_c W_c + \mu_s W_x = \mu_p W_p \]  
\[ \frac{y_P}{W_P} + \frac{y_X}{W_X} + \frac{1 - y_X - y_P}{W_N} = \frac{1}{W} \]  
\[ \frac{y_X}{W_X} + \frac{1 - y_X}{W_N} = \frac{1}{W_A} \].

The equations governing the solid and gas species are mass conservation laws. Equations (3.3)-(3.6) represent the conservation of the total gas phase, the total solid phase,
combustion product mass fraction and oxygen mass fraction respectively. Diffusion and advection are taken into account, along with the creation and consumption of gaseous reaction products and oxygen due to the chemical reaction. In the writing of these equations it is assumed that the diffusivity of the gas does not change between each gas, i.e.

\[ D_X = D_N = D_P = D. \]  \hfill (3.16)

As with other assumptions made in arriving at this model, movement of the solid through, for example, thermal expansion and high heat fluxes is not included as it is not essential to the basic phenomena. Thus a change to the solid density is determined by chemical conversion alone. The solid and gas densities are given in bulk form,

\[ \rho = \rho_{in} \phi \]
\[ \rho_s = \rho_{in} (1 - \phi). \]  \hfill (3.17)

Thus whilst porosity does not appear explicitly in the solid or gas density equations, it is included implicitly.

The conservation of energy equation is given in (3.7). It is assumed here that there is a local thermal equilibrium so that,

\[ T_g = T_s = T. \]  \hfill (3.18)

This assumption is usually considered valid in the case of smouldering combustion and has been found to hold for low forced velocity opposed combustion [90]. It is assumed that the thermal conductivity of the solid and gas phases occurs in parallel and that both work done by pressure changes and viscous dissipation are negligible. Radiation is not included in the model. This assumption is valid for porous media with a sufficiently small particle diameter where the effects of radiation have been found to be negligible [90]. Finally, there is heat release through chemical conversion, \( Q \), defined as the energy released per unit mass of solid consumed.

The equations governing the fluid motion are given by Darcy’s law (3.8) and the ideal gas law (3.9). Darcy’s law has been both determined experimentally and derived mathematically. The law gives a linear relationship between flow rate and a pressure gradient in a porous medium. Darcy’s law only holds for Newtonian fluids over a certain range of flow rates. As flow rates increase deviations from the law are found
due to factors such as inertia and turbulence [104]. However for the range of flow velocities found in smouldering combustion this relationship is taken to be sufficiently accurate. The ideal gas law is an approximation of gas behaviour which states that the density of gas is determined by its pressure, temperature and mean molecular mass. This approximation is usually taken to be reasonable over the range of conditions found in combustion [105].

The relationship between the reaction rate and temperature can be approximated by the Arrhenius equation, given in (3.11). Whilst this is not the only reaction rate equation which has been applied to smouldering combustion, for low temperature smouldering of peat it is sufficiently accurate (as discussed in Section 2.3). Here $T_A$ is the activation temperature, the temperature below which a decreasing proportion of molecules have sufficient energy for reactions to occur. This is defined as $T_A = E_A/R$. The activation temperature is used here, having a more physically recognisable meaning.

The porosity of the solid and the initial porosity are given by,

\[ \phi = 1 - \frac{V_s}{V} \quad \text{and} \quad \phi_0 = 1 - \frac{V_{s0}}{V} \]  

respectively. Here it has been assumed that the total volume occupied by the medium, $V$, remains constant. It is also taken that the intrinsic density of the solid remains constant. This assumption is valid in the present case where only one solid species is being considered. However for models where multiple solid species are used an alternative equation, such as that used by Rein [25], may be required. The intrinsic density, bulk density and initial bulk density of the peat are defined by

\[ \rho_{s_{in}} = \frac{m_s}{V_s} \quad \rho_s = \frac{m_s}{V} = \frac{V_s}{V} \rho_{s_{in}} \quad \text{and} \quad \rho_{s_0} = \rho_{s_{in}} \frac{V_{s0}}{V}. \]  

Combining the equations in (3.19) and (3.20) an equation for the evolution of the porosity can be derived.

\[ \phi = 1 - \frac{V_s}{V} = 1 - \frac{V_s}{V_{s_0}} (1 - \phi_0) = 1 - \frac{\rho_s}{\rho_{s_0}} (1 - \phi_0) \]  

(3.21)
3.3 Non-dimensionalising the Model

To simplify the problem the model is non-dimensionalised, removing units from the system of equations, with the definitions

\[
\begin{align*}
\varrho &= \varrho' \varrho_c \\
\rho_s &= \rho_s' \rho_{sc} \\
\mu &= \mu' \mu_c \\
p &= p' p_c \\
y_s &= Y_s y_{sc} \\
y_r &= Y_r y_{rc} \\
\omega &= \omega' \omega_c \\
T &= T_0 + T'T_c \\
t &= t't_c \\
x &= x' x_c \\
D &= D'D_c.
\end{align*}
\]

Substituting these definitions into equations (3.3)-(3.9) gives the equations,

\[
\begin{align*}
\left[ \frac{x_c}{t_c u_c} \right] \varrho' \varrho_c' + \nabla' \cdot (\varrho' \varrho_c' \bar{u}) &= \left[ \frac{\omega_c x_c}{\varrho_c u_c} \right] \omega' \\
\rho_s' &= - \left[ \frac{\omega_c x_c}{\rho_{sc}} \right] \omega' \\
\varrho' \left( \frac{x_c^2}{D_c t_c} \right) Y_{r'} + \left[ \frac{u_c x_c}{D_c} \right] \varrho_c' \nabla' Y_r &= \nabla' \cdot (\varrho' D' \nabla' Y_r) + \left[ \frac{\omega_c x_c^2}{\varrho_c y_{rc} D_c \mu_c W_c} \right] \omega' \\
\varrho' \left( \frac{x_c^2}{D_c t_c} \right) Y_{s'} + \left[ \frac{u_c x_c}{D_c} \right] \varrho_c' \nabla' Y_s &= \nabla' \cdot (\varrho' D' \nabla' Y_s) - \left[ \frac{\omega_c x_c^2}{\varrho_c y_{sc} D_c \mu_c W_c} \right] \omega' \\
\left( \frac{\rho_s c_s x_c^2}{t_c} \right) \rho_s' + \left[ \frac{\varrho_c c_g x_c^2}{t_c} \right] \varrho_s' \nabla' T' &= \left[ \frac{Q \omega_c x_c^2}{T_c} \right] \omega' \\
\left[ \frac{u_c x_c \bar{u}}{K p_c} \right] \varrho_c' &= - \left[ \frac{\varrho_c x_c \varrho_c}{p_c} \right] \frac{\tilde{\varrho}}{\phi} - \nabla' p' \\
\left[ \frac{R \varrho_c T_0}{W P_0} \right] (1 + \left[ \frac{T}{T_0} \right] T') \varrho' &= \phi \left( 1 + \left[ \frac{p_c}{p_0} \right] p' \right) \\
\phi &= 1 - \left[ \frac{p_c}{p_s} \right] \rho_s'(1 - \phi_0) \\
\omega' &= \left[ \frac{A p_n \varrho_c y_{sc}}{\omega_c} \right] \rho_s' \varrho_c' Y_s \exp \left( \frac{-T_A}{T_0 + T_c T'} \right) \
\end{align*}
\]

The following definitions can then be made

\[
\begin{align*}
\text{Le} &= \frac{\phi_0 \lambda_g + (1 - \phi_0) \lambda_s}{\rho_{sc} c_s D_c} \\
\varpi &= \frac{p_c}{P_0} \\
\delta &= \frac{\varrho_c}{\rho_{sc}} \\
\epsilon &= \frac{c_g}{c_s} \\
\nu &= y_{sc} \frac{\mu_c W_c}{\mu_s W_x} \\
\gamma &= \frac{T_c}{T_0} \\
v &= \frac{\lambda_s}{\lambda_g}.
\end{align*}
\]

The Lewis number, Le, is the ratio of thermal diffusivity to mass diffusivity. It is worth noting that the Lewis number in a single phase is usually used to characterize fluid flows where simultaneous heat and mass transfer occur. In this instance, with
mixed phases, the Lewis number is the effective bulk Lewis number of the porous medium as a whole. The solid density is much greater than the gas density \( \rho_s \gg \varrho \). Given the high intrinsic solid density of peat, this remains true even for a highly porous peat; the effective density of the solid species is approximately 25 times higher than that of the gas species for a peat with a porosity of 0.97. Thus the bulk Lewis number can be approximated by

\[
\frac{\phi \lambda_g + (1 - \phi) \lambda_s}{(\rho_s + \varrho) \left( \frac{\rho_s c_s \varrho c_g}{\rho_s c_s + \varrho c_g} \right) D_c} \approx \frac{\phi \lambda_g + (1 - \phi) \lambda_s}{\rho_s c_s D_c}.
\]

(3.25)

Thus the bulk Lewis number in the unburnt region, where \( \phi \equiv \phi_0 \) is that used in non-dimensionalising the model. The Lewis number is an important feature of this model, as it is this parameter which is key to the thermal-diffusive instabilities discussed in Section 2.5.

The remaining definitions are dimensionless ratios of either gas phase characteristics to solid phase characteristics, or of characteristic conditions to initial conditions. From here on it will be assumed that \( \varpi \approx 0 \) due to the fact that the pressure variation about the ambient pressure will be very small and that that diffusivity is constant, i.e. \( D' = 1 \).

The molecular weight of the total gas phase and air are given by,

\[
\frac{1}{W} = \frac{Y_r y_{r_c}}{W_P} + \frac{Y_s y_{s_c}}{W_X} + \frac{1 - Y_r y_{r_c} - Y_s y_{s_c}}{W_N}
\]

and

\[
\frac{1}{W_A} = \frac{y_{s_c}}{W_X} + \frac{1 - y_{s_c}}{W_N} \approx \frac{1}{29}
\]

respectively. Considering the ideal gas law equation, and taking \( \varrho_0 = \varrho_c \), a relationship between initial conditions can be found

\[
\phi_0 = \frac{R \varrho_c T_0}{W_A P_0}.
\]

(3.28)

The formula for the non-dimensionalised reaction rate, \( \omega' \), in (3.23) can be simplified by setting

\[
\alpha = \frac{T_c}{T_0 + T_c}, \quad \beta = \frac{T_A T_c}{(T_0 + T_c)^2}.
\]

(3.29)

Here \( \beta \) represents the Zeldovich number, a non-dimensional measure of the temperature sensitivity of the reaction rate, which is used as an expansion parameter in large activation energy asymptotics. This leads to a non-dimensionalised reaction rate of
the form

\[
\omega' = \left[ \frac{A \rho_s \theta_c y_{x_c}}{\omega_c} \right] \exp \left( \frac{-T_A}{T_0 + T_c} \right) \rho_s' \theta_s' Y_x \exp \left( \frac{\beta (T' - 1)}{1 + \alpha (T' - 1)} \right).
\] (3.30)

Setting,

\[
x_c^2 = \beta^2 \frac{\nu D_c}{A \rho_s \theta_c y_{x_c}} \exp \left( \frac{T_A}{T_0 + T_c} \right)
\] (3.31)

\[
\Omega = \beta^2 \rho_s' \theta_s' Y_x \exp \left( \frac{\beta (T' - 1)}{1 + \alpha (T' - 1)} \right),
\] (3.32)

the equation for \( \omega' \) reduces to

\[
\omega' = \left[ \frac{\nu \theta_c D_c}{\omega_c x_c^2} \right] \Omega.
\] (3.33)

Finally the following definitions are made

\[
t_c = \frac{x_c^2}{\text{Le} D_c} \quad y_{rx} = \frac{\mu_p W_p}{\mu_X W_X} y_{x_c} \quad p_c = \theta_c x_c g
\]

\[
u_c = \frac{D_c}{x_c} \quad K' = \frac{K \theta_c x_c g}{\mu D_c} \quad T_c = \frac{\delta \nu Q}{c_q \text{Le}}.
\] (3.34)

Once these definitions have been made the non-dimensional equations for the reaction product and oxygen mass fractions are found to only differ by the sign of the reaction term. In fact the differential equation for the reaction product mass fraction can be dropped and replaced by the relation

\[
Y_P = 1 - Y_X.
\] (3.35)

Using this and dropping primes leads to the full non-dimensional model.
The Non-Dimensional Model

\[ \frac{\text{Le} \rho_t + \nabla \cdot (\rho \mathbf{u})}{\text{Le} \rho_s} = \nu \Omega \]
\[ \text{Le} \rho_{st} = -\delta \nu \Omega \]

\[ \rho (\text{Le} Y_{st} + \mathbf{u} \cdot \nabla Y_{st}) = \nabla \cdot (\rho \nabla Y_{st}) - \Omega \]
\[ Y_{p} = 1 - Y_{X} \]

\[ (\rho_{s} + \delta \rho) T_{t} + \frac{1}{\text{Le}} \delta \rho \rho_{st} \cdot \nabla T = \nabla \cdot \left( \frac{\phi + (1 - \phi)}{\phi_{0} + (1 - \phi_{0})} \nu \right) \nabla T + \Omega \]
\[ \mathbf{u} = K' \left( -\frac{\phi}{\phi} - \nabla p \right) \]
\[ \phi = 1 - \rho_{s} (1 - \phi_{0}) \]
\[ \rho = \frac{W \phi}{W_{A} \phi_{0} + 1 \gamma T} \]
\[ \frac{1}{W} = \frac{Y_{p} y_{Pc} + Y_{X} y_{Xc}}{W_{P}} + \frac{1}{W_{X}} + \frac{Y_{X} y_{Xc}}{W_{N}} \]
\[ \Omega = \beta^{2} \rho_{s} \rho Y_{X} \exp \left( \frac{\beta (T - 1)}{1 + \alpha (T - 1)} \right) \]  

(3.36)

Characteristic Values

The set of characteristic values used to determine the non-dimensional equations are summarised below.

\[ \rho_{c} = \rho_{0} \quad u_{c} = \frac{D_{c}}{x_{c}} \quad t_{c} = \beta^{2} \frac{\nu}{\text{Le} A \rho_{X} y_{Xc}} \exp \left( \frac{T_{A}}{T_{0} + T_{c}} \right) \]
\[ \rho_{sc} = \rho_{s0} \quad p_{c} = \rho_{c} x_{c} y \quad T_{c} = \frac{\delta \nu Q}{\text{Le} c_{s}} \]
\[ y_{Xc} = y_{X0} \quad x_{c} = \sqrt{\text{Le} D_{c} t_{c}} \quad y_{Pc} = \frac{\mu_{P} W_{P}}{\mu_{X} W_{X} y_{Xc}} \]

The characteristic values for gas density, solid density and oxygen mass fraction are simply given by initial values. The characteristic product mass fraction is scaled such that one unit of gaseous product is created per unit of oxygen consumed in the reaction.

The characteristic time scale is given by the time scale of the reaction and the characteristic distance by the distance that heat diffuses during the characteristic time. The change in pressure due to gravity over the characteristic length in the vertical direction gives the characteristic pressure and the characteristic velocity is given by the speed at which gas diffuses over the characteristic length. It can be noted that this velocity is a factor \( \text{Le}^{-1} \) faster than the ratio \( x_{c}/t_{c} \) since \( u_{c} = \sqrt{D_{c}/\text{Le} t_{c}} \) while
\[ \frac{x_c}{t_c} = \sqrt{\frac{Le D_c}{t_c}}. \]

Thus \( u_c \) represents a gas-diffusion velocity and not one that arises directly from the scaling of length and time. Typically, for \( Le \ll 1 \) we have \( u_c \gg \frac{x_c}{t_c} \).

<table>
<thead>
<tr>
<th></th>
<th>( T_c ) (K)</th>
<th>( x_c ) (m)</th>
<th>( t_c ) (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>333</td>
<td>14</td>
<td>( 2 \times 10^8 )</td>
</tr>
<tr>
<td>CO(_2)</td>
<td>572</td>
<td>0.004</td>
<td>17</td>
</tr>
</tbody>
</table>

Table 3.1: Characteristic scales for carbon monoxide and carbon dioxide producing combustion. Values are calculated from those presented in Appendix A.

The characteristic temperature is given by the adiabatic temperature rise divided by the Lewis number, the temperature rise found in flame balls. Significant changes can be made to the dimensional solutions by simply varying the chemical reaction assumed to be dominant. Table 3.1 presents some of the approximate characteristic scales for the problem, when either carbon monoxide or carbon dioxide are assumed to be produced by the chemical reaction. Due to the exponential nature of the chemical reaction, raising the characteristic temperature by a factor of less than 2 is found to reduce the length scale by a factor of over 1000. This significant shift in the magnitude of the characteristic scales highlights the importance of studying non-dimensional equations.

Smouldering combustion is typically incomplete, as discussed in Section 1.4. Thus carbon monoxide producing combustion is considered for the majority of this thesis. In reality, however, a mixture of carbon monoxide and carbon dioxide is likely to be generated. The two chemical reactions are thus compared in Chapter 6. Whilst the reactions are found to predict significantly different dimensional results, the non-dimensional results are qualitatively similar.

The Simplified Model

Before the full problem is considered, the equations are reduced to a simplified form. This is required for analytical solutions to be found. From these simplified solutions assumptions can be dropped one-by-one, building up the model to its full form and assessing the impact of each assumption. It is initially assumed that \( \phi \approx \phi_0 \), as it is taken that the medium is very porous to begin with, and that \( \rho \approx 1 \) i.e. the density of the total gas phase does not change. The first equation of (3.36) is ignored if density is to stay constant. This assumption is much used in combustion literature, with a good level of qualitative success for processes that are not driven by density change,
even though it can only be formally justified for small heats of reaction. If no imposed airflow is considered the gas velocity equals zero with the pressure gradient balancing gravitational force. Hence the set of equations can be reduced to a simplified form.

\[
\begin{align*}
L \rho_s &= -\delta \nu \Omega \\
L Y_{x_t} &= \nabla^2 Y_x - \Omega \\
(\rho_s + \delta \epsilon) T_t &= \nabla^2 T + \Omega \\
\Omega &= \beta^2 \rho_s Y_x \exp\left(\frac{\beta (T - 1)}{1 + \alpha (T - 1)}\right).
\end{align*}
\]

Chapter 4 considers analytical solutions to these simplified equations in 1-dimensional spherical symmetry. The same equations are considered in 2-dimensional axisymmetry in Chapter 5, with the addition of an imposed gas velocity. Finally the full set of equations given in (3.36) are solved in Chapter 6. In this chapter, rather than considering an imposed gas velocity, the gas flow is determined by Darcy’s law.
Chapter 4

Spherically Symmetrical Combustion

In this chapter spherically symmetrical smouldering combustion is investigated. In Section 4.1 the problem is introduced. A slight amendment to the non-dimensional equations presented in the previous section is introduced in order to find a more general analytical solution. In Section 4.2 analytical solutions to the problem in the low solid consumption rate limit ($\rho_{st} \to 0$) are presented and compared to one-dimensional numerical solutions. In Section 4.3 the standard solid consumption rate is considered. Analytical solutions are presented along with one and two-dimensional numerical simulations. Two-dimensional instabilities which are suppressed by the one-dimensional simulation are found to arise leading to combustion propagation via fingering smouldering fronts. Conclusions are drawn in Section 4.4.

4.1 Introduction

Combustion of a near-spherical nature has been produced experimentally in gases in the form of both stationary and propagating fronts [27, 106]. Smouldering combustion of this form would not only be difficult to ignite, but it would also be difficult to view as the combustion would be taking place deep within a solid fuel. In addition to this, due to the static nature of solid fuels, smouldering combustion must propagate in order to be sustained. Thus stationary solutions analogous to flame balls cannot physically exist in solid combustion. Despite this, comparable modes of combustion
have been produced experimentally in solid fuels. Low Lewis number combustion of thin fuels has been found to lead to fragmentation of planar fronts resulting in cap-like combustion fronts burning towards an imposed oxygen flow [43]. Assuming this mode of solid combustion behaves in a comparable manner to gaseous combustion, as the imposed velocity reduced the combustion region would be expected to transition from a cap-shaped to a near spherical combustion zone. Thus whilst static, spherical combustion in a solid cannot exist, near-spherical smouldering combustion moving along an axis and analogous to self-travelling flame balls could exist and indeed are found to exist in Chapter 5. Analytical descriptions of travelling fingers are difficult to produce, although combustion of this form is addressed numerically in Chapters 5 and 6. The analytical spherically symmetrical solutions derived in this chapter can thus be compared to both stationary (this chapter) and self-travelling (Chapter 5) modes of combustion.

Later chapters will focus on superadiabatic combustion where the reaction zone temperature is of the order $T_{ad}/\text{Le}$, where $T_{ad}$ is the adiabatic combustion temperature. However, due to a slight change to the formation of the problem, in this chapter one set of equations can be solved to find analytical solutions for both superadiabatic and adiabatic combustion. Radially propagating combustion has previously been investigated in gases [102]. Both stationary superadiabatic combustion and propagating adiabatic combustion were found to occur, along with an intermediary form of combustion in which the temperature dropped as the flames spread and the radius grew with $\sqrt{t}$ behaviour. The solutions for both superadiabatic and adiabatic combustion can be sought by using the same equations, but altering the combustion sheet temperature. The propagation rate of the combustion front does not need to be imposed, but is rather found to arise naturally as the equations are solved.

Smouldering combustion is taken to occur deep within the peat and the combustion zone is considered as being centered at the origin. For this reason, as buoyancy driven forces are ignored, the problem can be considered as taking a spherically symmetrical form. Far from the combustion region both the oxygen mass fraction and the temperature are at ambient levels. This problem is given by the simplified equations
detailed in the previous chapter,

\[
\begin{align*}
Le\rho_{si} &= -\delta \nu \Omega \\
LeY_{xi} &= \nabla^2 Y_x - \Omega \\
(\rho_s + \delta \epsilon) T_t &= \nabla^2 T + \Omega \\
\Omega &= \beta^2 \rho_s Y_x \exp\left(\frac{\beta (T - 1)}{1 + \alpha (T - 1)}\right),
\end{align*}
\]

(4.1)
along with the boundary conditions

\[
\begin{align*}
\lim_{r \to \infty} (\rho_s, Y_x, T) &= (1, 1, 0), \\
\lim_{r \to 0} (\rho_s, Y_x, T) &= (0, 0, 0).
\end{align*}
\]

(4.2)

When seeking analytical solutions the large Zeldovich number limit is usually considered. The Zeldovich number, \(\beta\), is a non-dimensional measure of the temperature sensitivity of the reaction rate. As long as the temperature is not close to the maximum temperature the reaction rate is exponentially small. When the Zeldovich number is large the reaction zone is concentrated within a narrow region over which the temperature deviates from the maximum temperature by only \(O(\beta^{-1})\). As \(\beta \to \infty\) this zone reduces to a sheet and so the reaction rate can be assumed negligible except inside this thin reaction layer. The location of this combustion sheet at time \(t\) is denoted \(R(t)\). Thus \(r < R\) comprises of the burnt zone, \(r = R\) the combustion sheet and \(r > R\) the unburnt region. Throughout this chapter when analytical solutions are derived it is taken that the rise above the ambient temperature in the burnt zone is given by the characteristic temperature to leading order and that all oxygen is consumed at the reaction sheet. Thus,

\[
\begin{align*}
T &= 1 + O(\beta^{-1}) \quad \forall r < R \\
Y_x &= 0 \quad \forall r < R.
\end{align*}
\]

In fact throughout this chapter it will be assumed that the oxygen mass fraction in the burnt region is identically zero. The non-dimensionalisation presented in the previous chapter assumed the combustion sheet temperature to be the superadiabatic combustion temperature found in flame balls. In order to find a more general solution to the problem a flame sheet scalar, \(\bar{T}\), is now taken into account. The characteristic
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Temperature is now defined as

\[ T_c = \frac{\delta \nu Q \bar{T}}{Le \epsilon}. \]

Solutions to two particular combustion regimes will be sought: adiabatic combustion (with \( \bar{T} = Le \)) and superadiabatic combustion (with \( \bar{T} = 1 \)). Although the characteristic temperature varies substantially between the two forms of combustion, the characteristic scales remain constant with respect to each regime. A transitory form of combustion exists between stationary superadiabatic combustion and adiabatic propagating combustion. In this region the flame sheet scalar would be expected to decrease as the combustion radius increased and so time derivatives of the characteristic temperature would need to be taken into account. However, analytical intermediary solutions of this form are not sought here.

Due to the redefinition of the characteristic temperature the energy released by the chemical reaction must be scaled. The appropriate energy equation is now given by,

\[ (\rho_s + \delta \epsilon) T_t = \nabla^2 T + \Omega / \bar{T}. \] (4.3)

It is worth noting that both the characteristic length scale and the characteristic time scale are functions of the characteristic temperature. Thus comparisons between the superadiabatic solution and the adiabatic solution need to be made with care.

4.2 Solid Consumption Tending to 0

Initially the problem where the solid consumption rate tends to 0 is considered. Whilst this problem is not physically feasible, as fuel must be consumed by the reaction, solving this problem aids in understanding the limits of the problem. The density of the gas species far from the combustion region, \( \rho_c \), will be much lower than the solid density far from the combustion region, \( \rho_{nc} \). Thus,

\[ \delta = \frac{\rho_c}{\rho_{nc}} \ll 1. \]
Hence the problem is studied in the limit $\delta \to 0$, where $\rho_s \to 1$. In this limit the equations take the simplified form,

$$LeY_{xt} = \nabla^2 Y_x - \Omega$$
$$T_t = \nabla^2 T + \Omega/\bar{T}$$
$$\Omega = \beta^2 Y_x \exp\left(\frac{\beta (T - 1)}{1 + \alpha (T - 1)}\right)$$  \hspace{1cm} (4.4)

with boundary conditions,

$$\lim_{r \to \infty} (Y_x, T) = (1, 0)$$
$$\lim_{r \to 0} (Y_x, T_r) = (0, 0).$$  \hspace{1cm} (4.5)

Apart from constant factors and scalings of variables, these equations are the same as the flame-ball model studied by Buckmaster and Joulin [102], Buckmaster et al [98], Champion et al [107] and others. Because this problem has already been addressed in detail, only some of the broad features of the problem are highlighted here. Analytical solutions to the solid consumption problem are presented in Section 4.3. Numerical solutions to the cylindrically symmetrical problem are then considered in greater detail in Chapters 5 and 6.

Whilst the solid species no longer appears explicitly in the equations it remains an important feature of the model; the large bulk density of the solid species plays a key role in reducing the Lewis number.

### 4.2.1 Analytical Solutions

Considering the large Zeldovich number limit it is possible to split the problem into two regions: the inner region and the outer region. The inner region consists of the combustion sheet and the outer region consists of the rest of the domain. As chemical reactions are assumed to only occur at the combustion sheet, the reaction term in the outer region can be dropped. By matching solutions in the inner region to solutions in the outer region jump conditions can be found, describing the changes between the two sides of the flame sheet ($r = R^-$ and $r = R^+$). The equations can then be solved by using the jump conditions at the reaction sheet to determine unknown values found when solving the outer problem.
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Inner Problem

The reaction zone is concentrated in the vicinity of the moving surface \( r = R(t) \). A coordinate system attached to this front is now introduced along with the stretched variable

\[
\beta^{-1} \zeta = r - R(t).
\] (4.6)

The inner expansions for oxygen mass fraction and temperature are given by

\[
Y_{\text{inner}} = \beta^{-1} \psi(t, \zeta) + O(\beta^{-2})
\]

and

\[
T_{\text{inner}} = 1 - \beta^{-1} \phi(t, \zeta) + O(\beta^{-2})
\] (4.7)

respectively. This leads to the differential equations for \( \phi \) and \( \psi \)

\[
\text{Le} \left( \beta^{-1} \psi_t - R_t \psi_\zeta \right) = \beta \psi_{\zeta\zeta} + \left( \frac{2}{R + \zeta \beta^{-1}} \right) \psi_\zeta - \Omega - \beta^{-1} \phi_t + R_t \phi_\zeta = -\beta \phi_{\zeta\zeta} - \left( \frac{2}{R + \zeta \beta^{-1}} \right) \phi_\zeta + \Omega / \bar{T}
\]

\[
\Omega = \beta \psi \exp \left( \frac{-\phi}{1 - \alpha(\phi \beta^{-1})} \right),
\] (4.8)

with the boundary condition

\[
\lim_{\zeta \to -\infty} (\psi, \phi) = (0, \bar{\phi}(t)).
\] (4.9)

Where \( \bar{\phi}(t) \) is unknown. To leading order as \( \beta \to \infty \) this gives

\[
\psi_{\zeta\zeta} = \psi e^{-\phi} = \bar{T} \phi_{\zeta\zeta}.
\] (4.10)

Integrating twice and applying boundary conditions a relationship between \( \phi \) and \( \psi \) is found.

\[
\phi = \bar{\phi}(t) + \psi / \bar{T}
\] (4.11)

Substituting this relation into equation (4.10) the equation can be written in terms of \( \psi \) alone.

\[
\psi_{\zeta\zeta} = \psi \exp \left( -(\bar{\phi}(t) + \psi / \bar{T}) \right)
\] (4.12)

Multiplying by \( \psi_\zeta \), rearranging and integrating gives the equation

\[
\psi_\zeta = \bar{T} \sqrt{2e^{-\phi}(1 - e^{-\psi / \bar{T}})} (\psi / \bar{T} + 1) = \bar{T} \phi_\zeta.
\] (4.13)

From this the limits of \( \phi_\zeta \) and \( \psi_\zeta \) as \( \zeta \to \infty \) are found to be

\[
\lim_{\zeta \to \infty} \psi_\zeta = \bar{T} \lim_{\zeta \to \infty} \phi_\zeta = \sqrt{2} \bar{T} e^{-\bar{\phi} / 2}.
\] (4.14)
Matching Conditions

The outer solution must also be expanded before being matched with the inner solution. Only matching conditions for the oxygen mass fraction are shown in detail below. However, the same method is applied to find matching conditions for temperature, the result of which is stated. Expanding the outer solution for the oxygen mass fraction gives,

\[ Y_X^\pm(r, t) = Y_0^\pm(r, t) + \beta^{-1}Y_1^\pm(r, t) + O(\beta^{-2}), \]  

(4.15)

where \(-\) and \(+\) represent the burnt and unburnt sides of the reaction sheet respectively.

\[ Y_0(r, t) = (Y_0^\pm)_{r=R} + \left( \frac{\partial Y_0^\pm}{\partial r} \right)_{r=R} (r - R) + \ldots \]

\[ Y_0(r, t) = (Y_0^\pm)_{r=R} + \left( \frac{\partial Y_0^\pm}{\partial r} \right)_{r=R} (\beta^{-1}\zeta) + O(\beta^{-2}) \]

\[ Y_1(r, t) = (Y_1^\pm)_{r=R} + \left( \frac{\partial Y_1^\pm}{\partial r} \right)_{r=R} (\beta^{-1}\zeta) + O(\beta^{-2}) \]

From this the oxygen mass fraction can be written in terms of the inner variable \(\zeta\)

\[ Y_X^\pm = (Y_0^\pm(\zeta))_{r=R} + \beta^{-1}\left[ (Y_1^\pm)_{r=R} + \left( \frac{\partial Y_0^\pm}{\partial r} \right)_{r=R} \zeta \right] + O(\beta^{-2}) \]

Matching this with the inner solution given in equation (4.7) at \(O(1)\), \(O(\beta^{-1})\) and the gradients in the limit \(\zeta \to \pm\infty\) gives

\[ (Y_{x0}^\pm)_{r=R} = 0 \]

\[ \left[ (Y_0^\pm) \zeta + \psi \right]_{\zeta \to \pm\infty} = (Y_1^\pm)_{r=R} \]

\[ (\psi_\zeta)_{\zeta \to \pm\infty} = \left( \frac{\partial Y_1^\pm}{\partial r} \right)_{r=R} \]

(4.16)

Combining these conditions with the limits found in equation (4.14) and employing the exactly equivalent arguments for temperature reveals the jump conditions for \(Y_X\) and \(T\) as

\[ \text{JC1: } [Y_X]_{r=R} = [T]_{r=R} = Y_X = 0 \]

\[ \text{JC2: } [Y_X, T]_{r=R} = -\sqrt{2T}, \]

(4.17)

where \([f]_{r=R} = f(r = R^+) - f(r = R^-)\) represents the jump conditions at the flame sheet.
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Outer Problem

As chemistry is restricted to the inner region, in the outer region the profiles must satisfy,

\[ \text{Le} Y_{x_t} = \nabla^2 Y_x \]
\[ T_t = \nabla^2 T, \quad (4.18) \]

to exponentially small orders as \( \beta \to \infty \). To simplify the problem the equations are moved to a frame of reference such that the flame ball radius is normalised at 1. Letting \( \eta = \frac{r}{R(0)} \) the new equations are given by

\[
\begin{cases}
Y_x = 0 & \text{for } \eta < 1 \\
\text{Le} R^2 Y_{x_t} = \left(\frac{2}{\eta} + \text{Le} \eta R R_t\right) Y_{x_n} + Y_{x_{\eta\eta}} & \text{for } \eta > 1 \\
T = 1 + \beta^{-1} \tilde{\phi} & \text{for } \eta < 1 \\
R^2 T_t = \left(\frac{2}{\eta} + \eta R R_t\right) T_n + T_{\eta\eta} & \text{for } \eta > 1,
\end{cases} \quad (4.19)
\]

to an accuracy of order \( \beta^{-1} \).

Smouldering fires are by their very nature slow moving. Although the reaction sheet may propagate, it is taken that the speed at which it does so will be of significantly smaller magnitude than the rates at which heat and oxygen diffuse. Hence the temperature and oxygen mass fraction profiles might be expected not to depend explicitly on time, but rather on the location of the combustion sheet \( R \) and its spread rate \( R_t \). Under this assumption the problem can be considered as being quasi-steady, with this assumption being checked in retrospect against the solutions obtained.

For \( \eta > 1 \), initially only considering the problem for the oxygen mass fraction, the equation then simplifies to,

\[ Y_{x_{\eta\eta}} = -\left(\frac{2}{\eta} + \text{Le} \eta R R_t\right) Y_{x_n}, \]

in which \( Y_{x_t} \) is neglected with \( \eta \) fixed. Integrating twice and applying boundary conditions reveals the solution for \( Y_x \).

\[
Y_x = 1 - \frac{\sqrt{\frac{1}{2} \pi \text{Le} R R_t} \left[ \text{erf} \left( \eta \sqrt{\frac{1}{2} \text{Le} R R_t} \right) - 1 \right] + \exp \left( -\frac{1}{2} \text{Le} \eta^2 R R_t \right) / \eta}{\sqrt{\frac{1}{2} \pi \text{Le} R R_t} \left[ \text{erf} \left( \sqrt{\frac{1}{2} \text{Le} R R_t} \right) - 1 \right] + \exp \left( -\frac{1}{2} \text{Le} R R_t \right)}
\]
In order to simplify this solution two properties of the error function can be utilised. Given that as \( x \to 0 \), \( \text{erf}(x) \to 0 \) and \( \text{erf}(x) = 1 \) for \( x \gg 1 \), the solution can be simplified such that,

\[
Y_x \approx \begin{cases} 
1 - \frac{1}{\eta} \exp\left(-\frac{1}{2} \text{Le} R R_t (\eta^2 - 1)\right) & \text{for } \sqrt{\text{Le} R R_t} / 2 \ll 1 \\
1 - \frac{1}{\eta} \exp\left(-\frac{1}{2} \text{Le} R R_t (\eta^2 - 1)\right) & \text{for } \sqrt{\text{Le} R R_t} / 2 \gg 1,
\end{cases}
\]

leading to the same approximation in both limits. This assumption holds for both the stationary solution (\( R_t = 0 \)) and for large scale, adiabatic combustion (\( R \to \infty \)). However when \( \text{Le} R R_t \) is close to 2 this assumption may lead to discrepancies between numerical and analytical solutions. Returning to \( r \) from \( \eta \) an approximate solution for \( Y_x \) can be given by

\[
Y_x = \begin{cases} 
0 & r < R \\
1 - \frac{R}{r} \exp\left(-\frac{\text{Le} R_t}{2R} (r^2 - R^2)\right) & r > R.
\end{cases}
\]

Solved in an exactly analogous way, the solution for temperature can be approximated by

\[
T = (1 + \beta^{-1} \bar{T}) \times \begin{cases} 
1 & r < R \\
\frac{1}{r} \exp\left(-\frac{R_t}{2r} (r^2 - R^2)\right) & r > R.
\end{cases}
\]

which holds so long as \( R R_t \) is not close to 2. These equations can be used with the second jump condition detailed in equation (4.17) to reveal the equations for the temperature scalar and combustion sheet propagation rate.

\[
\bar{T} = \frac{1}{\sqrt{2}} \left( \frac{1}{R} + \text{Le} R_t \right)
\]

\[
R_t = \sqrt{2} - \frac{1}{R}
\]

These equations are solved for superadiabatic combustion (\( \bar{T} = 1 \)) in Section 4.2.2 and for adiabatic combustion (\( \bar{T} = \text{Le} \)) in Section 4.2.3.

### 4.2.2 Superadiabatic Numerical Solution

First the superadiabatic combustion problem where \( \bar{T} = 1 \) is considered. Using equations (4.23) and (4.24) superadiabatic combustion is found to occur when \( R = 1/\sqrt{2} \).
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Figure 4.1: A sketch of the stationary profiles of temperature and oxygen mass fraction are plotted against $r$.

and $R_t = 0$. It thus follows that the stationary solution is given by the profiles,

$$Y_X = \begin{cases} 
0 & r < 1/\sqrt{2} \\
1 - (\sqrt{2}r)^{-1} & r > 1/\sqrt{2}
\end{cases}$$

$$T = \begin{cases} 
1 & r < 1/\sqrt{2} \\
(\sqrt{2}r)^{-1} & r > 1/\sqrt{2},
\end{cases}$$

(4.25)

to leading order which are shown graphically in Figure 4.1. The solution derived here is essentially the standard flame ball solution, highlighting the similarities between smouldering combustion and gaseous combustion in the low fuel consumption limit.

As with all numerical simulations presented in this thesis, solutions are obtained using COMSOL Multiphysics. COMSOL is a finite element solver with the capability of solving coupled partial differential equations. All constant values used when solving equations numerically are presented in Appendix A. Whilst analytical models consider the limit $\beta \to \infty$, for numerical models a finite Zeldovich number is required. Using the values given in Appendix A an appropriate Zeldovich number for superadiabatic peat combustion would be expected to be of order 7 when carbon is being converted to carbon dioxide and of order 18 when carbon monoxide is being produced. Previous studies have found the Zeldovich number of cellulose (one of the main components of peat) to be approximately 15 [76]. In this thesis the Zeldovich number is taken to be 10 unless specified otherwise. Increasing the Zeldovich number reduces the width of the reaction sheet. Thus using a high Zeldovich number requires a more highly refined
mesh and hence more time is taken to find a solution. The value of 10 is chosen here as it lies towards the lower end of appropriate values and so increases computational efficiency.

When solving the equations numerically a suitable method needs to be determined to calculate the combustion sheet radius. The chosen method was to determine the location of the flame sheet by the equation,

\[ \int_0^\infty H(0.01 - Y_x) \, dr, \]  

(4.26)

where \( H \) is the Heaviside function which is defined by,

\[
H(x) = \begin{cases} 
0 & x < 0 \\
\frac{1}{2} & x = 0 \\
1 & x > 0 
\end{cases}
\]  

(4.27)

so that

\[
H(0.01 - Y_x) = \begin{cases} 
0 & Y_x > 0.01 \\
\frac{1}{2} & Y_x = 0.01 \\
1 & Y_x < 0.01.
\end{cases}
\]  

(4.28)

This assumes the flame sheet radius is given by the radius over which \( Y_x < 0.01 \). As the reaction is oxygen limited this would appear to be a valid assumption. Defining the radius as the location of the maximum reaction rate is an alternative option. However, this can not be evaluated easily within COMSOL and results need to be exported and analysed separately in order to obtain this information. It is thus taken that the Heaviside function will give the combustion sheet location to a sufficient degree of accuracy. The argument of the Heaviside function at which it switches between zero and one needs to be close to, but not equal to, zero. Choosing a value of 0.01 was found to lead to good agreement between the Heaviside method and the maximum reaction rate method, in a few cases where comparisons were made.

The equations are solved for a range of initial combustion radii and the results are presented in Figure 4.2. Numerical simulations of the stationary superadiabatic problem simply show how, much like flame balls, the combustion front is unstable. For all radii considered the combustion region either immediately collapses in on itself, or propagates outwards for a period before collapsing in. For the initial radii where combustion initially propagates outwards, the temperature at the flame-sheet falls as
the radius increases, as shown in Figure 4.2. The thickness of the reaction-sheet grows as a result until it is no longer small compared with the radius $R$. At this stage the chemistry is no longer vigorous enough to sustain the combustion. For a very small time interval after ignition (when the time interval is less than the diffusion time) the scaled radius would be expected to be 0 for all initial radii considered. However, as such small time steps are not shown in Figure 4.2, the scaled radius at the first time step is not 0.

Previous studies have found that a class of flame balls exists which propagates outwards, cooling as they do so, before reaching a steadily propagating adiabatic state. This form of combustion can, however, not be captured by the model as the combustion...
sheet temperature is assumed to be superadiabatic, of the order $T_{ad}/Le$. The model does, however, capture the initial behaviour of the combustion region. When the initial radius is greater than the stationary flame ball radius the combustion region initially propagates outwards. When the initial radius is lower than the flame ball radius the combustion region immediately collapses in on itself.

Although the combustion structure is unstable, the results presented here still have important implications. As discussed in Chapter 2, mechanisms such as heat losses and gas velocities can stabilise flame balls allowing them to be ignited experimentally under the correct conditions. Thus comparable structures would be expected to be stabilised by similar mechanisms in solid combustion. However, these structures can only be theoretical as stationary combustion in the limit $\rho_{si} \rightarrow 0$ cannot physically persist.

4.2.3 Adiabatic Numerical Solution

In general, adiabatic combustion of peat would be unlikely to occur due to insufficiently high combustion zone temperatures. However, the density of peat can vary significantly, with a range of 30 to 565 Kg/m$^3$ being reported [108]. Adiabatic combustion of peat would be likely to only physically occur in the low peat density limit. A reduction in peat bulk density results in an increase of the gas to solid bulk density ratio, $\delta$. This in turn serves to increase the adiabatic flame sheet temperature,

$$T_c = \frac{\delta \nu Q}{c_s}.$$

In this low peat density limit it is assumed that for the peat to maintain its structural integrity the solid bulk density remains significantly greater than the gas bulk density ($\rho_{sc} \gg \rho_c$). Thus, whilst the density ratio would be significantly higher than the value given in Appendix A, the assumption that $\delta \ll 1$ would remain. The constants given in Appendix A would suggest that even for peat of bulk density 30 Kg/m$^3$, combustion temperatures would be insufficiently high to allow for adiabatic combustion to occur ($T_c \approx 50$ and $T_c \approx 100$ for the carbon monoxide and carbon dioxide producing combustion respectively). The values given in Appendix A are, however, simply approximations of orders of magnitude. Experimentally determined values for thermal characteristics of peat cover a large range and little attention has been given to the
kinetic constants of peat combustion. Thus the low estimation of the flame sheet temperature by the values given in Appendix A does not completely preclude adiabatic smouldering combustion of peat, but rather it should be used to highlight the parameter range in which this form of combustion would lie. Even though adiabatic (large radius) combustion of peat might only be possible in an unrealistic limit, it is still of interest to investigate this limit. At the least, it helps to complete the picture of the range of combustion limits which are accessible via the model.

The Zeldovich number would also be expected to vary with the characteristic combustion sheet temperature. For adiabatic combustion this would result in a Zeldovich number approximately 3-5 times lower than the values stated previously, depending on the chemical reaction considered. However, in the same manner in which the characteristic temperature increases in the low fuel density limit, the Zeldovich number would also increase in this limit. Thus, when the solid density is sufficiently low so that adiabatic combustion can occur, the Zeldovich number would be of a comparable order to that of the superadiabatic problem. Hence for adiabatic combustion the Zeldovich number is again assumed to equal 10 in the numerical calculations.

In the adiabatic phase $\bar{T} = L e$. For equations (4.24) and (4.23) to hold $R$ must be large and the combustion sheet propagation rate is found to be constant. The reaction sheet location at a given time is given by the equation,

$$R = \sqrt{2t} + C,$$

(4.29)

where $C$ is an unknown constant. The constant does not equal the initial flame ball radius ($R = 1/\sqrt{2}$) found for superadiabatic combustion. This is due to the differing reference start times and scalings, and the fact that in equation (4.29) $t = 0$ does not correspond to superadiabatic combustion.

To solve the adiabatic combustion problem numerically, combustion is initiated at $R = 20$ using the profiles given in (4.31). As adiabatic combustion is being studied $\bar{T} = L e$ is set in the energy equation. The progression of the combustion front with time is presented in Figure 4.3. The propagation rate is found to tend towards a constant value in the large radius limit as predicted by the analytical solution. The numerical solution predicts the reaction sheet location at a given time to be given by

$$R = 1.37t + 151.$$

(4.30)
The numerical propagation rate is thus approximately 3% lower than that predicted analytically, where an error of the order $\beta^{-1}$ is to be expected.

![Graph of combustion front location over time](image)

Figure 4.3: Location of the combustion front with time for adiabatic combustion. A line of best fit (dashed red) is included for the upper half of the data.

As a constant propagation rate is only valid in the large radius limit, the profiles for oxygen mass fraction and temperature in this limit are also derived. Here a solution would be expected to take the form,

\[
Y_x = \begin{cases} 
0 & r < R \\
1 - e^{-L\sqrt{2}(r-R)} & r > R 
\end{cases}
\]

\[
T = \begin{cases} 
1 & r < R \\
e^{-\sqrt{2}(r-R)} & r > R 
\end{cases}
\] (4.31)

The profiles of the oxygen mass fraction and temperature at time intervals of 50, along with the initial ignition profile, are presented in Figure 4.4. As the combustion front propagates the profiles are found to move towards steady states as the analytical solution predicts. A comparison of the numerical and analytical profiles for the oxygen mass fraction and temperature is given in Figure 4.5. Analytical results are taken in the large radius limit, given by equations (4.31), and numerical results are those when $t = 1000$, $R \approx 1519$. The difference between the analytical and numerical profiles is small. Thus the analytical approximation captures the key features of the temperature and oxygen mass fraction profiles both qualitatively and, to a satisfactory degree, quantitatively.
Two-dimensional solutions in the low solid consumption rate limit are not shown here. The features found when these equations are solved are also found in the more complex solid consumption problem (Section 4.3.4). However, these features are more readily seen in the solid consumption model. Here the solid profile acts not only to highlight the activity of the combustion process at a given moment, but it also shows the history of the combustion front by mapping at which point chemical reactions have occurred, and to what extent.

Solving the equations for the low solid consumption rate limit highlights a number of interesting features of spherically symmetrical peat combustion. In this limit the combustion front behaves in a manner analogous to flaming combustion. In the large radius limit the combustion front tends to a planar wave exhibiting a constant spread rate, behaviour which has been experimentally found to occur in gases. In addition to this a stationary solution, exhibiting the key features of a flame ball, is also found to exist, albeit being unstable in the formulation studied here. However, due to the assumption that $\rho_{st} \to 0$, these solutions are purely theoretical.
4.3 Incomplete Solid Combustion

In this section the more complex, but physically realistic, problem where solid fuel is consumed by the reaction is considered. Whilst $\delta \ll 1$ as before, it is no longer appropriate to take the limit $\delta \to 0$ as this implicitly implies that $\rho_s \to 0$. However, given the small magnitude of $\delta$, so long as the combustion is not fuel limited it can be assumed that

$$\rho_s \gg \delta. \quad (4.32)$$

This allows simplifications to be made as they were in the previous section, whilst ensuring the reaction term is maintained in the solid species equation. The equations solved analytically in this section are thus,

$$\text{Le} \rho_{s_t} = -\delta \nu \Omega$$
$$\text{Le} Y_{X_t} = \nabla^2 Y_X - \Omega$$
$$\rho_s T_t = \nabla^2 T + \Omega/\bar{T}$$
$$\Omega = \beta^2 \rho_s Y_X \exp \left( \frac{\beta (T - 1)}{1 + \alpha (T - 1)} \right), \quad (4.33)$$

with the boundary conditions,

$$\lim_{r \to \infty} (\rho_s, Y_X, T) = (1, 1, 0),$$
$$\lim_{r \to 0} (\rho_s, Y_{X_r}, T_r) = (0, 0, 0). \quad (4.34)$$
4.3.1 Analytical Solutions

As before, the problem can be split into inner and outer regions and matching conditions between the two solutions can be applied. The profile of the solid species in the outer region is expected to be,

\[ \rho_s = \begin{cases} \bar{\rho} & r < R \\ 1 & r > R, \end{cases} \]  

(4.35)

where \( \bar{\rho} \) is the burnt peat density. In the inner region, both the temperature and the oxygen mass fraction are constant to leading order, however the peat density is not. As \( \beta \to \infty \) and the inner region reduces to a sheet, a jump in the peat density across the sheet is found. Hence the appropriate inner expansions are given by,

\[ T_{\text{inner}} = 1 - \beta^{-1} \phi(\zeta, t) + O(\beta^{-2}) \]

\[ Y_{\text{inner}} = \beta^{-1} \psi(\zeta, t) + O(\beta^{-2}) \]

\[ \rho_{\text{inner}} = \hat{\rho}(\zeta, t). \]  

(4.36)

As before these definitions are substituted into the equations given in (4.33) and the stretched variable is used to give,

\[ \text{Le} \left( \hat{\rho}_t - \beta R_t \hat{\rho}_\zeta \right) = - \delta \nu \Omega \]

\[ \text{Le} \left( \beta^{-1} \psi_t - R_t \psi_\zeta \right) = \beta \psi_\zeta + \frac{2}{(\beta^{-1} \zeta + R)} \psi_\zeta - \Omega \]

\[ \hat{\rho} \left( - \beta^{-1} \phi_t + R_t \phi_\zeta \right) = - \beta \phi_\zeta - \frac{2}{(\beta^{-1} \zeta + R)} \phi_\zeta + \Omega / \bar{T} \]

\[ \Omega = \beta \hat{\rho} \psi \exp \left( \frac{-\phi}{1 - \alpha \beta^{-1} \phi} \right). \]  

(4.37)

with

\[ \lim_{\zeta \to -\infty} (\hat{\rho}, \phi, \psi) = (\bar{\rho}, \bar{\phi}, 0) \]

\[ \lim_{\zeta \to \infty} (\hat{\rho}) = 1. \]  

(4.38)

Taking the limit \( \beta \to \infty \), as before, gives the leading order equations as

\[ \frac{\text{Le} R_t}{\delta \nu} \hat{\rho}_\zeta = \psi_\zeta = \bar{T} \phi_\zeta = \hat{\rho} \psi e^{-\phi}. \]  

(4.39)

Integrating with respect to \( \zeta \) and using the boundary conditions leads to the relations

\[ \bar{T} \phi_\zeta = \psi_\zeta = \frac{\text{Le} R_t}{\delta \nu} (\hat{\rho} - \bar{\rho}) \]

\[ \bar{T} \lim_{\zeta \to \infty} \phi_\zeta = \lim_{\zeta \to \infty} \psi_\zeta = \frac{\text{Le} R_t}{\delta \nu} (1 - \bar{\rho}). \]  

(4.40)
Integrating again gives,

$$\phi = \bar{\phi} + \psi / \bar{T},$$

(4.41)

giving an equation in terms of $\psi$ alone as

$$\psi_{\zeta} = \left( \frac{\delta \nu \psi_\zeta}{LeR_t} + \bar{\rho} \right) \psi \exp\left( -\left( \frac{\bar{\phi} + \psi / \bar{T}}{} \right) \right).$$

(4.42)

In order to solve this equation the fact that $\zeta$ does not appear explicitly in the equations can be utilised. One method to solve equations of this form is by rewriting the second derivative in terms of the first derivative and the original function.

$$\psi_{\zeta\zeta} = \frac{d\psi_{\zeta}}{d\zeta} = \frac{d\psi_{\zeta}}{d\psi} \frac{d\psi}{d\zeta} = \psi_{\zeta} \frac{d\psi}{d\zeta}.$$  

(4.43)

Substituting this and integrating leads to the relation

$$\psi_{\zeta} + \frac{LeR_t}{\delta \nu} \bar{\rho} \ln \left| \frac{\bar{\rho}}{\delta \nu \psi_{\zeta}} \right| = \frac{\delta \nu}{LeR_t} \bar{T}^2 e^{-\bar{\phi}} \left( 1 - e^{-\psi / \bar{T}} \right).$$

(4.44)

Finally, using the fact that as $\zeta \to \infty$, $\psi \to \infty$, and $\psi_{\zeta} \to \frac{LeR_t}{\delta \nu}(1 - \bar{\rho})$ the relation

$$1 - \bar{\rho} + 7 \ln|\bar{T}| = \left( \frac{\delta \nu \bar{T}}{LeR_t} \right)^2 e^{-\bar{\phi}}$$

(4.45)

is obtained. As in the previous section matching conditions are applied to reveal the jump conditions,

**JC1**: $[Y_\chi] = [T] = Y_\chi = 0$

$[\rho_s] = 1 - \bar{\rho}$

**JC2**: $[Y_{\chi_r}] = -\bar{T}[T_r] = \frac{LeR_t}{\delta \nu}(1 - \bar{\rho})$.

In the outer region the oxygen mass fraction and the temperature do not depend on the fuel density. Thus the profiles found in the previous section for $Y_\chi$ and $T$ remain unchanged. These can again be represented by the leading order quasi-steady approximations

$$Y_\chi = \begin{cases} 0 & r < R \\ 1 - \frac{R}{r} \exp \left( -LeR_t \frac{(r^2 - R^2)}{2R} \right) & r > R \end{cases}$$

(4.46)

$$T = \begin{cases} 1 & r < R \\ \frac{R}{r} \exp \left( -Rt \frac{(r^2 - R^2)}{2R} \right) & r > R. \end{cases}$$
In addition to this the jump conditions lead to the three relations,

\[ \bar{T} = \frac{LeRR_t + 1}{RR_t + 1} \tag{4.47} \]
\[ LeRR_t = \frac{\delta \nu}{1 - \bar{\rho} - \delta \nu} \tag{4.48} \]
\[ R_t = \frac{\delta \nu \bar{T} Le}{(1 - \bar{\rho} + \bar{\rho} \ln|\bar{\rho}|)^{0.5}} \tag{4.49} \]

4.3.2 Superadiabatic Numerical Solution

For combustion to reach the superadiabatic temperature found in flame balls, using equation (4.47), the propagation rate must be nearly 0. Whilst the value \( R_t = 0 \) is not physically feasible, as the combustion front must propagate in order to be sustained, the solution as \( \bar{T} \to 1 \) and \( R_t \to 0 \) can be examined. From equations (4.48) and (4.49) the stationary solution is found to exist only in the low solid consumption rate limit \( \delta \to 0 \). This result should be expected given that the peat cannot diffuse and so combustion can only occur in a given location for a finite period of time. Combining these equations and taking the limit \( \delta \to 0 \) reveals the equation

\[ R = \frac{\sqrt{1 - \bar{\rho} + \bar{\rho} \ln|\bar{\rho}|}}{1 - \bar{\rho}} \tag{4.50} \]

This equation predicts that the radius is 1 when all of the fuel is consumed, and \( 2^{1/2} \) when no fuel is consumed. Analytical results presented in the previous section assumed that no fuel was consumed and also found the the stationary radius to be \( 2^{1/2} \). Thus in the limit \( \delta \to 0 \) the two models agree on the characteristics of the stationary solution.

Whilst combustion in the limit \( \delta \to 0 \) is not physically feasible, these results still have important implications. Although stationary spherically symmetrical combustion cannot occur in solids, self-travelling, near-spherical combustion can occur, as will be seen. Numerical simulations of self-travelling combustion are presented in the following chapter along with comparisons to the analytical results presented here. Numerical simulations of superadiabatic combustion produce results which are very similar to the results presented in Section 4.2.2. Thus numerical simulations of this problem are not included here.
4.3.3 Adiabatic Numerical Solution

Solving equations (4.47)-(4.49) for adiabatic combustion \((\bar{T} = Le)\) leads to the relations,

\[
\bar{\rho} = 1 - \delta \nu \quad (4.51)
\]

\[
R_t = \delta \nu (\delta \nu + (1 - \delta \nu) \ln|1 - \delta \nu|)^{-0.5} \quad (4.52)
\]

valid for large \(R\). Relation (4.52) is plotted in Figure 4.6. When all fuel is consumed \((\delta \nu = 1)\) the propagation rate is 1 and when no fuel is consumed \((\delta \nu = 0)\) the propagation rate is \(\sqrt{2}\). Thus both the low solid consumption limit problem and the standard consumption rate problem share the same trends for adiabatic combustion as \(\delta \to 0\).

![Figure 4.6: Profile of the predicted propagation rate with fuel consumption.](image)

Numerical solutions are found by solving the equations given in (4.33) and setting \(\bar{T} = Le\). The equations are solved in spherical symmetry using the boundary conditions given in (4.34). The ignition mechanism is the same as that presented in the previous adiabatic section, with \(\rho_s = 1\) over the entire domain. The results presented in the previous section implicitly assumed that the peat density remained constant, with a value of 1. In this section, where peat consumption is considered, the results are almost identical to those presented in the previous section. Given that \(\delta \ll 1\), from Figure 4.6 it can be seen that the analytical solution predicts \(R_t\) should be expected to be close to, but slightly less than, \(\sqrt{2}\). When the equations are solved numerically the spread rate is found to be approximately 1.37 showing a satisfactory level of agreement between the two solutions. The relationship between radius and time is in fact found
to be almost identical to the relationship presented in Figure 4.3 and thus a plot of
the relationship in the standard consumption limit is not included here. In addition to
this, both the low fuel consumption limit and the standard consumption problem share
the same qualitative features, although quantitative differences would be expected to
arise for larger values of $\delta \nu$. Due to the assumption $\delta \rightarrow 0$ made in the low-solid
consumption problem, this term is not a feature of the simpler model. However, this
term can play an important role in determining the propagation rate (Figure 4.6).

In the large radius limit equation (4.51) predicts the quantity of fuel remaining in
the burnt zone to be

$$\bar{\rho} = 1 - \delta \nu \approx 0.9983.$$  

The profile of the peat at $t = 1000$ is shown in Figure 4.7. The quantity of burnt peat
remaining is approximately 0.9983, showing a very high level of agreement between
the analytical and numerical solutions.

![Figure 4.7: Profile of the solid species at t=1000. The dashed red line represents $\rho_s = \bar{\rho} = 0.9983$.](image)

Finally, as both the simplified model and the solid consumption model predict
the same profiles for oxygen mass fraction and temperature as the combustion radius
tends to infinity, it is interesting to compare both numerical solutions together with
the analytical solution. Figure 4.8 highlights how the the analytical solution captures
the profiles of the oxygen mass fraction and the temperature for both models to a
satisfactory degree of accuracy.
Figure 4.8: Comparison of analytical profiles of oxygen mass fraction and temperature with numerical profiles for both the solid consumption problem and the low-solid consumption limit. Both numerical results are taken at $t = 1000$, when $R = 1519$ and $R = 1520$ for the low-solid consumption limit and the standard consumption problem respectively.

### 4.3.4 Cylindrically Symmetrical Numerical Solution

Analytical solutions show a good level of agreement to one-dimensional numerical solutions. However considering the problem in one-dimension suppresses the impact that any two-dimensional instabilities may have. Thus two-dimensional, axisymmetrical simulations are also undertaken. Solving the equations in two-dimensions requires a large highly refined mesh. For this reason the time scale over which the equations can be studied is limited.

When the cylindrically symmetrical equations are solved a marked change from the predicted solution is seen. Figure 4.9 displays the temperature, oxygen mass fraction and peat density, ignited in the same manner as in the spherically symmetrical simulation, at $t = 15$. Low-lewis number instabilities cause the front to fragment and produce a complex fingering pattern. Fingering results in higher peak temperatures and lower burnt peat densities than those found in the one dimensional study.

As the equations can only be solved over a limited time period, in depth analysis of this complex fingering pattern is not conducted here. Despite this, individual fingers appear to all express similar characteristics, such as the burnt peat density and the combustion zone temperature. Before tip splitting occurs higher temperatures are found however, which can lead to higher levels of fuel consumption in these regions.
Figure 4.9: Profiles of temperature, oxygen mass fraction and peat density for adiabatic combustion at $t = 15$. The parameters employed are given in Appendix A, i.e $Le = 0.05$, $\beta = 10$. No heat loss term, $F$, is included.
4.4 Conclusions

Spherically symmetrical peat combustion has been investigated in both the low fuel consumption rate limit and for the standard consumption rate problem. Both nearly stationary superadiabatic combustion and propagating adiabatic combustion at large radii have been considered. When the combustion sheet temperature is the adiabatic temperature, analytical solutions show a satisfactory level of agreement to 1-dimensional numerical simulations.

Solid combustion must propagate in order to be sustained as only a limited quantity of fuel exists in a given location. Thus stationary smouldering combustion can not occur. However, this form of combustion can be studied in the limit $\delta \to 0$, i.e. in the low fuel consumption limit. In this limit spherically symmetrical peat combustion possesses the same key features as those found in gaseous combustion. It is also found to be unstable in the formulation studied here. Although stationary combustion of this form cannot occur in solid combustion, near-spherical smouldering combustion moving along an axis and analogous to self-travelling flame balls can exist. Self-travelling combustion of this form is addressed in the following chapter where numerical solutions are compared to the analytical solutions derived here.

Whilst one-dimensional numerical simulations of the adiabatic problem show a satisfactory level of agreement with analytical solutions, this solution is also found to be unstable. When the problem is studied in cylindrical symmetry the combustion front is found to fragment, leading to fingering combustion. Fingering enhances diffusive fluxes at the tip of each finger, thus superadiabatic temperatures are attained in this region. In addition to this, individual fingers appear to share a comparable peak combustion zone temperature and burnt peat density. Whilst the analytical adiabatic solutions derived are unstable they still have physical relevance. However, the solutions only apply to combustion occurring in a channel sufficiently narrow so that instabilities are suppressed.
Chapter 5

Combustion with an Imposed Gas Velocity

In this chapter travelling wave solutions of superadiabatic peat combustion propagating in the presence of an imposed air flow are presented. Low Lewis number instabilities promote curvature of the combustion front. Hence a propagating, near-spherical, combustion region analogous to a flame ball can be followed. The resulting burnt zone has a shape resembling that of a finger. In Section 5.1 the problem is introduced. The set of equations describing smouldering combustion with an imposed gas velocity and an additional heat loss term are detailed in Section 5.2. Methods used to identify a travelling wave solution and characteristics of the combustion profile are also presented. The effects of heat loss, gas velocity and Lewis number on the combustion profile are discussed and compared to experimental studies in Sections 5.3, 5.4 and 5.5 respectively. The effects of the constant density assumption are assessed in Section 5.6, where a constant and non-constant density model are compared. In Section 5.7 an equation estimating the distance between two neighbouring fingers is derived. Finally conclusions are drawn in Section 5.8.

5.1 Introduction

The 2-dimensional numerical simulations presented in the previous chapter highlighted a tendency for a radially propagating, adiabatic combustion front to fragment. Rather than a planar combustion front being observed, a complex fingering pattern was found
5.2 THE TRAVELLING WAVE MODEL

and combustion sheet temperatures were found to reach superadiabatic levels. This phenomena is caused by low Lewis number instabilities. In this chapter a superadiabatic, near-spherical, combustion region propagating in the presence of an imposed airflow is considered. This form of combustion has been observed experimentally in combustion of a thin solid fuel [43]. In addition to this, this form of smouldering combustion is analogous to flame balls in gaseous combustion, which have been studied much more intensively [27, 41, 42, 100].

In the physical problem, rather than a lone finger travelling against an imposed gas flow, a system of fingers may be found. This behaviour has been observed in experiments conducted by Zik and Moses [43]. Although the system can initially appear random and complex, the width of each finger was found to be independent of any surrounding finger. In addition to this, after tip-splitting occurred the width of each finger and distance between two neighbouring fingers was maintained. Thus results found when studying a single finger in axisymmetry would be expected to have applications to a system of fingers. The only feature of the system not identified by the single-finger problem would be the distance between any two neighbouring fingers, $d$. However, an equation estimating the value of $d$ is given in Section 5.7. Deep-peat combustion could persist in the form of a single finger, or as a group of fingers. The arguments provided in Section 5.7 suggest the range of parameters over which a single finger, a fingering regime, or a planar front might be expected to be observed.

5.2 The Travelling Wave Model

5.2.1 Identifying a Travelling Wave Solution

Before attempting to seek a travelling wave solution it was first necessary to determine the preferred direction of smoulder. In order to assess whether the smouldering front moved with or against an imposed air flow the equations were first studied as an ignition problem in a static frame of reference. The simplified equations detailed in equations (3.37) were returned to with an imposed airflow added. A 2-dimensional, axisymmetric model was considered, where the gas flows in the positive $z$ direction at
speed \( v \).

\[
\begin{align*}
\text{Le} \rho_s &= -\delta \nu \Omega \\
\text{Le} Y_{X_t} + \nu Y_{X_z} &= \nabla^2 Y_{X_t} - \Omega \\
(\rho_s + \delta \epsilon) T_t + \frac{\delta \epsilon}{\text{Le}} \nu T_z &= \nabla^2 T + \Omega \\
\Omega &= \beta^2 \rho_s Y_{X_t} \exp \left( \frac{\beta (T - 1)}{1 + \alpha (T - 1)} \right)
\end{align*}
\] (5.1)

Boundary conditions were given by \( \rho_s = 1 \), \( Y_X = 1 \) and \( T = 0 \) on all external boundaries with axisymmetry at \( r = 0 \). In order to initiate combustion initial conditions were set by the temperature and oxygen mass fraction profiles,

\[
T = \begin{cases} 
1 & X < R \\
R/X & X > R 
\end{cases}
\]

\[
Y_X = \begin{cases} 
0 & X < R \\
1 - R/X & X > R, 
\end{cases}
\]

where \( X = \sqrt{r^2 + z^2} \). The initial peat density was set to equal one over the entire domain. Temperature and oxygen profiles of this form were identified as stationary solutions to the spherically symmetrical equations in Chapter 4, with no flow velocity and no solid consumption. Travelling wave solutions should be expected to have a broadly comparable structure, except with a skew in the \( z \) direction.

The progression of the combustion front when \( v = 1 \), ignited by a temperature and oxygen profile with \( R = 1 \), is presented in Figure 5.1. Opposed smouldering is found to be preferential. Due to the nature of smouldering combustion within a porous medium, fuel is generally more abundant than oxygen. As oxygen is being supplied to the burning region from below, combustion is promoted in this region. Thus a cap shaped reaction region propagates downwards, towards the oxidiser supply. This behaviour has also been observed experimentally in fingering combustion in microgravity [60]. A range of combinations of values for \( R \) and \( v \) were trialled. All successful ignitions were, however, found to lead to fronts with an expanding width. These fronts resulted in spherical or egg-shaped burnt zones depending on the magnitude of the imposed velocity, as illustrated by Figure 5.1, rather than a branch of fixed-term travelling wave solutions.
5.2. **THE TRAVELLING WAVE MODEL**

In order to isolate a branch of travelling wave solutions an artificial heat loss term was added. Buckmaster et al found that dimensionless heat loss functions of the form \( f(T)\beta^{-1} \) act to stabilise flame balls [98]. In addition to this, experimental investigations of fingering instabilities in smouldering combustion found increased heat losses lead to a reduction in tip-splitting [43]. In this study, for simplicity, the dimensionless heat loss function \( FT\beta^{-1} \) is considered, where \( F \) is a constant. In this work adding this term as a temporary measure serves two purposes. Firstly, as initial attempts to identify a solution proved unfruitful, including this term stabilised the problem further allowing a point of access to a travelling wave solution. Secondly, in the physical problem heat would be lost to mechanisms such as pyrolysis and evaporation. Whilst the inclusion of these processes is beyond the scope of this study, including a heat loss term serves as a simple method to identify the effects such heat losses may have on a combustion finger. As the effects of heat losses on fingering combustion have also been investigated experimentally, theoretical results found by varying the heat loss parameter, \( F \), can also be compared to experimental results.

---

*Figure 5.1: Contour plots of \( \rho_s = 0.99 \) depict the progression of the smouldering front with time. The gas velocity and ignition radius are given by \( v = 1 \) and \( R = 1 \) respectively.*
CHAPTER 5. COMBUSTION WITH AN IMPOSED GAS VELOCITY

Figure 5.2: Ignition of a stable, travelling combustion front. The heat loss parameter and imposed velocity are $F = 0.82$ and $v = 1$ respectively. Contour plots of $\rho_s$ depict the progression of the front with time.

Initially the heat loss term and imposed velocity were both set to equal one. A solution could not be found under these parameters, however, and so the heat loss parameter was reduced. Maintaining the velocity at one and reducing the heat loss to 0.82 was found to lead to the successful ignition of a travelling wave solution for a range of values of $R$. A travelling wave solution ignited by the profiles given in equations (5.2), with $R = 1$, is presented in Figure 5.2.

Once a travelling wave solution had been identified, the problem was moved to a frame of reference attached to the combustion front. The frame of reference was set such that it moved at speed $S$, maintaining the position of the tip of the combustion front at the point $(0,0)$. It can be noted that the finger-tip speed, $S$, and gas velocity,
5.2. THE TRAVELLING WAVE MODEL

$v$, are not measured against the same scale of speed. While $S$ is measured against $x/c/\sqrt{LeDc/\tau_c}$ the gas velocity is measured against $Dc/x_c = \sqrt{Dc/\tau_c} = Lc^{-1} x_c/\tau_c$ as outlined in Section 3.3. The equations thus take the form,

$$
Lc_\rho_s + Lc_S\rho_s = -\delta \nu \Omega
$$

$$
LcY_x + (LcS + v)Y_x = \nabla^2 Y_x - \Omega
$$

$$(\rho_s + \delta \epsilon) T_1 + \left( (\rho_s + \delta \epsilon)S + \frac{\delta \epsilon}{Le} v \right) T_z = \nabla^2 T + \Omega - FT\beta^{-1}
$$

$$
\Omega = \beta^2 \rho_s Y_x \exp \left( \frac{\beta (T - 1)}{1 + \alpha (T - 1)} \right).
$$

(5.3)

The boundary conditions were set as $Y_x = 1$, $T = 0$ on all external boundaries. For the solid species, $\rho_s = 1$ was set on the lower and right hand boundaries with $\rho_{ss} = 0$ along the upper boundary. Axisymmetry was set for all variables along $r = 0$. The domain needed to be sufficiently large so that the chemical reactions occurring in the combustion zone did not affect the solution at the domain edge. For a finger of radius 1, a width and height of approximately 500 and 1000 respectively were taken to be appropriate. The mesh was refined in the combustion region and along the profile of the burnt finger. Elsewhere a coarse mesh was sufficient. Thus the problem could be solved over a large domain without significantly impacting the time taken to reach a solution.

In order to identify the propagation rate, $S$, an integral along the boundary $r = 0$ was used. Due to the choice of location of the finger in the frame of reference, the profile of the peat density along the $z$ axis can be approximated by,

$$
\rho_s = \begin{cases} 
1 & z < 0 \\
\bar{\rho} & z > 0,
\end{cases}
$$

(5.4)

where $\bar{\rho}$ again represents the density of the peat in the burnt zone. Thus an integral of the form,

$$
\int_{-L}^{L} \rho_s - \frac{1}{2}(1 + \bar{\rho}) \, dz = 0,
$$

(5.5)

can be used to determine the appropriate value for $S$, by setting $S$ to be the propagation rate required so that equation (5.5) holds. The burnt peat density is, however, unknown and is found to vary as parameters of the problem are changed. Thus an integral that is independent of the burnt peat density is required. This was arrived at by way of a Heaviside function. A Heaviside function was defined such that where
the peat density was identically 1, the function took a value of 1. In the burnt region, where \( \rho_s \neq 1 \), the function took a value 0. Equation (5.5) could then be used with the Heaviside function replacing \( \rho_s \), and setting \( \bar{\rho} = 0 \). This produced an integral which set the finger tip at the point \((0,0)\) without requiring knowledge of the burnt peat density. The only conditions on \( L \) in equation (5.5) are that it is much greater than the size of the reaction region and that both \( L \) and \( -L \) lie within the domain over which the equations are applied.

### 5.2.2 Profiles of the Travelling Wave Solution

Before parametric studies are addressed later in this chapter, a number of interesting characteristics of the solution profiles will be discussed. These characteristics apply to the majority of the solutions in the following sections. In some limits of the problem notable changes to this profile are found, which will be discussed in the following sections as they arise. The profiles shown here thus act as a reference point for comparisons with later results. For illustration the solutions when \( F = 0 \) and \( v = 1 \) are presented.

The existence of steady travelling wave solutions when \( F = 0 \) will be discussed in the following section.

The profiles of temperature, oxygen mass fraction and peat density are shown in Figure 5.3. The profiles of oxygen and temperature are comparable to the near-spherical profiles with logarithmic tails found in flame balls [42]. Hot gas, with a high combustion product mass fraction, is advected in the positive \( z \) direction towards the hot burnt zone. Hence temperatures are higher and less oxygen is found behind the combustion zone.

A higher fraction of peat is consumed towards the edge of the finger, rather than at the centre of the finger where higher temperatures are attained. Figure 5.4 shows that whilst the reaction rate is highest at the tip of the finger, combustion in the interior of the finger is limited. This can be attributed to a lack of oxygen in this region. Along the edge of the finger, whilst less intense, reactions occur for a longer period of time due to the increased availability of oxygen. Hence peat continues to be consumed in this region. As the reaction rate is an exponential function of temperature, logarithmic steps of the reaction rate are also shown in Figure 5.4. This plot highlights the spherical nature of the combustion zone. Although the reaction is most intense in a cap shape
Figure 5.3: Temperature, oxygen mass fraction and peat density profiles displaying the travelling wave solution when \( v = 1 \) and \( F = 0 \).
region at the tip of the finger, the reaction rate is still at a significant level over a spherical region.

In Chapter 4 appropriate values of the Zeldovich number were discussed. In this chapter a value of $\beta = 10$ was again chosen as being representative whilst conserving computational power. In order to determine whether there were any significant implications of using a reduced Zeldovich number a parametric study was performed. Values of 0 and 1 for $F$ and $v$ respectively were used. The profiles of the peat density along $z = 5$ and $r = 0$ are shown in Figure 5.5. A value of $z = 5$ was deemed appropriate as in this region chemical reactions were negligible, yet the mesh was highly refined, ensuring accurate results.

Changing the Zeldovich number leads to only quantitative changes to the peat density profile. Higher values lead to steeper gradients between unburnt and burnt regions. This is due to the fact that increasing the Zeldovich number serves to decrease the thickness of the reaction zone. This narrowing of the combustion zone limits the region in which combustion can occur. Thus at higher Zeldovich numbers a higher density of peat remains in the burnt zone. The peat density in the centre of the
finger ranges from approximately 0.59 to 0.74. Whilst this is a significant quantitative increase, no qualitative changes to the combustion profile arise due to alterations of the Zeldovich number. The model presented here aims to capture the qualitative features of fingering smouldering combustion, rather than the quantitative features. Thus a Zeldovich number of 10 is deemed suitable.

5.3 The Effects of Heat Loss

In the physical problem heat would be lost from the combustion zone by both evaporation and pyrolysis reactions. Inclusion of a pyrolysis reaction and the addition of water are beyond the scope of this study. However, the addition of a heat loss term in the energy equation acts as a simplified method by which to study the effects of heat losses from the combustion zone. Whilst this term will not produce quantitatively the same results as including further equations to describe evaporation or pyrolysis, the trends identified in this section highlight qualitative changes heat losses would be expected to have.

A parametric study of the heat loss term, \( F \), is undertaken whilst maintaining the imposed velocity at \( v = 1 \). Above a critical heat loss of approximately \( F = 0.82 \) no solutions exist. For heat losses above this value, quenching occurs as there is
insufficient energy for sustained combustion. Below this critical value is a multivalued solution. Whilst the lower branch could be studied in full, due to the rapidly growing width of the finger on the upper branch (Figure 5.7), this branch could only be studied over a limited range of values.

Figure 5.6: Profiles of the propagation speed and finger radius as a function of heat loss.

In order to determine the finger radius an approach similar to that when determining the propagation rate, $S$, was used. A Heaviside function was defined such that where the peat density was identically one, the Heaviside function equalled zero. For the rest of the domain, where some peat had been consumed, the Heaviside function equalled one. Thus this again acted as a switch, giving a value only to the areas where combustion had occurred. Integrating this across $z = C$ thus determines the finger radius. The value $C$ is chosen so that it lies within a region far enough from the tip so that the reaction rate is negligible, yet close enough so that the mesh is well refined. The scale of the solution changes significantly as parameters are varied and so $C$ is not
constant, but rather assigned an appropriate value for a given problem. For a finger of radius one, an appropriate value of $C$ was taken to be approximately 5. Here the value $L$ was set to be the width of the domain over which the equations were solved. However, any value greater than the finger radius would produce the same result.

![Graph of Maximum Temperature vs Heat Loss](image1)

![Graph of Burnt Peat Density vs Heat Loss](image2)

Figure 5.7: Profiles of the maximum temperature and burnt peat density as a function of heat loss.

In addition to the finger radius and the propagation speed, maximum temperature and burnt peat density are plotted in Figure 5.7. Due to the curved nature of the combustion front, the density of peat in the burnt zone depends on its location within the finger. Returning to Figure 5.5(a), the two values which appear best able to represent the burnt peat density are the density in the centre of the finger and the minimum peat density. Thus it is these two values which are used throughout this chapter to characterise the density of the peat in the burnt zone.

From Figure 5.7 it is apparent that when the heat loss term is zero, there are two solutions: an infinitely wide finger and a finger with a radius of approximately one. An analogous finding to this has also been found in the study of flame balls.
[42]. As the flame ball study did not include a gas velocity, and did not take into account the presence of a solid fuel, this multivalued solution must be due to diffusive mechanisms. These mechanisms result in increased heat losses widening a small finger and narrowing a large finger. In gases the lower branch has been found to be unstable to 1-dimensional perturbations and a portion of the upper branch is unstable to 3-dimensional perturbations. In this study, in the presence of an imposed airflow and a solid fuel, the lower branch is stable. Stability is determined by solving the time-dependent equations over a large time scale ($t = 10,000$ was used here). This is done at the limits ($F = 0$ on the lower branch and approximately $F = 0.46$ on the upper branch) along with several intermediary values. If no change was found to the solution after running the time-dependent simulations the solution was taken to be stable. Three-dimensional instabilities, found to occur in flame balls of a large radius, have not been investigated here, although these might only arise for wide enough fingers with $F > 0$.

Figures 5.7 and 5.6 highlight that an increase in the finger radius corresponds to a cooler combustion profile, which propagates at a faster speed and consumes a lower proportion of the fuel. Both an increase in the combustion zone temperature and a reduction to the propagation rate would be expected to lead to a reduction in the peat density in the burnt region. This relationship can be observed by returning to the non-dimensional equations. For the steady-state travelling wave problem, the quantity of peat in the burnt zone is determined by the equation,

$$\rho_{s_z} = -\frac{\delta \nu}{LeS} \Omega.$$  

The term $\delta \nu/Le$ is constant. Thus the density of the peat in the burnt region is determined by the reaction rate and the propagation speed. As the reaction rate is an exponential function of temperature, the effect of a small increase in temperature can dominate over a large increase to the propagation speed. In this section a reduction in the peak reaction temperature corresponds to an increase in propagation speed. Hence this cooler, more quickly propagating combustion would be expected to, and indeed does, correspond to an increase in the burnt peat density.

The finger radius is plotted against the peak reaction temperature in Figure 5.8. When the peak combustion temperature is 1, the finger radius is approximately 4. As the combustion temperature increases from 1, the finger radius slowly decreases. However, as the peak combustion temperature decreases from 1, the finger radius
increases substantially. This relationship is found throughout this chapter, and is discussed further in the concluding section.

Experiments conducted by Zik and Moses concluded that the width of a smouldering finger was determined by the ability of the front to release heat [43]. The effects of heat losses were investigated by increasing the flow of cooling nitrogen gas whilst maintaining the flow of oxygen. Higher heat losses were found to result in narrower, more slowly propagating fingers. This result corresponds to the upper branch of the multivalued solution shown in Figure 5.7. It is interesting to note that it is the upper branch which is found to be stable in gases, and also appears to replicate the behaviour of fingering combustion experiments. Thus, whilst the numerical simulations suggest two stable solutions exist, in the physical problem it may be the upper branch on which solutions are found to lie.

The results presented in this section highlight the similarities between smouldering combustion fingers in a porous media and flame balls. The introduction of a heat loss parameter, $F$, results in a multivalued solution and leads to results analogous to those found in gaseous combustion. The equations solved in this section differ from the classical flame ball equations by both the inclusion of a solid fuel and an imposed gas velocity. These additions serve to stabilise the problem so that both branches of the solution are stable. The narrowing, and slowing, of the finger with increased heat
loss on the upper branch also agrees with experiments conducted by Zik and Moses [61, 43].

5.4 The Effects of Gas Velocity

In a naturally occurring underground peat fire the gaseous velocity field would not be planar as it is here. However, studying planar flow allows general trends to be identified along with the limits of the problem. In this section the effects of the imposed gas velocity on propagation speed, finger radius and burnt peat density are investigated. Here, as in all following sections, the heat loss parameter is taken to be zero. The imposed velocity is studied from $v = 0$ to the low-fuel extinction limit found at $v = 106$.

![Graph 1: Propagation speed and finger radius as a function of gas velocity.](image1)

- Figure 5.9: Propagation speed and finger radius as a function of gas velocity, $v$.

The propagation rate is predicted to initially increase with gas velocity, before reaching a plateau. A small decrease in the propagation speed is then observed before
the extinction limit is reached. Experimental studies of a planar combustion front conducted by Torero et al found the propagation speed increased, reached a peak, then decreased [65]. The initial increase in the propagation rate was attributed to the increased supply of oxygen to the reaction zone. As the velocity increased further, however, the effect of advective heat losses dominated the effect of an increased oxygen supply and the propagation rate slowed. Zik and Moses made similar findings when studying fingering combustion [61, 43]. Whilst increasing the oxygen flux increased the propagation rate, increasing the nitrogen flux decreased it.

The key features of the relationship between propagation speed and gas velocity are thus captured for low gas velocities. At high gas velocities, however, the model does not predict the reduction in propagation rate which has been experimentally observed. In addition to this, at high imposed velocities the model predicts that some oxygen remains in the burnt zone. The minimum oxygen mass fraction found in the combustion region is shown in Figure 5.10. This figure highlights that the plateauing of the propagation rate corresponds to an increase in the fraction of oxygen remaining in the burnt zone. Planar smouldering combustion experiments have, however, found that the oxygen concentration in the burnt zone remains essentially zero for combustion occurring near the high gas velocity extinction limit [91].
The finger radius is predicted to reduce with gas velocity. The characteristic velocity is given by the diffusion velocity. Thus, when the velocity is of order one the gas diffusion rate and advection rate are of the same order. As thermal diffusivity is approximately 20 times lower than the gas diffusivity, when the gas velocity is of order 0.05 conduction and convection are of the same order. As the gas velocity increases, and convection begins to play an important role in the transportation of heat, the finger radius declines significantly. Zik and Moses found that the finger radius increased slightly with increased oxygen flow, but decreased significantly with increased nitrogen flow [61, 43]. Thus increasing the flow of air, which consists mainly of nitrogen, would be expected to reduce the finger radius. Hence the predicted relationship between gas velocity and finger radius shows a good level of qualitative agreement with experimental data.

![Figure 5.11: Burnt peat density and maximum temperature as a function of velocity.](image)

The profiles of maximum combustion temperature and burnt peat density are presented in Figure 5.11. The model predicts that the maximum combustion temperature
increases with gas velocity. The initial rise of temperature with gas velocity has been found to occur in planar filtration combustion. However, much like the propagation speed, the temperature reaches a peak before decreasing [65]. The decreasing temperature resulted in an extinction limit due to excessive advective heat losses. The fingering model, however, predicts that extinction only occurs in the low-fuel limit.

In general, higher velocities result in higher combustion temperatures leading to higher levels of fuel consumption. In the low gas velocity limit, however, this is not the case. As the gas velocity increases from 0, the propagation rate increases rapidly. The effect of the increase in propagation rate dominates the effect of the increase in temperature and hence, for low gas velocities, an increase in the gas velocity leads to an increase in the burnt peat density.

The model captures a number of the key features found experimentally in low-velocity planar filtration combustion and in low-velocity fingering combustion. At high gas velocities use of a one-step, global temperature model is known to lead to discrepancies between predicted and experimental results in planar combustion (as discussed in Section 2.4). These discrepancies are also found here although, due to a lack of experimental evidence, it is not clear whether deep-peat combustion does behave in a comparable manner to planar combustion in this limit. The work of Zik and Moses would suggest that at high imposed gas velocities the distance between two fingers reduces to 0 and a planar front is observed [61, 43]. Experiments performed by Hadden et al also appear to suggest that this behaviour may be found in peat combustion [64]. The model presented here considers the problem in cylindrical symmetry. Hence tip-splitting is not observed and the distance between fingers is not known. However, this is addressed in Section 5.7.

5.4.1 Self-travelling Combustion

A stable, self-travelling solution was identified when $v = 0$, with no heat loss ($F = 0$). Due to the lack of a gas velocity the combustion region is of a more spherical manner than that found in advection-driven combustion. When an imposed airflow is included, as the combustion is oxygen limited, peak reaction rates are found at the point where the oxygen rich gas flow meets the combustion region. In self-travelling combustion, as the far-field oxygen supply is isotropic, peak reaction rates are found at the interface.
between the combustion region and the burnt region (Figure 5.12).

![Figure 5.12: Profile of the reaction rate for self-travelling combustion.](image)

To study the self-travelling solution further, the frame of reference is shifted so that the combustion region is centered at (0,0). The profiles of temperature and oxygen mass fraction along both the positive and negative $z$ axis and along $z = 0$ are shown in Figure 5.13. An analytical (flame ball) approximation has also been included for comparison. This is given by the profiles,

$$
Y_x = \begin{cases} 
0 & X < 1 \\
1 - 1/X & X > 1 
\end{cases}
$$

$$
T = \begin{cases} 
1 & X < 1 \\
1/X & X > 1,
\end{cases}
$$

where $X = \sqrt{r^2 + z^2}$. These are the profiles of spherically symmetrical combustion found in the previous chapter. Only a small portion of peat remains in the burnt region in self-travelling combustion. Thus the analytical solution when all peat is consumed, $R = 1$, is used. It is worth noting that the analytical solution was derived for stationary combustion, not self-travelling combustion, it is simply interesting to see how the two profiles compare.
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The oxygen mass fraction profile is very nearly radially symmetrical. The temperature profile, however, shows a higher level of anisotropy due to the propagating nature of the combustion zone. At a given distance from the centre of the combustion region, the temperature is highest in the burnt region and coolest ahead of the finger in the fresh fuel. The analytical (flame ball) profiles highlight that the same order of magnitude of the solution is maintained in the self-travelling solution. In addition to this, aside from the anisotropy, the analytical profiles do still capture the main qualitative features of the temperature and oxygen mass fraction profiles.

Figure 5.13: Profiles of the temperature and oxygen mass fraction for self-travelling combustion are plotted with the analytical solution to the spherically symmetrical problem.

Brailovsky and Sivashinshky developed a model which considered both stationary and self-travelling flame balls with a heat loss term [42]. A parametric study of the heat loss term unveiled a multivalued solution, as was found in Section 5.3. A bifurcation point was, however, found to exist on the upper branch. This point corresponded to a move from stationary to self-travelling combustion and could occur as either a conventional or inverted bifurcation depending on the parameters considered. For a range of heat losses, three separate solutions could thus be found: two stationary and one self-travelling. In the present work, due to the inclusion of a solid fuel, stationary solutions are not possible. However, repeating the parametric study for $F > 0$, with the gas velocity set at zero uncovers a multivalued solution for self-travelling smouldering combustion.

The results, shown in Figure 5.14, reveal a notable difference between self-travelling
and advection-enhanced combustion. Although the relationship between heat loss and both the maximum temperature and finger radius remain as they did in the previous section (for $v = 1$), the propagation speed now increases with reduced radius. The gas velocity thus plays an important role in determining how heat losses affect the propagation speed of a finger. In order to assess this relationship, a parametric study of gas velocity for a small heat loss ($F = 0.01$) is undertaken. This result is then compared to the results when the same study is undertaken for no heat loss. The difference between the two propagation speeds at a given velocity, $(S_{F=0} - S_{F=0.01})$, thus indicates whether an increase in heat loss results in an increase, or decrease of
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the propagation speed on the lower branch.

Figure 5.15: $S_{F=0} - S_{F=0.01}$ is plotted to depict how an increase in heat loss affects the propagation speed for a variety of imposed gas velocities. Positive values indicate that $F$ and $S$ increase together on the upper (large radius) branch, while negative values indicate that they have opposite trends.

Figure 5.15 shows how, for velocities less than approximately 0.5, an increase in heat loss on the lower (small radius) branch results in a decrease in the propagation rate. For velocities above 0.5 an increase in heat loss on the lower (small radius) branch results in an increase in the propagation rate. Assuming physical solutions lie on the upper branch, where the trends are reversed, additional heat losses thus slow the advection-driven combustion and increase the speed of diffusion-driven combustion. At a critical velocity of approximately $v = 0.5$ the effects of advection and diffusion balance and the propagation speed does not change with heat loss.

The self-travelling solution highlights the similarities between flame balls and fingering combustion in solid fuels. The numerical solutions capture the same trends found in the analogous flame ball problem, and are comparable to the analytical stationary solution derived in Chapter 4. In the physical problem, however, a buoyancy-driven velocity field would sustain combustion. Self-travelling smouldering combustion thus only has applications to combustion regimes where the buoyancy driven velocity field is essentially negligible. Buoyancy-driven combustion is investigated in the following chapter.
CHAPTER 5. COMBUSTION WITH AN IMPOSED GAS VELOCITY

5.5 The Effect of the Lewis Number

The Lewis number is a key feature of the model, as it is this value which causes the thermal-diffusive instabilities leading to ball-like structures. In order to assess the impact that varying the Lewis number has upon the profile of the solution, the definition of the Lewis number is returned to,

\[ Le = \frac{\lambda_g \phi_0 + \lambda_a (1 - \phi_0)}{D_c c_s \rho_s c}. \]

It is taken that the diffusivity of the gas, \( D_c \), remains constant and is defined by an intrinsic characteristic of oxygen behaviour in air. Thus, changes to the Lewis number must be accounted for by changes to the thermal diffusivity of the peat,

\[ \frac{\lambda_g \phi_0 + \lambda_a (1 - \phi_0)}{c_s \rho_s c}. \]

Figure 5.16: Propagation speed and finger radius as a function of the Lewis number for \( v = 1 \) and \( F = 0 \).
5.5. THE EFFECT OF THE LEWIS NUMBER

The thermal diffusivity is taken as a stand alone value, and will not impact any other value. Whilst changes to the thermal conductivity and specific heat capacity would in fact alter either the values $\nu$ or $\epsilon$, the former does not appear in the equations when constant porosity is assumed and the latter only appears in the equations multiplied by the gas to solid density ratio, $\delta$, which is very small. Thus changes to either of these values would not be expected to have a significant impact on the solution.

![Graph showing finger radius plotted against propagation speed.](image)

*Figure 5.17: Finger radius is plotted against propagation speed*

The characteristic temperature is a function of the Lewis number. In addition to this, the characteristic length and time scales are functions of the characteristic temperature. Thus results found when solving the dimensionless equations must be returned to dimensional form before being presented to avoid misinterpretation. Parametric studies are undertaken for an imposed gas velocity of 1. The equations are solved for $0.015 \leq Le \leq 1$.

Both the propagation speed and the finger radius depend heavily on the Lewis number, with both varying by approximately 10 orders of magnitude over the range studied (Figure 5.16). In fact when the propagation rate and finger radius are plotted against each other, in logarithmic form, a near linear relationship is found to exist (Figure 5.17). This relationship can be approximated by the equation $R = 10^{-7.3}S^{-1.1}$.

The density of peat remaining in the burnt zone decreases as the maximum combustion temperature increases. It is worth noting that the combustion temperature increases above the ambient by a factor of approximately 67 as the Lewis number
reduces from 1 to 0.015 whilst the propagation speed increases by approximately 9 orders of magnitude. It is, however, the effect of the increased temperature which dominates the effect of the increased propagation speed. Thus the burnt fuel density reduces with increasing temperature. Hence as the Lewis number reduces towards 0, combustion becomes fuel limited.

The leading order temperature at the combustion sheet is approximately the adiabatic combustion temperature divided by the Lewis number. Thus the increase of the peak combustion temperature above the ambient temperature ($T_0$) should be very nearly proportional to the inverse of the Lewis number. This relationship is plotted in Figure 5.19. The dependence of the propagation rate and combustion zone temperature on the Lewis number has previously been experimentally observed in thermally thin porous media by Zhang et al [94].

An interesting feature of the numerical simulations is that the solution is found to be stable, in the cylindrically symmetrical formulation studied, for the full range of
5.6. THE CONSTANT DENSITY ASSUMPTION

Lewis numbers considered. However, for large Lewis numbers the combustion sheet temperature would be unlikely to be sufficiently high to sustain combustion. Thus, whilst a stable solution theoretically exists, it will not physically exist unless the Lewis number is sufficiently small.

Whilst the Lewis number is a key feature of fingering combustion, so long as combustion is within the fingering regime, changes to the Lewis number are likely to only lead to quantitative changes to the combustion profile. That is, increasing the Lewis number from 0.015 to 0.05 only changes the scale of the solution and serves to move the combustion regime away from the low-fuel limit. However, the Lewis number must be much less than one to lie within the fingering regime.

5.6 The Constant Density Assumption

Until this point a constant density assumption has been held. This will now be dropped and an equation for gas density will be included. In order to assess the impact of the constant density assumption the parametric study of $v$ undertaken in the Section 5.4 is repeated using a variable density model. It is worth noting that the equation for density does not take into account gas density consumption or production at the reaction zone, and that the density variations do not affect the velocity field in any way. In addition to this, the assumptions $W = W_A$ and $\phi = \phi_0$ are still held in this section. Thus, the inclusion of a gas density change is made in a rather simplistic way.
at this stage. A fuller consideration of all of the effects of density change, including buoyancy is addressed in the following chapter.

\[
\begin{align*}
Le \rho_s + Le S \rho_s &= -\delta \nu \Omega \\
\rho (Le Y_{xt} + (Le S + \nu) Y_{xz}) &= \nabla \cdot (\rho \nabla Y_x) - \Omega \\
(\rho_s + \delta \epsilon \rho) T_t + (\rho_s + \delta \epsilon \rho) ST_z + \frac{\delta \epsilon \rho}{Le \nu} \nabla T &= \nabla^2 T + \Omega \\
\theta &= \frac{1}{1 + \gamma T} \\
\Omega &= \beta^2 \rho_s \rho Y_x \exp\left(\frac{\beta (T - 1)}{1 + \alpha (T - 1)}\right). 
\end{align*}
\]

(5.7)

Here \(\gamma = T_z/T_0 \approx 1\) for carbon monoxide producing combustion, as shown in Appendix A.

![Graph](image)

Figure 5.20: Propagation speed and finger radius as a function velocity with \(\gamma = 1\).

The propagation speed and finger radius are plotted against gas velocity in Figure 5.20. The results show little qualitative change between the constant and non-constant
5.6. THE CONSTANT DENSITY ASSUMPTION

density models. However, the inclusion of a non-constant gas density reduces the propagation rate by a factor of approximately 2 (for \( \gamma = 1 \)), and increases the diffusion-driven finger radius by a factor of approximately 6.

![Figure 5.21: Profiles of burnt peat density and maximum temperature with velocity, for \( \gamma = 1 \).](image)

The differences found between the two models can be accounted for by considering the inclusion of a non-constant gas density term in the reaction equation. The gas density is lower in the hot combustion region, resulting in a reduction in the reaction rate. This in turn results in a slower propagation rate and a lower diffusion-driven combustion temperature (and hence a wider finger radius), as shown in Figure 5.21. When the gas velocity is high, the reduction in the reaction rate serves to increase the burnt fuel density, allowing combustion to be sustained at higher imposed velocities.

The constant density model predicted that the propagation rate increased and reached a plateau, before reducing slightly near the low-fuel limit. The non-constant
density model predicts the same behaviour for low velocities, but rather than reaching a plateau the propagation rate is predicted to peak before reducing, showing a higher level of agreement with experiments. However, experiments would also suggest that in the physical problem advective heat losses cause extinction before the low-fuel extinction limit is reached [65], behaviour which is not predicted by either model.

The model also predicts, unlike the constant density model, that very little oxygen remains in the burnt zone. The minimum oxygen mass fraction is plotted against imposed gas velocity in Figure 5.22. The oxygen mass fraction in the burnt zone remains of order $10^{-3}$ or below for imposed gas velocities of approximately 140 and below. An imposed gas velocity of approximately 140 also corresponds to the velocity above which all peat is consumed at the edge of the finger. Hence, aside from the low-fuel limit, the non-constant gas density model predicts that no significant amount of oxygen remains in the burnt zone. This is in contrast to the constant density model where a minimum oxygen mass fraction of order $10^{-2}$ is found when approximately one-third of the fuel in the combustion finger remains unburnt. Thus the non-constant density model shows a higher level of agreement with the planar combustion experiments of Torero et al [65] than the constant density model.

The constant and non-constant density models both capture the main qualitative features of low-velocity smouldering combustion. The only qualitative differences between the two models occur at high gas velocities where, due to the 1-step chemical reaction and global temperature assumptions, both models show disparities between predicted and experimental results in as far as experimental findings are available. In
addition to this, it is possible that at high velocities fingering combustion may also be suppressed, if the distance between two neighbouring fingers reduces to 0.

5.7 The Distance Between Neighbouring Fingers

The experiments conducted by Zik and Moses found that the onset of fingering occurred at relatively low gas velocities. When the imposed oxygen velocity was of the order 10 cm/s, cellular or planar fronts were found. As the velocity was reduced combustion moved to a fingering regime and lateral diffusion became increasingly important. When the gas velocity was of the order 1 cm/s fingering with tip-splitting occurred and when it was of the order 0.1 cm/s fingering without tip-splitting occurred. As the imposed oxygen velocity increased the distance between two neighbouring fingers, $d$, thus decreased with a planar front corresponding to $d = 0$ [61, 43].

Zik and Moses also found that combustion only occurred in the tip of each finger; as was found in the numerical simulations presented in this chapter, combustion did not occur along the profile of the finger. Fingers which were closer to the oxygen supply were found to screen neighbouring fingers. The screened fingers extinguished due to a lack of oxygen and the tip of the screening finger was found to split. After tip-splitting the distance between neighbouring fingers was maintained. Whilst Zik and Moses did not identify the mechanism for tip-splitting, they did predict the widening of the finger prior to the tip-splitting would give insight into the problem. At a certain point tip-splitting ceased and after this point sparse fingers were found. Zik and Moses concluded that the instability was not a collective effect, but a local feature involving a single finger.

The experiments of Zik and Moses considered a line ignition. Under the correct conditions the planar front fragmented to a fingering regime [61, 43]. The experiments of Olson et al performed in microgravity, however, considered ignition in the centre of a piece of paper [60]. A radiant heater was used to produce a circular ignition zone. This zone appeared to be larger than the natural length scale of the fingering instability. Thus shortly after ignition a number of small fingers began to propagate towards the imposed airflow. These fingers then began to split, leading to a fingering regime with tip-splitting like that found by Zik and Moses. Point ignitions which are sufficiently
small as to produce a single finger do not appear to have been conducted. However, it would seem possible that when the gas velocity is sufficiently small so that tip-splitting is suppressed, that a point ignition could produce a single finger propagating against an imposed flow. Thus, the single-finger model presented here may physically occur given the correct ignition mechanism and gas velocity. However, the distance between neighbouring fingers would be a key feature of the tip-splitting fingering regime.

The model presented here only considers a single finger; tip-splitting is suppressed by the cylindrically symmetrical model and the distance between two neighbouring fingers is not captured. For high imposed gas velocities the model predicts combustion to take the form of a narrow finger. Experiments would suggest, however, that at large velocities fingering may not be found as \( d \to 0 \), resulting in a planar front [61, 43, 64].

In this section, using some broad considerations based on the ideas of Zik and Moses [61, 43], an estimation for the mean distance between any two fingers is made. Fingers are considered as taking a hexagonal distribution, with neighbouring fingers centered a distance \( d \) away from one another. A sketch of this regime is shown in Figure 5.23. Following the work of Zik and Moses an hypothesis is that the distance between neighbouring fingers adjusts itself so that almost all of the oxygen is consumed, leaving little leakage between fingers. Zik and Moses confirmed experimentally that, within 10\% experimental error, all oxygen was consumed by the combustion front. Whilst this finding was confirmed for the tip-splitting regime it is, however, unclear whether it was also confirmed for the sparse-finger regime. Despite this, an equation derived by Zik and Moses using this idea showed a good level of quantitative agreement with experimental results. Although both the experimental and theoretical work of Zik and Moses considers the smouldering problem as essentially two-dimensional, using this hypothesis seems to be a natural way of extending the arguments for three-dimensional fingering.

Given this hypothesis, the flux of oxygen relative to each moving finger is approximately the amount of oxygen consumed per unit area. The rate of oxygen consumption per finger (in dimensional terms) is thus approximately

\[
\Gamma_X \approx \frac{1}{2} \sqrt{3} d^2 \varrho_0 (S + v) y_{X_0},
\]

given that the hexagon associated with each finger has an area of \( \frac{1}{2} \sqrt{3} d^2 \). The solid, on the other hand, is only consumed within the finger which has a radius \( R \). The rate
of solid consumption per finger can thus be given by,

$$\Gamma_S \approx \pi R^2 S(\rho_s - \tilde{\rho}),$$  \hfill (5.9)

where $\tilde{\rho}$ is a suitable mean value of the burnt solid density. Given that the mass of gas consumed by reacting with a unit mass of solid is

$$\frac{\mu_x W_x}{\mu_c W_c},$$

it follows that,

$$\frac{\mu_c W_c}{\mu_x W_x} \Gamma_X = \Gamma_S$$

$$\frac{\mu_c W_c}{\mu_x W_x} \frac{\sqrt{3}}{2} d^2 \varrho_0 (S + v) y_{x_0} \approx \pi R^2 S(\rho_{s_0} - \tilde{\rho}).$$  \hfill (5.10)

Non-dimensionalising using the characteristic scales given in chapter 3, and recalling the differing scales of the propagation rate and the gas velocity, this leads to the dimensionless equation

$$\left(\frac{\sqrt{3} \delta v}{2\pi Le}\right) d^2 (Le S + v) \approx R^2 S(1 - \tilde{\rho})$$  \hfill (5.11)
giving,

\[
\frac{d}{R} = \sqrt{\frac{2\pi}{3} \frac{1 - \rho}{\delta \nu \mathrm{Le}} \frac{\mathrm{Le}}{\rho_s(r=0)}} - \frac{v}{\delta v \mathrm{Le} + v/S}.
\]  

(5.12)

The predicted distance between neighbouring fingers is plotted against gas velocity in Figure 5.24. The results are analogous to the two-dimensional results found by Zik and Moses [61, 43]. As the imposed velocity increases, or rather the ratio $v/s$, the distance between fingers decreases, with sparse fingers predicted at low gas velocities. In addition to this, Zik and Moses found experimentally that tip-splitting occurred for $d \lesssim 2R$. This corresponds to velocities above approximately 3.

![Figure 5.24: The predicted finger spacing, $d$, is plotted against velocity. Two values of $\bar{\rho}$ are used, the peat density in the centre of the finger and the minimum peat density, with values of $R$ and $S$ determined by the numerical solutions for each value of $v$.](image)

The equation does, however, predict that the distance between neighbouring fingers is greater than 0.4 for the full range of values studied. Zik and Moses confirmed a movement from a fingering to a planar front in the combustion of paper [61, 43]. A similar relationship appears to have been found in peat by Hadden et al [64] (shown in Figure 2.2). However, this relationship was not discussed by the author. Thus whilst equation (5.12) does capture a number of the key features of the relationship between velocity and finger spacing, it does not predict a point at which fingering moves to a more continuous cellular or planar front.
5.8 Conclusions

Travelling wave solutions of fingering combustion in peat with an imposed gas velocity have been investigated. Parametric studies have been undertaken for a heat loss term, $F$, the imposed gas velocity, $v$, and the Lewis number, $Le$. Little research has been conducted into fingering combustion in three-dimensions. Thus, rather than comparing results to experiments of fingering combustion in peat, they are compared to results of planar filtration combustion experiments and fingering combustion experiments of a piece of paper. Although these experiments are not considering the same problem, the numerical solutions found here show a good level of agreement to the experiments. When the imposed gas velocity is high a number of discrepancies are found between predicted results and experimental results. In filtration combustion these discrepancies have been accredited to simplifications made in considering one-step reaction, global temperature models (as discussed in Chapter 2). Whilst this may also be the case for fingering peat combustion, more experimental evidence is required before firm conclusions can be drawn.

The density of peat remaining in the burnt zone is dependent on the term, $\frac{\delta \nu}{LeS}$. As the reaction rate is an exponential function of temperature, the burnt peat density is highly dependent on peak reaction temperatures and it is usually this which is the dominant factor in determining the burnt peat density. However, when the propagation speed varies significantly whilst the temperature remains relatively constant, it can be this which has the greatest effect on the burnt peat density. In the parametric studies this was only found at low imposed gas velocities (Section 5.4).

A trend found throughout this chapter was that a rise in the maximum combustion temperature was accompanied by a decrease in finger radius. The length scale of the problem, the distance heat diffuses in the characteristic time, is an exponential function of the combustion sheet temperature.

\[ x_c^2 = \beta^2 \frac{\nu D_c}{\rho c y c} \exp\left(\frac{T_A}{T_0 + T_c}\right) \]

Thus a small decrease in the combustion temperature results in an exponential increase in the length scale of the problem. This is highlighted by the dimensional results presented in Section 5.5, where an increase in the peak combustion temperature above
ambient by a factor of approximately 67 leads to a reduction in the finger radius by a factor of $10^9$. In the other, dimensionless, sections when the maximum temperature is greater than one an increase in temperature leads to a small decrease in the finger radius. When the maximum temperature is less than one a small decrease in temperature leads to a significant increase to the finger radius. The only time this relationship does not hold is in the large gas velocity limit where combustion is fuel limited. Here the model predicts that the finger radius increases slightly despite the fact that the temperature is also increasing. However, as discussed earlier, in this limit one-step global temperature models are generally found disagree with experiments.

When studying the heat loss parameter, $F$, the propagation speed of the finger on the upper (large radius) branch was found to decrease with increased heat loss for advection-driven combustion, whilst the opposite occurred for diffusion-driven combustion. Thus the propagation speed is decoupled from combustion temperature and finger radius. The findings of Zik and Moses suggested that the propagation speed of a finger was dependent on the availability of reactants [43]. This finding is also made in this study. When fuel or oxygen is the limiting factor of the reaction, an increase in the limiting substance causes the propagation rate to increase. In addition to this, when the availability of oxygen remains constant, a narrower finger results in a decrease in the propagation rate in advection-driven combustion and an increase in propagation rate in diffusion-driven combustion. This can again be accredited to the increased availability of oxygen in each regime. Smaller fingers enhance the diffusional flux, whilst large fingers provide a larger surface area over which the gas and fuel intersect. The propagation rate does not depend solely on the availability of reactants though. Increasing the flow of a cooling non-reacting gas has been shown to slow fingering combustion [43] and, as was shown in Section 5.5, the Lewis number can also play a significant role in determining the propagation rate.

The results presented in this section show a good level of agreement with experimental studies of both filtration combustion and fingering combustion, and the findings are analogous to those found in the study of flame balls. Fingering combustion also has unique features not found in planar combustion. Thus predicted trends of fingering combustion features, such as the propagation speed, should not necessarily be expected to replicate those trends found in planar combustion.
As no experimental data exists on fingering combustion of peat, planar smouldering studies are, at present, the best resource available to highlight possible weaknesses in the model presented here.
Chapter 6

Buoyancy-Driven Combustion

In this chapter combustion driven by buoyant oxidiser flow is considered. In deep-peat combustion, rather than the planar velocity field considered in the previous chapter, Darcy’s law would determine the gaseous velocity field. The permeability of the solid is a key parameter of this form of problem, thus appropriate permeability values are discussed in depth in this chapter. In Section 6.1 the problem is introduced. In Section 6.2 experimental values for the permeability of peat are discussed. A parametric study investigating the effect of permeability on the combustion profile is undertaken and the constant molecular weight assumption is assessed. The constant porosity assumption held thus far is dropped in Section 6.3. Equations describing the relationship linking porosity and permeability are discussed and the effects of altering the initial solid porosity are investigated. Finally, conclusions are drawn in Section 6.4.

6.1 Introduction

The previous chapter studied the effects of planar oxidiser flow on the profile of the combustion front. Whilst this work produced useful information, in the natural world a planar velocity field would be unlikely to exist. In deep-peat fires the velocity field would be determined by Darcy’s law, leading to buoyancy-driven combustion. Thus it is important to compare and contrast the simpler planar flow model with the more complex buoyant flow model.

The onset of buoyant flows inside a porous medium depends strongly on the permeability of the material [109]. For this reason finding an appropriate order of magnitude...
of the permeability of peat is important. In addition to this it needs to be taken into account that in the burnt zone the porosity, and thus the permeability, of peat may be significantly higher. A number of equations have been put forward linking permeability and porosity. Whilst the equations do not produce quantitatively the same results they do all share the same qualitative features. Permeability is not a linear function of porosity, but rather is found to increase singularly as the porosity tends to one. Thus the permeability of the burnt peat may be significantly higher than the permeability of the fresh peat.

In this chapter the full model presented in equations (3.36) is considered. The equations, written in a frame of reference moving with the combustion front, are given by

\[
Le \rho_t + Le S \rho_z + \nabla \cdot (\rho \mathbf{u}) = \nu \Omega \tag{6.1}
\]

\[
Le \rho_t + Le S \rho_z = -\delta \nu \Omega \tag{6.2}
\]

\[
\rho (Le \dot{Y}_X + Le SY_X + \mathbf{u} \cdot \nabla Y_X) = \nabla \cdot (\rho \nabla Y_X) - \Omega \tag{6.3}
\]

\[
Y_p = 1 - Y_X \tag{6.4}
\]

\[
(\rho_s + \delta \rho) T_t + (\rho_s + \delta \rho) ST_z + \delta \sigma \frac{\mathbf{u} \cdot \nabla T}{Le} = \nabla \cdot \left( \left( \frac{\phi + (1 - \phi)}{\phi_0 + (1 - \phi_0)} \right) \nabla T \right) + \Omega \tag{6.5}
\]

\[
u = K' (-p'_r) \tag{6.6}
\]

\[
\phi = 1 - \rho_s (1 - \phi_0) \tag{6.8}
\]

\[
Y_p \frac{Y_p}{W_P} + \frac{Y_X y_{Xc}}{W_X} + \frac{1 - Y_p y_{Pc} - Y_X y_{Xc}}{W_N} \tag{6.10}
\]

\[
\Omega = \beta^2 \rho_s \rho \frac{\rho_0}{\Phi_0} \exp \left( \frac{\beta (T - 1)}{1 + \alpha (T - 1)} \right) \tag{6.11}
\]

In order to simplify the equations the variable \( p' \) has been introduced. This is defined by

\[
p = p' - \frac{\rho_0}{\phi_0} z = p' - \frac{z}{\phi_0} \tag{6.12}
\]

This amendment changes the appropriate boundary conditions for pressure on all external boundaries to \( p' = 0 \). Here \( \rho_0 \) represents the nondimensional gas density far from the combustion zone and thus \( \rho_0 = 1 \). The relations in (6.4) and (6.8)-(6.11) do
not require boundary conditions. The velocity equations \( (6.6) \) and \( (6.7) \) are merged with the continuity equation \( (6.1) \) in COMSOL and requires the pressure formulation detailed in \( (6.12) \). Finally, equations \( (6.2), (6.3) \) and \( (6.5) \) use the boundary conditions given in the previous chapter.

It is initially assumed that the gas molecular weight and porosity remain constant (i.e. \( W = W_A, \phi = \phi_0 \)), but these assumptions are dropped in Sections 6.2 and 6.3 respectively. Finally, as in the previous chapter the finger propagation speed, \( S \), and the gas velocity, \( u \), are measured on velocity scales that differ by a factor of \( Le \).

### 6.2 The Permeability of Peat

Soil permeabilities cover a large range of values. Permeability can be as low as \( 10^{-20} \text{ m}^2 \) in clay up to \( 10^{-9} \text{ m}^2 \) in fibrous peat [110, 111]. However, the permeability of peat can also vary significantly depending on its geographical location and degree of decomposition.

A common method used to find the permeability of soil is to fully saturate a sample with water before applying a hydraulic pressure difference. Darcy’s law is used to determine the flow though the media, and the hydraulic conductivity is expressed in terms of a velocity [112]. The hydraulic conductivity is also known as the coefficient of permeability, although many authors abbreviate the term to permeability [113, 114]. Thus, most literature discussing the permeability of peat presents a value in terms of a velocity, not an area. Typical values for the hydraulic conductivity of peat cover a range of approximately \( 10^{-4} \) to \( 10^{-8} \text{ m/s} \) [112, 114].

An assumption that peat is isotropic has been held to this point. Studies investigating the isotropy of peat permeability have, however, produced contrasting results. The horizontal hydraulic conductivity has been found to be greater than the vertical hydraulic conductivity by a factor of 300 [114], a factor of 10 [115] and to show no significant change [116]. The permeability of soil is also often thought to decrease with depth, although this is not necessarily the case. Experiments undertaken in permafrost terrain in Canada found that below 20 cm the hydraulic conductivity of peat remained approximately constant, with a value close to \( 5.8 \times 10^{-6} \text{ m/s} \) [117]. Between 10 cm and 20 cm, however, the permeability decreased by three orders of magnitude. Studies of
6.2. **THE PERMEABILITY OF PEA T**

peat taken from the Pennines in the UK echoed this result. Hydraulic conductivity was not found to vary significantly with depth maintaining a value of approximately $3 \times 10^{-8}$ m/s between depths of 10 cm and 80 cm [118]. In this chapter isotropy of peat will continue to be assumed. This is, in part, due to difficulties in applying anisotropic permeability in COMSOL. However, as permeability is not found to change with depth below approximately 20 cm and as the vertical and horizontal permeabilities have been reported to be the same in undecomposed peat, this assumption does seem reasonable for the present study.

It is usually taken that hydraulic conductivity is linearly related to permeability by the equation,

$$\kappa = \frac{K \rho f \phi g}{\mu},$$  \hspace{1cm} (6.13)

where $\kappa$ is the hydraulic conductivity (m/s) and $\rho_f$ is the density of the fluid (Kg/m$^3$) [117]. Taking $g \approx 10$ m/s$^2$, $\mu \approx 10^{-3}$ kg/ms [119], $\rho_f \approx 1000$ kg/m$^3$ [120] and $\phi \approx 1$ the relationship between hydraulic conductivity and permeability can be approximated by,

$$K \ [m^2] \approx 10^{-7} \kappa \ [m/s],$$

an equation which is used by Bear [110]. As most studies investigating the permeability of peat use water based tests, this relation is commonly used to calculate the intrinsic permeability of peat. Using this method the estimated range in which the permeability of peat would be expected to lie is $10^{-15}$ to $10^{-11}$ m$^2$.

Whilst this equation does provide an approximation of the relationship between the hydraulic conductivity and the permeability of peat, it should be used with caution. Calculating the permeability of fibrous media using hydraulic conductivity can lead to errors due to its highly compressible and easily deformable nature [121]. In addition to this, when using water to calculate the permeability of peat it should be taken into account that water molecules can bind to soils. This creates a film approximately one molecule thick and reduces the effective diameter of channels through which the water can flow. Moreover, the fibres of peat themselves expand when wet, further constricting the pores through which water can flow. Hence lower measurements of permeability are found when using water based tests rather than air [122, 123].

Although the majority of values for the permeability of peat are given in terms of hydraulic conductivity, a few experiments have been conducted using air as the fluid
within the pores. The permeability of peat has been found to vary from approximately $10^{-14}$ to $10^{-12}$ m$^2$ in peats with a low air filled porosity, up to approximately $10^{-10}$ to $10^{-9}$ m$^2$ in more porous peats [124, 111]. The upper range of these values corresponds to the permeability of a humus layer, which has a permeability of approximately $10^{-12}$ to $10^{-9}$ m$^2$ as the porosity ranges from 0.1 to 0.8 [124]. The range of permeabilities found using air thus appears to be approximately 2 orders of magnitude higher than those found using water based tests. Despite this, studies using water are still of importance. Experiments investigating the isotropy of peat have relied on results from water based tests and these results would be expected to be applicable to the gas permeability of peat.

![Finger radius and propagation speed as a function of permeability.](image)

As appropriate values for the permeability of peat cover a large range, a parametric study of permeability is used to determine the role the peat permeability plays in determining the combustion profile. Initially results in this section are given in terms of the dimensional permeability, $K$, as opposed to the dimensionless permeability, $K'$. 
This is in order to clearly represent how the combustion profile corresponds to known permeability values. Later data is, however, presented in terms of the dimensionless permeability.

A parametric study is performed from $K = 10^{-14}$ m$^2$ to a low-fuel extinction limit found at approximately $10^{-9.3}$ m$^2$. The propagation speed and finger radius are plotted against permeability in Figure 6.1. The results are found to be analogous to those presented in Section 5.6, where the effects of an imposed gas velocity on a non-constant gas density model were studied. As the results are analogous, peak temperature and burnt peat density profiles are not presented in this chapter. The similarities between the two models is discussed further at the end of this section where the two models are compared in terms of the gas velocity at the finger tip.

![Figure 6.2: Profiles of the combustion zone for advection-driven ($K = 10^{-10}$ m$^2$) and diffusion-driven ($K = 10^{-14}$ m$^2$) combustion. The magnitude and direction of the gas flow is given by the surface plot and arrow plot respectively. The burnt region is represented by a contour of $\rho_s = 0.99$.](image)

When the permeability of peat is low, gaseous flow through the medium is restricted. Thus at low permeabilities combustion is diffusion-driven. This results in large, slowly propagating fingers. As the permeability increases the ease with which oxygen can flow through the medium increases. Thus the magnitude of the buoyant
forces also increases. Hence more oxygen is available in the combustion zone, but
advective heat losses also increase. This leads to an increase in the propagation speed
and reduction in the finger radius, the same trends identified in the previous chapter.

![Graph](image.png)

Figure 6.3: The gas velocity at the point (0,0).

Surface plots of the velocity field at $K = 10^{-10}$ and $K = 10^{-14}$ m$^2$ are presented in
Figure 6.2. When the permeability of the solid is high a buoyancy driven velocity field
is found. When the permeability is low, however, the velocity field is of a more radial
nature. This results in a negative gas velocity at the tip of the finger, albeit with a
very low magnitude (Figure 6.3). This is discussed further in the following section.

In order to assess how permeability affects the combustion profile further, a carbon
dioxide producing reaction ($C + O_2 \rightarrow CO_2$) is considered. Modeling this reaction
requires changes to a number of constant values. The values used are again presented
in Appendix A. Changing the chemical reaction in this manner also alters a number of
length scales of the problem. Theoretically, the Zeldovich number will vary with the
length scale of the problem and should thus take a different value for the two reactions.
In Section 5.2.2, however, no significant qualitative changes to the combustion profile
were found when a parametric study of Zeldovich number was undertaken. Thus the
assumption that $\beta = 10$ held thus far will continue to be held for the carbon dioxide
reaction. The results are plotted, along with the results for carbon monoxide producing
combustion, against the dimensionless permeability $K'$ in Figure 6.4. Results are
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plotted in logarithmic form in order to aid comparison at low values.

Figure 6.4: Carbon dioxide and carbon monoxide producing reactions are plotted against the dimensionless permeability $K'$.  

When plotted in this dimensionless form both reactions exhibit the same qualitative features as the permeability changes. The range of dimensional permeabilities which correspond to the results presented in Figure 6.4 does, however, vary significantly between the two reactions. The permeability covers a range of approximately $10^{-13.65}$ to $10^{-9.3}$ m$^2$ for carbon monoxide producing combustion and $10^{-9.8}$ to $10^{-5.3}$ m$^2$ for carbon dioxide producing combustion. Thus the identified trends occur in carbon dioxide producing combustion at permeabilities approximately 4 orders of magnitude higher than in carbon monoxide producing combustion. As discussed earlier, a typical permeability of a porous peat is approximately $10^{-10}$ m$^2$. This value corresponds to
advection-driven combustion in carbon monoxide producing combustion and diffusion-driven combustion in carbon dioxide producing combustion. Hence kinetics are of great importance when determining the range of permeabilities over which fingering combustion is likely to occur.

The dimensionless permeability is given by the formula,

\[ K' = \frac{K \theta \cdot g \beta}{\mu} \sqrt{\frac{\nu}{\nu}} \exp \left( \frac{T_A}{T_0 + T_c} \right). \]

The fraction \( T_A/(T_0 + T_c) \) is dependent on the chemical kinetics of combustion. This fraction has a value of approximately 34 for carbon monoxide producing combustion and 10 for carbon dioxide producing combustion. Taking into account that this fraction appears in an exponential function explains the shift in the range of dimensional permeabilities over which the trends identified in Figure 6.4 occur. The chemical kinetics of peat are not well determined [25], thus the exact relationship between \( K \) and \( K' \) is not known. In addition to this, different peats can possess significantly different chemical kinetics. Cancellieri et al found that whilst the elementary composition of peats of differing origins were relatively similar, small differences could lead to significantly different degradation behaviour [125]. For this reason the exact range of permeabilities over which fingering combustion occurs is not clear, and in fact differing peats with differing chemical kinetics are likely to express the fingering regime over different ranges of permeabilities. However, the results suggest that the fingering regime can arise in the range of permeabilities known to occur naturally in peats.

Both carbon monoxide and carbon dioxide are produced by smouldering peat combustion [126]. Thus the carbon monoxide model can be considered to act as an approximate lower bound and the carbon dioxide model an approximate upper bound in terms of an appropriate range of permeabilities over which fingering combustion arises. The characteristic values presented in Table 3.3 also suggest these two values may act as bounds. Carbon monoxide producing combustion is predicted to lead to relatively cool combustion, with fingers of a large radius. Carbon dioxide producing combustion on the other hand seems likely to over predict the combustion temperature, resulting in a predicted finger radius of a few millimeters. Hence it seems reasonable to assume that physical values lie somewhere between these two combustion regimes.

Finally, the similarities between the planar flow model and the buoyancy-driven
flow model will be discussed. The models are compared in Figure 6.5, along with the constant density model, where results are presented in terms of the gas velocity at the finger tip, \(v(0,0)\). It should be noted that this quantity is dependent on exactly where the finger-tip is defined to be. Here the point \((0, 0)\) corresponds to the point where fuel is first consumed by the chemical reaction. However, different definitions of the finger-tip location may lead to different results. Negative velocities, found in the buoyancy driven model at low permeabilities, are omitted because only positive gas velocities were considered in the planar flow model; gas production in the combustion region was not considered for planar flow, here negative gas velocities would correspond to forward smouldering, not reverse.

All three models capture the same qualitative features of the relationship between gas velocity and the combustion profile. However, the constant density assumption
Figure 6.6: The vertical component of the gas velocity at the finger tip is plotted as a function of permeability, with numerical approximations.

is found to lead to a significant quantitative deviation from the other two models. The quantitative differences between the buoyant flow model and the planar flow, non-constant gas density model can be accounted for by considering the velocity fields for buoyancy driven combustion and returning to the velocity profiles presented in Figure 6.2. When the peat is highly permeable and combustion is advection-driven, inward radial gas flow increases the availability of oxygen at the reaction site. Thus the buoyant flow model predicts narrower, more quickly propagating fingers for advection-driven combustion than the planar flow model. When combustion is diffusion-driven buoyant forces decrease and radial flow away from the combustion region becomes more prominent. This in turn leads to wider, more slowly propagating fingers being predicted by the buoyant flow model. Although radial flow does lead to quantitative changes between the two models, the simple planar flow model does capture the key
features of buoyancy-driven combustion.

The gas velocity at the finger tip is plotted as a function of permeability in Figure 6.6. Data is plotted in both standard and logarithmic form. A linear line of best fit is calculated for the standard plot and is also included in the logarithmic plot. The linear line of best fit is found to be appropriate for gas velocities of approximately 1 and above. As discussed in Chapter 5, velocities of greater than approximately one correspond to advection-driven combustion, with velocities less than approximately one corresponding to diffusion-driven combustion.

![Buoyant Flow and Planar Flow Models](image1)

![Buoyant Flow and Planar Flow Models](image2)

Figure 6.7: Finger radius and propagation speed as predicted by the buoyant flow model are compared with the results predicted by the planar flow, non-constant density model using \( v = 0.58K' \)

In order to find an analytical approximation to the best fit lines presented in Figure
6.6, the equation for the vertical velocity component is considered,

\[ v = K' \left( -p_z + \frac{1 - \phi}{\phi_0} \right) = K' \left( -p_z + \frac{\gamma T}{1 + \gamma T} \right). \]  \hspace{1cm} (6.14)

Assuming the temperature at the finger tip is close to 1 and that the pressure gradient is small, this leads to approximations for the gas velocity at the finger tip as,

\[ v_{CO} = 0.58K' \text{ and } v_{CO_2} = 0.72K'. \]

This approximation requires a number of assumptions to be made and results in an error in the constant of approximately 20%. Despite this, the relationship does allow an estimate of the order of magnitude of the gas velocity at the finger tip to be found in terms of the solid permeability and the combustion kinetics.

The two models are compared for carbon monoxide producing combustion in Figure 6.7. Whilst the two models do not predict the same quantitative results, they do both predict the same key qualitative trends. Hence the planar flow model, used with equation (6.14), is sufficient to capture the key qualitative features of buoyant smouldering combustion.

### 6.2.1 The Constant Molecular Weight Assumption

Thus far it has been assumed that the molecular weight of the gas phase remains constant, taking the value of air. Now this assumption is dropped and a constant and non-constant molecular weight model are compared. The non-constant molecular weight model replaces the assumption \( W = W_A \) with the relation

\[ \frac{1}{W} = \frac{Y_P y_{P_C}}{W_P} + \frac{Y_X y_{X_C}}{W_X} + \frac{1 - Y_P y_{P_C} - Y_X y_{X_C}}{W_N}. \]  \hspace{1cm} (6.15)

Using this, along with the equations for the molecular weight of air \( (W_A) \), the gas product mass fraction \( (Y_P) \) and the characteristic product mass fraction \( (y_{P_C}) \) given by equations (3.27), (3.35) and (3.34) respectively, the molecular weight ratio can be written as,

\[ \frac{W_A}{W} = 1 + (1 - Y_X)\overline{W}, \]  \hspace{1cm} (6.16)

where

\[ \overline{W} = y_{X_C} \frac{W_A}{W_N} \left( \frac{\mu_P W_N}{\mu_X W_X} - \frac{W_N}{W_X} - \frac{\mu_C W_C}{\mu_X W_X} \right). \]  \hspace{1cm} (6.17)
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The sign of the term $\overline{W}$ depends on the chemical reaction assumed to occur. As the combustion product mass fraction is less than that of oxygen for carbon monoxide producing combustion, and greater than that of oxygen for carbon dioxide producing combustion, $\overline{W}$ takes a positive value (approximately 0.027) for the former and a negative value (approximately -0.08) for the latter.

In order to assess the impact of the constant molecular weight assumption, a parametric study of permeability is carried out for both the constant and non-constant molecular weight models. The study is performed for both carbon monoxide and carbon dioxide producing combustion, and the results are presented in Figures 6.8 and 6.9.

![Graphs showing the impact of constant vs. non-constant molecular weight models on permeability and finger radius.](image)

Figure 6.8: A constant and non-constant molecular weight model are compared over a range of permeabilities.

There is no qualitative impact to the results when the non-constant molecular weight assumption is made, and only a small quantitative impact. Figure 6.8 thus shows that the constant molecular weight assumption is sufficient to capture the key
qualitative features of both reactions. In addition to this, if the peat is sufficiently porous so that combustion is advection-driven, there is no significant quantitative difference between the results predicted by the two models.

Figure 6.9: Velocity fields for low permeability combustion (taken at \( \log|K'| = -3 \)) where combustion is diffusion driven. Both carbon monoxide and carbon dioxide producing combustion are shown, for both the constant and non-constant molecular weight models.

The velocity fields of the two reactions for both the constant and non-constant molecular weight models are shown in Figure 6.9. This again highlights how, whilst the results are quantitatively different when combustion is diffusion-driven, there is little qualitative impact of making the constant molecular weight assumption. It also shows that when combustion is diffusion-driven, gas is advected away from the reaction zone for all of the situations considered.
In order to investigate the velocity field further, the gas density equation is considered.

\[ \rho = \frac{W \phi}{W_0 \phi_0} \frac{1}{1 + \gamma T} \]  

(6.18)

It is assumed that the porosity remains constant so that \( \phi \equiv \phi_0 \). Given this, and using equations (6.16) and (6.17) the gas density can be written as a function of temperature and oxygen mass fraction.

\[ \rho (1 + (1 - Y_X)W)(1 + \gamma T) = 0 \]  

(6.19)

Taking the Lagrangian derivative of this gives,

\[ \dot{\rho} - \frac{Y_X W}{1 + (1 - Y_X)W} \frac{\gamma \dot{T}}{1 + \gamma T} = 0 \]  

(6.20)

where \( \dot{\rho} = \text{Le} \partial_t + \mathbf{u} \cdot \nabla \). The continuity, oxygen mass fraction and energy equations can also be rewritten so that

\[ \rho \nabla \cdot \mathbf{u} = \nu \Omega \]

(6.21)

\[ \rho Y_X = \nabla \cdot (\rho \nabla Y_X) - \Omega \]

\[ \rho_0 T_i + \frac{\delta \rho}{\text{Le}} T = \nabla \cdot \left( \left( \frac{\phi + (1 - \phi)v}{\phi_0 + (1 - \phi_0)v} \right) \nabla T \right) + \Omega \]

where it has been taken that the frame of reference is stationary, i.e. \( S = 0 \). Substituting these equations into equation (6.20) gives,

\[ \left[ \rho \nabla \cdot \mathbf{u} + \frac{W \nabla \cdot (\rho \nabla Y_X)}{1 + (1 - Y_X)W} \right] \delta \epsilon + \frac{\gamma \text{Le}}{(1 + \gamma T)} \left[ \rho_0 T_i \nabla \cdot \left( \frac{\phi + (1 - \phi)v}{\phi_0 + (1 - \phi_0)v} \nabla T \right) \right] \]

\[ = \left[ \nu + \frac{W}{1 + (1 - Y_X)W} \right] \delta \epsilon + \frac{\gamma \text{Le}}{(1 + \gamma T)} \Omega. \]

(6.22)

This shows that \( \nabla \cdot \mathbf{u} \) depends on (a) diffusion of \( Y_X \) (b) imbalances from the simple solid heat equation with reaction and (c) the chemical reaction. The reaction rate, \( \Omega \), is strong where \( Y_X \approx 0 \). Thus the terms

\[ \nu + \frac{W}{1 + W} \]

(6.23)

are important in the reaction zone. The value of (6.23) can take a positive or negative value depending on which chemical reaction is assumed to occur. Thus whilst the full picture involves a balance of many effects, the choice of chemical reaction can alter whether the terms given in (6.23) act as a source or a sink. The case in which molecular
weight is constant, with \( \bar{W} = 0 \) has already been simulated and shown to generate a source of volume (divergence of velocity) around the finger tip at low permeabilities for both the carbon monoxide and carbon dioxide producing reactions. However, in order to assess the effects of altering \( \bar{W} \) a parametric study is undertaken. Given that,

\[
\nu = y_X \frac{\mu_C W_C}{\mu_X W_X} \\
\text{and} \quad \bar{W} = y_X \frac{W_A}{W_N} \left( \frac{\mu_P W_N}{\mu_X W_X} - \frac{W_N}{W_X} - \frac{\mu_C W_C}{\mu_X W_X} \right) \tag{6.24}
\]

reducing \( \frac{\mu_C W_C}{\mu_X W_X} \) serves to reduce \( \nu \) but increase \( \bar{W} \). In addition to this, alteration of \( \nu \) would serve to alter the characteristic temperature and thus a number of length scales of the problem. Given that \( W_N, W_C \) and \( W_X \) are constants, to reduce the value of (6.23) the fraction \( \mu_P / \mu_X \) must be reduced. Considering the reaction

\[
2C + O_2 \rightarrow \mu_P W_P \tag{6.25}
\]

and setting \( W_P = (2W_C + W_X) / \mu_P \) a parametric study of \( \mu_P \) can be undertaken. Here \( \mu_P = 2 \) corresponds to a carbon monoxide producing reaction. Reducing this value corresponds to a reaction which produces fewer molecules, but molecules which have a higher density. This physically would represent a non-integer amount of molecules consisting of fractions of oxygen and carbon molecules. Although this is not physically possible it does demonstrate the effects of altering \( \bar{W} \). Reducing \( \mu_P \) will reduce \( \bar{W} \). Thus for for a sufficiently low value of \( \mu_P \) (6.23) will take a negative value.

The results of the parametric study are shown in Figure 6.10. As \( \mu_P \) decreases, \( \nu + \frac{\bar{W}}{1 + \bar{W}} \) decreases and becomes negative as expected. Thus this serves to act as a sink term in the reaction zone. However, the velocity at the finger tip decreases with \( \mu_P \). Thus other factors, such as diffusion of oxygen and imbalances for the simple heat equation can play a key role in determining the velocity field.

As there is no qualitative impact, and little quantitative impact, of assuming the gas molecular weight to be constant this assumption will be held for the remainder of this chapter. In addition to this, as the carbon monoxide and carbon dioxide producing reactions are analogous when presented in terms of the dimensionless permeability, henceforth the carbon monoxide reaction alone will be considered and results will be presented in terms of \( K' \).
6.3 The Effect of Porosity

A weakness of the model studied thus far is that it does not take into account that the burnt peat will be more porous and hence more permeable than fresh peat. When the peat is highly porous, a constant porosity model is likely to be sufficient. For a less porous peat, however, discrepancies may be found between the constant and non-constant porosity models. In Section 6.3.1 the impact of the constant porosity assumption is assessed over a range of permeabilities. Appropriate equations linking permeability and porosity are discussed in Section 6.3.2. Finally, Section 6.3.3 compares a non-constant permeability (and thus non-constant porosity) model with the simpler constant porosity model.

6.3.1 The Constant Porosity Assumption

It was previously assumed that the porosity remains constant, i.e. \( \phi \approx \phi_0 \), by taking into account that the porosity of unburnt peat is already very close to 1. Now this assumption is dropped and replaced by equation (6.8). The constant and non-constant...
porosity models are compared over a range of permeabilities in Figure 6.11. Including an equation for non-constant porosity leads to no significant qualitative change and only a small quantitative change to the predicted results.

\[ \phi = 1 - \rho_s (1 - \phi_0) \]

The non-constant porosity equation serves to increase the gas density in the burnt region as \( \rho = f(\phi/\phi_0) \). When the initial porosity is close to 1, \( \phi/\phi_0 \) must also be close to one and hence there is little impact of taking the porosity to be constant.

The constant porosity assumption not only needs to be tested over a range of permeabilities, it should also be tested over a range of initial porosities. As the porosity of the peat reduces the oxygen available in the soil reduces. Flow of the oxidiser would be aided in the burnt region where the peat is both more porous and more permeable. Hence in a dense peat changes to the permeability and porosity of burnt peat may be an important feature of combustion. However, at this stage performing a parametric study of the initial peat porosity would not capture how the permeability of the peat
6.3. THE EFFECT OF POROSITY

is affected by the porosity. Thus a relationship linking porosity and permeability must first be determined.

6.3.2 The Relationship Between Porosity and Permeability

The existence of a relationship between permeability and porosity is well known; as porosity increases permeability increases accordingly. Thus burnt peat is both more porous and more permeable than fresh peat. Many different equations linking porosity and permeability have been put forward but only the most commonly used, and most applicable to this study, will be discussed here. For a more full review of these equations see Dullien [127].

The equation most commonly used to define the relationship between porosity and permeability is the Kozeny-Carman equation. This equation considers flow through a porous medium by considering flow through non circular pipes or holes [127, 121]. The equation is given by,

\[ K = \frac{\phi^3}{C}\left(\rho_{\text{m}}S_A(1 - \phi)\right)^2 \]

where \( C \) is the Kozeny-Carman constant and \( S_A \) is the specific surface area per mass of solid. The equation gives satisfactory results for media that consist of spherical particles lying within a narrow range of diameters. For other cases the equation is often not valid, however it is still widely used as it appears to be the best simple expression available [128]. In practice the relationship is thought to apply to sandy soils but not to clay soils, and for hydraulic conductivities within the range of approximately \( 10^{-11} \) to \( 10^{-1} \) m/s [129].

Quinton et al investigated the applicability of the Kozeny-Carman equation to peat [117]. A reasonably good match was found between estimated and observed data. The Kozeny constant was, however, required to change by more than one order of magnitude to remain applicable for the upper surface of the peat where the soil was more porous. The weakness of the Kozeny-Carman equation at high porosities is due to the fact that the so called Kozeny constant is in fact not constant. Whilst for porosities between 0.55 and 0.86 it remains approximately constant with a value close to 5, for porosities above this it increases substantially as the porosity tends to one [130]. The weakness of this equation is thus especially prominent in highly porous media such as dry peat.
A number of equations approximating the dependence of the Kozeny constant on porosity have been put forward (see Mauret and Renaud [131]). One of the most commonly used is that by Ingmanson [132] cited in Mauret and Renaud [131].

\[
C = 3.5 \frac{\phi^3}{(1 - \phi)^{0.5}} (1 + 57(1 - \phi)^3)
\] (6.26)

Substituting this into the Kozeny-Carman equation leads to an equation for permeability which holds for the range of porosities found naturally within peat.

\[
K = \frac{1}{3.5(\rho_s S_A)^2(1 - \phi)^{3/2}(1 + 57(1 - \phi)^3)}
\] (6.27)

The weakness found in the Kozeny-Carman equation at high porosity is due to the fact that it is based on flow through tubes. At high porosities models based on flow around submerged objects are found to produce more accurate results. One such model has been put forward by Kyan et al [133]. When evaluated against the Kozeny-Carman equation for a highly porous fiberglass ($\phi \approx 0.97$) Kyan’s equation produced significantly more accurate results [121]. Whilst experimental results agreed with the value predicted by Kyan’s equation, the Kozeny-Carman equation used with Ingmanson’s equation produced values three times lower than experimental data. Although Kyan’s equation does lead to a more accurate estimation for permeability, for this study it has a major drawback. The equation contains a number of constants which need to be determined experimentally. As no experimental results have been published giving these figures for peat, and experimental work is beyond the scope of this study, Kyan’s equation is not a feasible choice here.

The final model that is worth noting is Brinkman’s equation [127]. Like Kyan’s equation, Brinkman’s equation is also based on flow around submerged objects.

\[
K = \frac{D_p^2}{72} \left( 3 + \frac{4}{1 - \phi} - 3 \left( \frac{8}{1 - \phi} - 3 \right)^{1/2} \right)
\]

As this equation predicts the permeability to be zero when the porosity is 0.3, it is not appropriate for materials with low porosity. Hence whilst the equation is appropriate for a highly porous dry peat, it may not be appropriate if a moist peat were to be considered. This equation only requires a characteristic particle or fiber diameter, $D_p$. Thus, unlike Kyan’s model experiments are not required to use this model as such data already exists in literature. Plotting the modified Kozeny-Carman equation
against Brinkman’s equation shows both equations lead to qualitatively the same results (Figure 6.12). In fact both equations produce quantitatively comparable results if the relation

\[
D_p = \frac{6}{\rho_s S_A}
\]  

(6.28)
is satisfied [127]. Whilst Kyan’s model predicts permeabilities which are qualitatively the same as experimental results, both the Kozeny-Carman equation and Brinkman’s equation correctly predict all the key qualitative features of the relationship. For this study it is taken that both equations would be sufficient in capturing the relationship between porosity and permeability to a suitable degree of accuracy. The Kozeny-Carman equation will be used here simply for the reason that it is the most commonly used.

The Kozeny-Carman equation requires knowledge of the geometry of the porous medium in question. A value for either the specific surface or a value for the particle diameter (used in conjunction with equation (6.28)) is required in order to use the equation. The specific surface can be calculated using geometrical properties of the medium or found experimentally, although the method used to calculate the specific area of peat needs to be chosen with care. Using microscopic analysis to determine the specific surface leads to values of approximately 50 m²/kg [134]. Using nitrogen isotherms, however, leads to values of approximately 1000 m²/kg with carbon dioxide isotherms leading to values 100 times larger [135, 136, 137]. The differences in these

**Figure 6.12:** Brinkman’s equation and the Kozeny-Carman equation relating permeability and porosity are compared. For illustration \(\rho_s = 1000 \text{ Kg/m}^3\), \(S_A = 10 \text{ m}^2/\text{Kg}\) and \(D_p = 0.0006 \text{ m}\) are used.
values do not show that one method is superior to the other, they are simply measuring the surface area of the peat accessible to different molecules.

The range of particle diameters found in peat is significantly lower than the range over which specific surface values lie. Most studies find the value to lie within the range $1.5 \times 10^{-4}$ to $10^{-3}$ m [138, 139]. Using these values with equation (6.28) predicts a lower range of values for the specific surface than those found experimentally, approximately 6 to 40 m$^2$/Kg.

Figure 6.13: The Kozeny-Carman equation, modified with Ingmanson’s equation, is used with specific surface values of 50 m$^2$/Kg (dotted line) and 1000 m$^2$/Kg (dashed line). The lines are superimposed over a plot comparing the relationship between the porosity and permeability of known soils, produced by Lauren et al [124].

The modified Kozeny-Carman equation given in equation (6.27) is plotted against known soils in Figure 6.13. This is done for specific surfaces of 50 and 1000 m$^2$/Kg in order to confirm the appropriate range of values. Many, if not all, soils contained liquid water. Thus air-filled porosity values are lower than the range found in dry peat. The higher of the two specific surface values corresponds well with compacted peat, with the lower displaying a closer correlation to pine hummus. The latter also agrees with experiments by Unno [111], which found permeabilities of order $10^{-9}$ m$^2$. 
in peat when $\phi = 0.8$. The values of peat permeability found by McAfee can also be seen to lie in the middle of this range.

### 6.3.3 Non-Constant Permeability Model

The constant porosity model will now be compared to a non-constant permeability model (including equations (6.6) and (6.27)). As discussed in the previous section, appropriate values for the specific surface of peat cover a large range of values. A parametric study of the specific surface of peat is thus initially carried out. However, permeability is also dependent on the initial porosity of the peat, $\phi_0$. Thus a parametric study of the initial porosity is also performed for a fixed specific surface.

#### Specific Surface and Permeability

A parametric study of the specific surface is performed with $\phi_0 = 0.9$. The maximum permeability in the burnt zone and the permeability in the fresh fuel zone are plotted in Figure 6.14. Results are presented in terms of the dimensionless permeability in the unburnt zone $K'_\infty$. Although the parametric study was undertaken for the specific surface, presenting the results in terms of permeability aids comparisons with other sections of this chapter. The plot highlights the degree to which the permeability of the burnt peat varies between the constant porosity model and the non-constant permeability model. Although there is little change in permeability between the burnt and unburnt regions for the mid range of values studied, a more significant difference is found at the upper and lower specific surface limits, where the burnt peat density is lower (results are analogous to those presented in Figure 5.21).

The range of permeabilities presented in Figure 6.14 corresponds to a range of specific surfaces of approximately 250 to 25,000 m$^2$/Kg. These values are towards the upper end of values discussed in the previous section. However, for carbon dioxide producing combustion these results would be expected to correspond to an approximate range of 1.5 to 750 m$^2$/Kg. These are towards the lower end of values found experimentally. Again this finding suggests that the two forms of reaction may act as bounds in terms of how a simple one-step reaction corresponds to peat combustion.

The non-constant permeability model predicts that a multivalued solution exists in highly permeable peat. This is investigated further by identifying the relationship
between the unburnt permeability and both the finger radius and the propagation speed. Results are plotted in Figure 6.15, where the non-constant permeability model is compared to the constant porosity model.

For the mid-range permeabilities, where there is little difference between the permeability in the burnt and unburnt zone, there is no significant difference between the results predicted by the two models. At low permeabilities, when combustion is diffusion-driven, the inclusion of the non constant permeability equation also has little impact. At high permeabilities, however, a more notable discrepancy between the two models is found. The non-constant permeability model predicts combustion to extinguish before the low-fuel limit is reached, unlike the results predicted by the constant porosity model. A similar transition from a single-valued to a multivalued solution was found by Schult et al [103], who considered uniformly propagating planar smoulder waves. The study found that altering the kinetic function describing the dependence of the reaction rate on the concentration of unburnt solid could induce a multivalued solution. When the reaction rate equation took the form $\Omega = f(\rho_s)$ a single valued solution was found, whilst a reaction rate of the form $\Omega = f(\rho_s)^{3/2}$ led to a multivalued solution. The study attributed extinction before the low-fuel limit was reached to the combustion front having difficulty consuming all available oxygen. As
6.3. THE EFFECT OF POROSITY

Figure 6.15: A constant porosity model is compared to a non-constant porosity, non-constant permeability model over a range of permeabilities.

As a result, the propagation rate slowed slightly before reaching the turning point.

For a highly porous peat, there is no significant implication of making a constant porosity assumption so long as combustion is not near the high permeability (and hence the high gas velocity) limit. However, this may not necessarily be the case for a less porous peat where the differences between the burnt and unburnt porosity and permeability may be more pronounced. Thus the same parametric study is performed for $\phi_0 = 0.7$. This change of initial porosity alters the length scales of the problem which should be taken into account when the results for the two initial porosities are compared; dimensionless unburnt permeabilities do not correspond to the same specific surface values for differing initial porosities.

The maximum permeability in the burnt zone is plotted against the unburnt permeability in Figure 6.16. Whilst both initial porosities of 0.9 and 0.7 produce the same qualitative trends, the latter predicts a greater difference between unburnt and burnt permeabilities for the full range of values studied. In order to assess how this
Figure 6.16: The maximum permeability in the burnt zone is plotted against the unburnt permeability for both $\phi_0 = 0.9$ and $\phi_0 = 0.7$. A dashed line is included, plotting unburnt permeability against itself, in order to compare the burnt and unburnt permeabilities with greater ease.

The results when the initial porosity is 0.7 are qualitatively the same as those found when the initial porosity is 0.9. However, a higher level of discrepancy between the constant porosity model and the non-constant permeability is found when the unburnt peat permeability is high. A comparison of the velocity fields for both models at $\phi = 0.7$, $\log |K'_\infty| = 1$ is shown in Figure 6.18. When a non-constant permeability equation is considered, the burnt peat is more permeable aiding flow through this region. This aids vertical flow through the finger. When combustion is advection-driven this results in an increased gas velocity at the finger tip. The increased gas velocity again serves to reduce the finger radius and increase the propagation speed.

The constant porosity model predicts more quantitatively accurate results in a highly porous peat. However, aside from the upper extinction limit, it is also sufficient to capture the key qualitative features of the combustion profile for a peat with a low porosity. In addition to this, the most significant quantitative differences are found near the high permeability (and thus high gas velocity) limit. For low and mid-range values the quantitative difference between the two models is less pronounced.
6.3. THE EFFECT OF POROSITY

Figure 6.17: A constant porosity model is compared to a non-constant porosity, non-constant permeability model over a range of permeabilities for $\phi_0 = 0.7$.

Initial Porosity and Permeability

Much like the parametric study of the Lewis number undertaken in Section 5.5, when the initial porosity of peat is varied various length scales and values appearing within the dimensionless equations are found to change accordingly. The characteristic peat bulk density and the characteristic gas bulk density are dependent on porosity and vary as the initial porosity is changed. This is important to note because although these values do not appear explicitly in the model, they do appear implicitly inside the constants $\text{Le}$, $\delta$, $\alpha$, $\beta$ and $K'$. In addition to these values, characteristic scales also vary as a number of these implicitly depend on initial bulk densities of the fuel. Whilst both $\alpha$ and $\beta$ vary with $\phi_0$, both values are found to be constant to leading order for $0.7 \leq \phi_0 \leq 0.97$. Thus the assumption that both values take the constant values given
Figure 6.18: Comparison of the velocity fields at $\phi_0 = 0.7$, $\log|K'_\infty| = 1$ for the constant porosity and non-constant permeability models. The magnitude and direction of the gas flow is given by the surface plot and the arrow plot respectively. The finger radius is given by a contour plot of $\rho_n = 0.99$

in Appendix A is held for this study.

A value of $\phi = 0.9$ has been used to this point, however, experiments have shown the value to range between approximately 0.73 and 0.97 [140, 12]. The assumption that $\phi \approx \phi_0$ is based on the fact that both values are close to 1. Thus as the initial porosity decreases a higher level of discrepancy between the constant and non-constant porosity models may be found.

A parametric study of $0.7 \leq \phi_0 \leq 0.97$ is undertaken. The profiles of the finger radius and propagation speed with initial porosity are presented in Figure 6.19. Results are standardised by dividing values by the characteristic length and propagation rate at $\phi_0 = 0.9$; thus results are dimensionless. For the full range of porosities found to naturally occur within dry peat the results suggest there is no significant implication of making the constant porosity assumption. However, the non-constant permeability model again captures the turning point which is not predicted by the simpler constant porosity model. This turning point is found at approximately $\phi_0 = 0.955$, although the lower branch is not followed for practical reasons.
The parametric study used a specific surface value of 500 m$^2$/Kg, which corresponds to a dimensionless permeability of $\log|K'_\infty| \approx 1.1$ at a porosity of 0.9. This corresponds to advection-driven combustion where there is little difference between the fresh peat porosity and the burnt peat porosity. When a larger fraction of the fuel is consumed, however, the constant porosity assumption may no longer be valid and discrepancies may arise when the two models are compared. Thus a parametric study of the initial porosity is also undertaken for diffusion-driven combustion where approximately half of the fuel is consumed by the reaction. A specific surface of $10^{3.8}$ m$^2$/Kg was used, corresponding to a fresh peat permeability of $\log|K'_\infty| \approx -1$ at a porosity of 0.9.

The results of the parametric study of the initial porosity for diffusion-driven combustion are shown in Figure 6.20. There is no significant impact on the predicted propagation rate or finger radius when the constant porosity assumption is made. Although the results of the models are quantitatively different, both models predict the same qualitative trends over the range of initial porosities studied.

Figure 6.19: Finger radius and propagation rate with initial porosity; advection-driven combustion.
6.4 Conclusions

Fingering combustion sustained by buoyant oxidiser flow has been investigated. The results are found to be analogous to the planar flow problem considered in the previous chapter, with permeability taking the place of an imposed velocity; an increase in permeability acts to increase the gas velocity at the tip of the finger. In fact a near linear relationship exists between the solid permeability and the gas velocity at the tip of the finger. Thus this relationship can be used with the simple planar flow model to predict the combustion profile for a given solid permeability.

Combustion is dependent on the dimensionless permeability,

\[ K' = \frac{K \rho_c g \beta}{\mu D_c} \sqrt{\frac{\nu D_c}{\bar{\rho}_c \bar{u}_c}} \exp \left( \frac{T_A}{T_0 + T_c} \right) \]

which is highly dependent on the kinetics of combustion. As these values are not well
determined, using different approximations for kinetic constants can lead to a significantly different range of dimensional permeabilities over which fingering combustion is expected to occur. However, the model predicts that for a range of dimensionless permeabilities combustion can be sustained. For permeabilities above a critical dimensionless permeability, which is likely to lie between $10^{1.5}$ and $10^2$, the results suggest that an over-blowing limit may be attained (Figure 6.16). For dimensionless permeabilities below approximately $10^{-1}$ combustion is diffusion-driven and combustion sheet temperatures may be insufficient for sustained combustion. The fingering regime is thus likely to be found between these two limits. For a certain range of dimensional permeabilities both the carbon monoxide and the carbon dioxide producing reactions are predicted to lie within this range.

Equations for permeability, porosity and gas molecular weight have been investigated, to identify the impact of setting each of these variables as a constant. The non-constant permeability model predicts that combustion is extinguished before reaching the low-fuel limit, capturing a feature of combustion known to occur in filtration combustion. However, whether fingering combustion behaves in the same manner is not clear due to a lack of experimental evidence. Aside from this there are no qualitative differences between the trends predicted by the simple model where porosity and molecular weight are assumed constant and their more complex counterparts. In addition to this, quantitative differences between the models are small and are only of a significant magnitude when the porosity of the peat is low.
Chapter 7

Conclusions

A one-step, global temperature model for the combustion of dry peat has been presented. Low Lewis number instabilities result in the fragmentation of a planar combustion front, leading to fingering combustion. Previous studies have found that when an experiment is set up in such a way as to force a single finger, this single finger possesses the same characteristics as those fingers found in the multi-finger system. Thus a single finger can reasonably be studied independently of any other finger. This simplifies the problem significantly, but this formation does not account for the distance between neighbouring fingers and hence does not distinguish between sparse fingering, fingering with tip-splitting or planar combustion. However, given the correct ignition mechanism and imposed gas velocity (or ignition mechanism and dimensionless permeability for buoyant combustion) it may be possible to ignite a single travelling finger. In addition to this, an equation estimating the distance between two neighbouring fingers has been derived. This equation captures a number of the qualitative features of the relationship between finger spacing and imposed gas velocity found experimentally in the fingering combustion of paper.

When reduced to its simplest form, and studied in the low fuel consumption limit, spherically symmetrical peat combustion is found to be analogous to a flame ball. However, smouldering combustion can not be stationary as only a finite quantity of solid fuel is available in a given location. Theoretical solutions to stationary spherically symmetrical combustion have been compared to numerical solutions of self-travelling combustion. Whilst the analytical solution does not capture the asymmetry of the solution which arises due to its propagating nature, it does still capture some of the
key features of the self-travelling problem.

Numerical solutions to adiabatic propagating combustion have been compared to analytical solutions. As adiabatic combustion temperatures are significantly lower than the superadiabatic temperatures found in flame balls and fingering combustion, combustion of this form is only likely to be observed in the low solid density limit. Analytical and spherically symmetrical numerical solutions show a good level of agreement in terms of oxygen and temperature profiles, propagation speed and burnt fuel density. However, two-dimensional instabilities arise when the equations are solved numerically in cylindrical symmetry. Rather than a smooth combustion front being found, the front fragments and results in a fingering regime. Superadiabatic temperatures are attained and as a result of this the burnt peat density is lower than that predicted analytically.

A single finger, propagating against an imposed oxidiser flow, was studied in cylindrical symmetry as a travelling wave problem. The effects of heat losses, gas velocity and Lewis number were identified. The propagation speed depends on the availability of reactants in the combustion zone, and the finger radius is dependent on heat losses. An artificially imposed heat loss term, $F$, is found to alter the characteristics of the combustion profile in a manner which is analogous to a flame ball. A multi-valued solution is found. Whilst only the upper branch is stable in flame balls, both branches are stable in the cylindrically symmetrical solid formulation. In addition to this, results on the upper branch agree with fingering combustion experiments suggesting increased heat losses lead to fingers of a smaller radius. Despite the simplified equations studied, results found when performing a parametric study of the imposed gas velocity for a non-constant density model show a good level of agreement with planar combustion experiments.

When the gaseous velocity field is determined by Darcy’s law the dimensionless permeability is found to be a key feature of the model.

\[ K' = \frac{g \beta K}{\mu D_c} \sqrt{\frac{\nu D_c}{\rho_y y_c}} \exp \left( \frac{T_A}{T_0 + T_c} \right) \]

The dimensionless permeability is highly dependent on the solid permeability and the combustion kinetics (which determine the value of $\exp \left( \frac{T_A}{T_0 + T_c} \right)$), as varying these
parameters within the range in which peat soils lie can alter the dimensionless permeability by several orders of magnitude. The results suggest that buoyant fingering combustion can arise naturally. However, given the varied nature of peats of different ages and locations an exact range of parameters over which fingering occurs can not be provided.

Constant porosity, permeability and molecular weight assumptions have been tested. There is no significant impact on the predicted results when molecular weight is assumed to be constant. Inclusion of a non-constant porosity equation also leads to only a small impact on the predicted results. However, when an equation relating porosity and permeability is included with the non-constant porosity equation a high permeability (and thus high gas velocity) extinction limit is found before all fuel is consumed. This captures a feature of smouldering combustion which has experimentally been determined in filtration combustion. The results indicate that the “over-blowing” extinction limit is reached at a dimensionless permeability between approximately $10^{1.5}$ and $10^2$, but varies depending on the chosen parameters. In addition to this, it may be possible that fingering is suppressed at high permeabilities as the distance between neighbouring fingers tends to 0. If combustion temperatures are insufficient when combustion is diffusion-driven, there would also be a lower limit on the dimensionless permeability. Thus this parameter is a key feature of buoyant smouldering combustion.

Increasing the permeability serves to increase the gas velocity at the finger tip. An approximately linear relationship between permeability and the velocity at the finger tip has been found, which is dependent on the kinetics of combustion. Whilst this approximation is based on a number of simplifications, it does provide a good estimate of the order of magnitude of the gas velocity. Thus the simple imposed oxidiser flow model presented in Chapter 5 can be used with this approximate relationship to capture the key features (aside from the over-blowing extinction limit) of buoyancy-driven combustion which were found in Chapter 6.

The results presented in this thesis show a good level of agreement with experimental results of both fingering combustion of a thin fuel and of filtration combustion of polyurethane foam. In addition to this, key trends predicted to occur in flame balls are also identified. However, no detailed experiments have been conducted into fingering combustion in a block of porous fuel. Thus when discrepancies do arise between
predicted and experimental results (such as in the high gas velocity limit) it is unclear whether it is the model, or the experiments which are correctly predicting the fingering behaviour. Thus more detailed experiments investigating this phenomenon in peat are required.

It is also worth considering the implications of the results in terms of the physical problem. As discussed in Chapter 2, low Lewis number curvature increases the robustness of the combustion zone allowing combustion to be sustained at heat losses which would extinguish a planar front. When peat fires occur in the wild they will often occur in the presence of water. Thus curvature would aid propagation, despite heat losses to mechanisms such as pyrolysis and evaporation. As combustion would only be occurring in a small region, heat generation would be minimal and only a small amount of gas combustion products (and smoke) would be produced. In fact as additional heat losses serve to decrease the finger radius, increased heat losses could make combustion even more difficult to detect. Thus it is perhaps this low Lewis number curvature which plays a key role in causing some peat fires to be so difficult to detect and extinguish.

There are a number of natural extensions to the work presented in this thesis. The model presented here aimed to capture the key qualitative features of the fingering phenomenon. A higher level of quantitative accuracy could be found by considering further chemical reactions, such as the full scheme presented at the start of Chapter 3. However, such a model would still be limited by the lack of experimental data with which to compare results. In addition to this water could be included in the equations. In naturally occurring wildfires peat is unlikely to be completely dry and the interaction between the combustion region and adsorbed water could play an important role in determining the combustion characteristics.
Appendix A

Constant Values

The characteristics of peat can vary significantly depending on its age and degree of decomposition. Hence rather than using exact values for the characteristics of peat, approximate orders of magnitude are given below. Values for both a carbon monoxide producing reaction and a carbon dioxide producing reaction are included. Unless stated otherwise, values for the carbon monoxide producing reaction are used.

- \( \alpha \) 0.9
- \( \beta \) 10
- \( c_g \) 1005 [J/KgK] Air at 20°C [141]
- \( c_s \) 1000 [J/KgK]
- \( D_c \) \( 2 \times 10^{-5} \) [m²/s] Oxygen in air at 38°C [142]
- \( \lambda_g \) 0.026 [W/mK] Air at 20°C [141]
- \( \lambda_s \) 0.1 [W/mK]
- \( \rho_{\text{atm}} \) 1000 [Kg/m³] Can vary significantly [8, 143, 144]
- \( \rho_{\text{ac}} \) 100 [Kg/m³] Can vary significantly [145, 8]
- \( \varrho_{\text{in}} \) 1.2 [Kg/m³] Air at 25°C [141, 140]
- \( \varrho_{\text{c}} \) 1.1 [Kg/m³] Air at 25°C assuming \( \phi \approx 0.9 \) [141, 140]
- \( y_{\text{Xc}} \) 0.21 Approximately 21% oxygen in air [146]
- \( \phi_0 \) 0.9 Varies between 0.73 and 0.97 [140, 12]
- \( \bar{\mu} \) \( 2 \times 10^{-5} \) [Kg/ms] Dynamic viscosity of air at 300K [147]
- \( \mu_{\text{XW}} \) (CO) 32 \( 2\text{C}+\text{O}_2 \rightarrow 2\text{CO} \)
- \( \mu_{\text{C}} \) (CO) 24 \( 2\text{C}+\text{O}_2 \rightarrow 2\text{CO} \)
- \( \mu_{\text{r}} \) (CO) 56 \( 2\text{C}+\text{O}_2 \rightarrow 2\text{CO} \)
Approximate Non-Dimensional Constant Values

\[ \delta = \frac{\rho_c}{\rho_{sc} c_s} \approx 0.01 \]
\[ \epsilon = \frac{c_s}{\lambda_s} \approx 1 \]
\[ \nu = \frac{\lambda_s}{\lambda_g} \approx 3.9 \]
\[ \text{Le} = 0.05^2 \]
\[ \nu_{CO} = y_N \frac{\mu_c W_c(CO)}{\mu_x W_x(CO)} \approx \frac{1}{6} \]
\[ \nu_{CO_2} = y_N \frac{\mu_c W_c(CO_2)}{\mu_x W_x(CO_2)} \approx \frac{1}{12} \]

\[ A(CO) = 4.44 \times 10^7 \text{ [s}^{-1}] \quad 2C+O_2 \rightarrow 2CO \quad [148] \]
\[ T_A (CO) = 21530 \text{ [K]} \quad 2C+O_2 \rightarrow 2CO \quad [148] \]
\[ Q (CO) = 9.6 \times 10^6 \text{ [J/Kg]} \quad 2C+O_2 \rightarrow 2CO \quad [148] \]
\[ \mu_x W_x (CO_2) = 32 \quad C+O_2 \rightarrow CO_2 \]
\[ \mu_c W_c (CO_2) = 12 \quad C+O_2 \rightarrow CO_2 \]
\[ \mu_p W_p (CO_2) = 44 \quad C+O_2 \rightarrow CO_2 \]
\[ A (CO_2) = 1.1 \times 10^4 \text{ [s}^{-1}] \quad C+O_2 \rightarrow CO_2 \quad [148] \]
\[ T_A (CO_2) = 8900 \text{ [K]} \quad C+O_2 \rightarrow CO_2 \quad [148] \]
\[ Q (CO_2) = 3.3 \times 10^7 \text{ [J/Kg]} \quad C+O_2 \rightarrow CO_2 \quad [148] \]

---

\(^1\) Little data exists on the intrinsic thermal characteristics of peat as most studies focus on bulk properties. Here values are assumed to be comparable to that of wood. The specific heat capacity of dry wood and wood char at 300K are 1300 J/KgK and 715 J/KgK respectively [149]. The specific heat capacity of dry peat at 300K is a comparable value to this, 951 J/KgK at 300K [57]. In this study an approximate order of magnitude of 1000 J/KgK is used. The thermal conductivity of softwoods and hardwoods are approximately 0.12 and 0.16 W/mK respectively [150]. Due to the high porosity of peat and the low thermal conductivity of air the bulk thermal conductivity of dry peat is lower than these values, approximately 0.04-0.07 W/mK [14, 151]. Here it is taken that an approximate order of magnitude for the intrinsic thermal conductivity of peat can be taken as 0.1 W/mK.

\(^2\) Using the values presented here the Lewis number, \((\phi_0 \lambda_g + (1-\phi_0) \lambda_c)/(\rho_c c_s D_c)\), is approximately 0.017. Using this value in chapters 5 and 6 results in combustion close to the low-fuel extinction limit. Hence a higher value of 0.05 is used throughout this thesis to move the solution away from this limit. This is discussed further in Section 5.5.
Appendix B

Ember Storm Model

A form of fire spread that has been referred to as an “ember storm” is examined. This work is based on the model derived by Sanders [152] and has been presented at the 19th International Congress on Modelling and Simulation [153]. In an ember storm, rather than the transport of heat and oxygen, the dominant mechanism determining the spread-rate of the fire is the lofting and landing of embers. Assuming that individual spotfires grow in an elliptical manner under the influence of the wind, the processes determining the spread of the fire can be assembled into an averaged continuum model. When an ember storm is spreading at a steady speed, its spread rate is found to be described by a single similarity solution.

Nomenclature

- $E$: lofted burning embers per unit area
- $b$: sum of all $n$ fire areas per unit area (without deducting overlaps)
- $B$: proportion of area actually burnt
- $f$: sum of all $n$ fire perimeters per unit area (without deducting overlaps)
- $F$: actual fire perimeter per unit area
- $n$: potential ignitions per unit area
- $R_h$: head-fire spread-rate
- $R_f$: flank-fire spread-rate
- $R_b$: backing-fire spread-rate
- $R_e$: overall spread rate of the ember storm
B.1. INTRODUCTION

Embers are relatively small pieces of burning or glowing debris. A large number of embers can be generated during wildfires. In the right conditions these embers can be lofted into the air and carried large distances by the wind, a process known as spotting [6]. In the absence of spotting a strong wind can produce a continuous, elliptical, fire perimeter [154, 155]. When spotting occurs, however, lofted embers are carried downwind and have the potential to cause discontinuous advances of the fire if they land and ignite fresh vegetation [156, 157]. New fires would also grow in an elliptical manner and would, in turn, generate more embers.

Under the correct conditions spotting can be the primary mechanism by which the fire progresses. This form of fire has been referred to as an “ember storm” [158]. As spotting is the main mechanism determining the progression of an ember storm, the transport mechanisms of oxygen and heat only play a small role in governing how the combustion front spreads. The effective average spread rate of the fire is instead
determined by factors such as the ember production rate, the extinction rate of embers in the air and the probability that a landing ember will ignite a new spotfire.

## B.2 Elliptical Fire Growth

Before considering the spread of an ember storm it is first necessary to consider the growth of a single spotfire. When considering an individual fire, started at a point and burning under a strong wind, it can be assumed that the fire front would take the shape of an ellipse [155]. The semi-major axis of the ellipse points in the direction of the wind, as shown in Figure B.1.

![Figure B.1: On the left is a sketch of an elliptical fire with head-fire spread-rate $R_h$, backing-fire spread-rate $R_b$ and flank-fire spread-rate $R_f$. The fire is ignited at the yellow dot. The red arrow marks the movement of the centroid (at speed $c$) during the time that the front of the fire sweeps through the orange area. On the right the increase in burnt area per unit length of fire perimeter ($s$) and the rate of increase in fire perimeter with time ($S$) are plotted against aspect ratio $r$. When the aspect ratio is 1, fires grow as circles with $S = s$ and $c = 0$.](image)

Considering the geometry of an ellipse, the equations for the semi-major axis, semi-minor axis and the centroid speed at time $t$ after ignition are given by

- semi-major axis: $\frac{1}{2}(R_h + R_b)t$
- semi-minor axis: $R_f t$
- centroid speed: $\frac{1}{2}(R_h - R_b) = c$.

In addition to this, taking that aspect ratio of the ellipse is $r = 2R_f/(R_h + R_b)$, equations
for the perimeter and area of the fire at time $t$ after ignition are given by

\[
\text{perimeter : } 2\pi St = 2t(R_h + R_b) \int_0^{\pi/2} \sqrt{1 - (1 - r^2) \cos \theta} \, d\theta
\]

\[
\text{area : } \pi St^2 = \pi t^2 \frac{1}{2} (R_h + R_b) R_f.
\]

Here $S$ is the mean spread-rate of the fire perimeter and $s$ is the mean spread-rate of the fire area. For a circular fire $S = s$ as shown in Figure B.1. Dividing the equations presented in (B.1) by time reveals formulae for $S$ and $s$ which depend only on the head, flank and backing spread-rates of the fire. Using an approximation for the integral in (B.1) reveals the equations for the perimeter and area spread rates.

\[
S = \frac{1}{4} (R_h + R_b) (3(1 + r) - \sqrt{(3 + r)(1 + 3r)}) (1 + \frac{1}{216} e^{-16r}) \pm \frac{1}{100} \%
\]

\[
s = \frac{1}{2} (R_h + R_b) R_f / S
\]

Although an ellipse is considered here, the profile of a fire burning under the presence of wind has also been likened to teardrops, ovoids and double ellipses [155]. Spotfires which do not grow as an ellipse, but as another self-similar shape, could be treated in a similar manner to that presented here. Whilst the equations for other geometry would not be quantitatively the same, they would share the same qualitative features to the equations derived here.

### B.3 Ember Storm Model

A continuum model is considered so that, rather than following the path of individual embers, the expected number of spotfires, $n$, per unit area is considered. In addition to this the number of lofted embers, the burnt area and the fire perimeter per unit area are also considered. A sketch of an ember storm is shown in Figure B.2. For convenience, fires which would have ignited a fire had they not landed on a burnt area (virtual ignitions) are also considered. In addition to this, overlap of two neighbouring spotfires is not deducted when considering the total burnt zone, $b$, or the total fire perimeter, $f$. However these values are later related to the actual burnt area and actual fire perimeter, $B$ and $F$, in a simple way, as will be seen.

As overlaps in perimeter and area are initially ignored, using equations (B.1), their growth rates can be given by

\[
f_t + cf_x = 2\pi Sn \quad b_t + cb_x = sf.
\]

(B.3)
The perimeter grows in sole proportion to the number of fires $n$ and the area grows in sole proportion to the perimeter $f$, for constant values of $S$ and $s$. The term $c\partial_x$ is needed to account for the movement of the centre of each elliptical spotfire.

![Figure B.2: Elliptical fires of equal aspect ratio and orientation, distributed randomly. Yellow dots represent $n$ ignitions (and virtual ignitions) per unit area. Orange areas mark out the vegetation that is actually burnt over a short time interval during which the arrows mark the movement of each centroid.](image)

The lofted burning ember density per unit ground area is denoted $E$. Embers are taken to land at the rate $\eta$ with $\kappa$ probability of igniting a new spotfire. Thus the rate at which new spotfires (including virtual spotfires) form is

$$n_t + cn_x = \kappa \eta E.$$  \hspace{1cm} (B.4)

The characteristic spotfire ignition time per lofted ember, $t_i$, is thus given by $1/\kappa \eta$.

It is assumed that embers are produced by the active fireline. Thus the rate at which embers are produced must take into account the actual fireline perimeter, $F$, rather than the total fire perimeter including overlaps, $f$. The rate at which vegetation is actually burnt per unit area is $sF$. If $\varepsilon$ embers are produced per unit area burnt, the rate embers are produced per unit area is thus $\varepsilon sF$. Taking into account that the embers are transported at an effective wind speed, $w$, the evolution of burning embers can be expressed by the equation

$$E_t + wE_x = \varepsilon sF - (\eta + \zeta)E = \varepsilon sF - E/t_e.$$  \hspace{1cm} (B.5)
Here \( \zeta \) represents the rate at which lofted embers are extinguished. The rate at which embers are lost is thus \( \eta + \zeta \) and its reciprocal, \( t_e = 1/(\eta + \zeta) \), is the mean lifetime of burning embers.

Finally, an assumption needs to be made to link \( f \) and \( F \). In addition to this, the actual burnt zone, \( B \), is linked to the total burnt zone including overlaps, \( b \). It is assumed that the proportion of fuel burnt changes slowly with distance, on a length scale which is large when compared to the average size of a spotfire. This assumption is valid for an ember storm where many spotfires are formed and embers are transported a distance which is significantly larger than the size of the average spotfire. If the total burnt area including overlaps, \( b \), is increased by a small amount, \( db \), the probability of increasing the actual burnt area \( B \) is proportional to the area that remains unburnt, \( 1 - B \). The increase in \( B \) is thus

\[
\text{d}B = (1 - B)\text{d}b \quad \text{so that} \quad 1 - B = e^{-b}.
\]

In a similar manner, the probability that a part of the total perimeter, \( f \) is not in a burnt area is also \( 1 - B \). It thus follows that

\[
F = (1 - B)f = e^{-b}f.
\]

The full set of equations can now be written in terms of \( B, E, F \) and \( n \). The frame of reference is set such that it moves with the ember storm at speed \( R_e \), the mean spread rate of the storm. This gives the equations,

\[
n_t - (R_e - c)n_x = \kappa \zeta E \tag{B.8}
\]

\[
F_t - (R_e - c)F_x = 2\pi S n(1 - B) - s F^2/(1 - B) \tag{B.9}
\]

\[
B_t - (R_e - c)B_x = s F \tag{B.10}
\]

\[
E_t + (w - R_e)E_x = \varepsilon s F - (\eta + \zeta)E. \tag{B.11}
\]

An ember storm travelling to the right would also require the boundary conditions

\[
\lim_{x \to \infty} (E, F, n, B) = (0, 0, 0, 0) \quad \text{and} \quad \lim_{x \to -\infty} (E, F, n_x, B) = (0, 0, 0, 1).
\]

**Analysis of the Model**

The model is first non-dimensionalised by making the following definitions,

\[
n = n_n n', \quad F = F_s F', \quad E = E_s E', \quad x = x_n x', \quad t = t_s t'. \tag{B.12}
\]
The proportion of fuel actually burnt, \( B \), is not nondimensionalised because this quantity is already dimensionless. By setting,
\[
\eta_s = \frac{\kappa \zeta \varepsilon}{\eta + \zeta}, \quad F_s = \frac{1}{st_s}, \quad E_s = \frac{\varepsilon}{\eta + \zeta}t_s, \quad x_s = (R_e - c)t_s, \quad t_s = \left( \frac{\eta + \zeta}{\pi_S S \kappa \zeta \varepsilon} \right)^{1/2}
\]
and defining,
\[
\lambda = \frac{w - R_e}{R_e - c}r, \quad \tau = \frac{1}{(\eta + \zeta)t_s},
\]
the dimensionless model is obtained.

\[
\begin{align*}
n_{t'} - n_{x'} & = E' \\
F_{t'} - F_{x'} & = 2(1 - B)n' - F'^2/(1 - B) \\
B_{t'} - B_{x'} & = F' \\
\tau E_{t'} + \lambda E_{x'} & = F' - E'
\end{align*}
\]

From the equations presented in (B.1), \( \pi_S S t_s^2 \) is known to be the area of any elliptical spotfire at time \( t_s \). As \( \varepsilon \) is the number of embers lofted per unit area burnt, this spotfire will have released a total of \( \varepsilon \pi_S S t_s^2 \) embers. The proportion of embers that fall back to the ground, still burning, with the ability to ignite a new fire is given by \( \kappa \zeta/(\eta + \zeta) \). This means that if
\[
\pi_S S t_s^2 \varepsilon \frac{k \zeta}{\eta + \zeta} = 1
\]
then the fire that has grown in the time \( t_s \) ignites, on average, exactly one new fire. Thus \( t_s \) is the time in which a new fire is formed from any one single elliptical fire. The time scale can also be written in terms of the geometry of the problem, requiring no knowledge of the values \( S \) and \( s \).

\[
t_s = \left( \frac{\eta + \zeta}{\pi_S S \varepsilon \kappa \zeta} \right)^{1/2} = \left( \frac{2t_i}{\pi(R_h + R_b)\varepsilon t_e} \right)^{1/2}
\]

The length scale \( x_s = (R_e - c)t_s \) is the extra distance the storm has travelled above the centroid movement distance during the spotting time. It can thus be thought of as the average spotting displacement distance. Relative to the frame of reference moving with the storm, embers are transported a mean distance of \( x_e = (w - R_e)/(\eta + \zeta) \) by the wind. The two values appearing in the dimensionless equations, \( \tau \) and \( \lambda \), can thus be written in terms of ratios of characteristic scales.

\[
\tau = \frac{t_e}{t_s} = \frac{1}{(\eta + \zeta)t_s} \quad \text{and} \quad \lambda = \frac{x_e}{x_s} = \frac{w - R_e}{R_e - c}r.
\]
These values represent the ember lifetime measured in units of the spotting time, and the ember transport distance measured in units of the spotting displacement distance respectively.

**B.4 Spread of a Steady-State Ember Storm**

A steady-state ember storm is now considered where the storm spreads at the speed \( R_e \). Here all time derivatives become zero giving the dimensionless equations,

\[
\begin{align*}
-n'_x &= E' \\
-B_x &= F' \\
-F'_x &= F'^2/(1 - B) - 2n'(1 - B) \\
\lambda E'_x &= F' - E',
\end{align*}
\]

with boundary conditions,

\[
\lim_{x' \to \infty} (E', F', n', B) = (0, 0, 0, 0) \quad \text{and} \quad \lim_{x' \to -\infty} (E', F', n'_x, B) = (0, 0, 0, 1).
\]

These equations are solved using COMSOL. In order to solve the equations it is found useful to return from the actual fire perimeter, \( F \), to the total perimeter without deductions, \( f \). Solving the equation for the actual fire perimeter leads to division by 0 when all the fuel is burnt. However, the relation detailed in (B.7) provides a simple link between the values \( f \) and \( F \). Whilst equations are solved in terms of \( f \), results are presented in terms of the more physically relevant value \( F \). In the steady-state ember storm equations only the parameter \( \lambda \) remains. In order to allow COMSOL to allocate an appropriate value to \( \lambda \) an additional constraint must be added. This constraint is given by,

\[
\int_{-L}^{L} B - 0.5 \, dx' = 0,
\]

where \(-L \leq x' \leq L\) represents the domain over which the equations are solved. This equation sets the frame of reference such that at the point \( x = 0 \), approximately half of the fuel has been burnt. The appropriate value of \( \lambda \) is then determined by COMSOL so that this equation holds. Numerically solving the equations this parameter is found to have the fixed characteristic eigenvalue

\[
\bar{\lambda} \approx 0.3051\ldots
\]
The spread rate of a steady ember storm is thus determined by this characteristic value of $\lambda$ and the scalings used to arrive at the dimensionless form of the model.

The shapes for the dimensionless functions $\bar{E}(x')$, $\bar{n}(x')$, $\bar{B}(x')$ and $\bar{F}'(x')$ are shown in Figure B.3. Far ahead of the storm there are no fires, and hence no land is burnt. Far behind the storm all fuel is burnt and $n'_n = \kappa \zeta \epsilon / (\eta + \zeta)$, i.e. the number of potential ignitions is equal to the number of embers lofted per unit area, which fall to the ground with the ability to ignite new fires. The fire perimeter and the number of embers both peak near the point $x' = 0$, where half the fuel is burnt, and are zero a long way from the storm.

![Figure B.3: The dimensionless profiles of $\bar{E}(x')$, $\bar{n}(x')$, $\bar{B}(x')$ and $\bar{F}'(x')$](image)

Whilst the spread-rate, $R_e$, and the characteristic time scale ratio, $\tau$, do not appear explicitly in the steady-state equations they can be calculated using the equations given in (B.18). The spread-rate adjusts itself so that the spotting displacement distance and ember transport distance have the fixed ratio, $x_e / x_s = \bar{\lambda}$. Thus, using equation (B.14),

$$R_e = \frac{w \tau + c \bar{\lambda}}{\tau + \lambda} = \frac{w t_e + c \bar{\lambda} t_s}{t_e + \lambda t_s}.$$

The lifetime of the lofted burning embers, $t_e$, is likely to be insensitive to wind-speed. The spotfire self replication time on the other hand, $t_s$, does depend on wind speed through the head, backing and flank-fire spread-rates. Thus the characteristic time scale ratio, $\tau = t_e / t_s$, should increase as the wind increases, causing the ember storm spread rate to approach the wind-speed $w$. The relationship between the storm
spread-rate, $R_e$, and the characteristic time scale ratio, $\tau$, is plotted in Figure B.4.

When $\tau$ is small, the model predicts that the storm spread-rate tends to the centroid speed, $c$. However, given that $c = \frac{1}{2}(R_h - R_b)$, the model thus predicts that the ember storm spreads at a rate which is slower than the head-fire spread-rate. Thus the model fails when $\tau$ is small. In this instance the fire front could be considered to remain mostly continuous, except when an occasional spotfire is produced ahead of it. The original fire front would gradually catch up with the tail end of this new fire until they merged, and the fire front would be moved forwards. Under the assumptions presented here the model is thus not appropriate for combustion regimes where only occasional spotting is observed.

**B.5 Conclusions**

A continuum model considering the key features of an ember storm has been investigated. The model assumes self-similar elliptical growth of spotfires, although amending the work to consider an alternative geometry is relatively straightforward. When a steady-state ember storm is considered the spread rate is found to be determined only by the characteristic value $\bar{\lambda}$ and the scalings used to arrive at the dimensionless model. The model as presented here has not been designed to deal with conditions when $\tau$ is small, and only occasional spotting is observed.
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