STARx Technology for Waste Oil Sludge Treatment Investigated with Numerical Modelling

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Abstract

Growing stockpiles of industrial liquid waste stored in lagoons are an outstanding problem worldwide. Self-sustaining Treatment for Active Remediation (STAR) is an emerging technology based on smouldering combustion that has been successfully deployed for in situ remediation of field sites (Grant et al., 2016). STAR is currently being developed as an ex situ treatment system (STARx) for industrial wastes by intentionally mixing them with sand. One engineering concept for STARx is the “hotpad”, for which some initial experiments have been conducted. However, a thorough experimental investigation is challenging due to the cost and time associated with each experiment. This work employed a two-dimensional (vertical cross-section) numerical model to systematically explore sensitivity of STARx hotpad performance to system design, operational parameters, and environmental factors. The phenomenological model that was used uniquely combines a multiphase flow code and a front expansion routine (MacPhee et al., 2012; Hasan et al., 2015). The model was first calibrated and validated against pilot-scale (~ 2 m width) hotpad experiments, providing confidence that the rate and extent of treatment were correctly predicted. Pilot-scale simulations then investigated the sensitivity of system performance to: injected airflow rate, organic liquid concentration, hotpad configuration, system dimensions, heterogeneity of intrinsic permeability, and heterogeneity of organic liquid concentration. The expected performance of two field-scale configurations (~ 10 m width) was also explored. Hotpad performance is predicted to be most sensitive to the injected air flux, with higher air fluxes achieving higher rates of organic liquid destruction and treating larger fractions of the initial mass. The uniformity of the advancing smouldering front was predicted to be highly dependent on the effective permeability ratio between untreated and treated materials. As a result, increased heterogeneity – of intrinsic permeability in particular – is predicted to degrade remedial performance. Full-scale systems were predicted to achieve treatment rates an order of magnitude higher than the pilot-scale for a similar organic liquid concentration and injected air flux. It is anticipated that this work will increase understanding of several key processes that impact STARx performance and help optimize hotpad design and operation.

Keywords

smouldering combustion, ex situ, remediation, numerical modelling, waste oil sludge
Co-Authorship Statement

This thesis was written in accordance with the guidelines and regulations for integrated-article format as stipulated by the Faculty of Graduate and Postdoctoral Studies at the University of Western Ontario. The candidate conducted all simulations, data analysis and interpretation under the close guidance and supervision of Dr. Jason Gerhard. Permeability testing was completed by the candidate with the assistance of Amanda Bastos. All hotpad experiments were conducted by Savron, a company located in Guelph, Ontario. Dr. Gavin Grant (Adjunct Professor at Western) and Grant Scholes, both Savron employees, contributed to the selection of simulations and provided feedback on the analysis of results conducted by the candidate.

Chapter 3: Numerical Modelling of the STARx Hotpad for Waste Oil Sludge Treatment

This chapter will be submitted to a peer-reviewed journal after the thesis has been completed. Proposed authorship: Rebecca L. Solinger, Jason I. Gerhard, Gavin Grant, and Grant Scholes

Contributions:

Rebecca L. Solinger: conducted permeability testing, simulations, analysis and interpretation of the results, and wrote the draft chapter.

Jason I. Gerhard: supervised model simulations and permeability testing, assisted in data interpretation, reviewed and revised the draft chapter.

Gavin Grant and Grant Scholes: led the team that conducted the hotpad experiments, provided hotpad experimental results to be interpreted by the candidate, provided input on simulations to conduct, and provided feedback on simulation results analyzed by the candidate.
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Chapter 1

1 Introduction

1.1 Introduction

Stockpiles of excavated contaminated soils and waste oil sludge stored in lagoons are a growing problem worldwide (Hu et al., 2013). As these materials are often landfilled or incinerated, alternative technologies that are economically competitive but more environmentally sustainable are needed (da Silva et al., 2012). One promising alternative technology is Self-Sustaining Treatment for Active Remediation (STAR) which destroys liquid contaminants embedded in a porous medium via smouldering combustion. Multiple laboratory studies and successful in situ field applications have proven that STAR performs well under a range of conditions and achieves near complete contaminant removal (Pironi et al., 2009; Switzer et al., 2014; Grant et al., 2016). The STAR technology is currently being adapted for ex situ applications (STARx), and will be well suited to treat waste oil sludge, which is intentionally mixed with sand for treatment, or stockpiles of excavated contaminated soils. Few STARx experiments are available because of the cost and time required. Numerical modelling is a time and resource efficient tool that can be applied to predict STARx system performance under a range of conditions. An existing numerical model was previously proven to correctly predict the rate and extent of treatment from small-scale STAR experiments (MacPhee et al., 2012; Hasan et al., 2015). However, the model has never been applied as a research or design tool for STARx systems.

1.2 Research Objectives

The overall goal of this thesis was to provide insight into expected behaviour of STARx systems under a realistic range of conditions. These conditions include both controlled parameters (i.e., design and operation) and environmental factors (i.e., heterogeneity).

The specific objectives of this work were to: 1) implement a measured relative permeability-saturation constitutive function in the model; 2) complete the first model calibration and validation against pilot-scale STAR experimental results; 3) identify design conditions and operational parameters that are anticipated to maximize batch treatment mass and minimize batch treatment time; 4) evaluate the influence of environmental factors on expected system
performance; and 5) approximate treatment masses and times that can be expected at the field-scale for a system operated under similar conditions. Additionally, this work aims to provide strengthened confidence in the model’s usefulness as a low cost, efficient design tool.

The findings from the numerical modelling study complement pilot-scale experimental results and are anticipated to be highly valuable when informing the design and operation of future STARx systems, including treatment of waste oil sludge and excavated contaminated soils.

1.3 Thesis Outline

This thesis was written in Integrated Article Format. Each chapter is briefly described below.

Chapter 2 presents a review of literature related to smouldering combustion; particularly smouldering of organic liquids in porous media. Emphasis was placed on previous experimental studies that have explored smouldering as a soil remediation technology and on previous work with the numerical model used in this research. Advantages and limitations of the model are discussed.

Chapter 3 presents results from pilot-scale hotpad experiments, permeability testing, and a comprehensive numerical modelling study. All five research objectives listed in Section 1.2 are addressed in this chapter. Following intrinsic and relative permeability testing, model calibration and validation were conducted. Then a suite of simulations was completed to infer the effects of injected air flux rate, contaminant pack saturation and configuration, heterogeneity in contaminant pack saturation, heterogeneity in intrinsic permeability, and system scale on predicted system performance (i.e., the rate and extent of treatment). Modelling results were used to approximate expected treatment times and masses for a full-scale system. An adaptation of this chapter is expected to be submitted to a refereed journal following the submission of this thesis.

Chapter 4 presents a summary of the research conducted in this thesis, including key conclusions and a series of recommendations for future modelling and experimental work.

A series of nine appendices are provided. These include supplementary, detailed results from the experiments and modelling study discussed in Chapter 3 that are intended to provide additional
support for the analysis and conclusions presented in this thesis. Appendix A contains additional pilot-scale STARx experimental data that was used for model calibration and validation. This includes thermocouple and emission data, calculations of experimental average vertical smouldering velocities, and supporting evidence that the experimental average vertical smouldering velocity was not constant with contaminant pack height. Appendix B details the results of the intrinsic and relative permeability testing, as well as the curve fitting process that was completed to implement a measured relative permeability-saturation constitutive function in the model. Appendix C summarizes the selection process for model calibration parameters. Appendices D and E provide supporting figures from the numerical modelling study, including the predicted initial air flux distributions, final extents of treatment, and smouldering front evolution for all simulations whose figures were not included in Chapter 3. Appendix F illustrates how the two-dimensional nature of the simulated configurations affects local air flux magnitudes along the contaminant pack centerline. Appendix G includes results from additional simulations that altered the tortuosity exponent in the relative permeability-saturation constitutive function to confirm the importance of the effective permeability ratio between untreated and treated material. Appendix H illustrates the effects of removing the clean sand cap from the system, and Appendix I provides the results of two additional full-scale hotpad configurations that were simulated.

1.4 References


Chapter 2

2 Literature Review

2.1 Introduction

Treatment and disposal of waste oil sludge is an outstanding problem worldwide (da Silva et al., 2012; Hu et al., 2013). A by-product from oil extraction and processing in the petroleum hydrocarbon industry (Xu et al., 2009), waste oil sludge is an emulsion of petroleum hydrocarbons, water, solids, and metals (Mazlova and Meshcheryakov, 1999). While the amount of sludge generated varies between operations, approximately 1 tonne of sludge is generated for every 500 tonnes of processed crude oil (Oudenhoven et al., 1995). Globally, this amounts to a current sludge generation rate of 60 million tonnes per year, in addition to the estimated 1 billion tonnes of sludge previously generated (da Silva et al., 2012). Historically, sludge was often stored in unlined lagoons, resulting in soil and groundwater contamination. The physical and chemical properties of waste oil sludge depend on the crude oil source and how it was processed, creating a large variation between sludge from different sources (Hu et al., 2013). Waste oil sludge typically has high concentrations of toxic substances, including polycyclic aromatic hydrocarbons (PAHs) and heavy metals, posing serious human and environmental health risks (Mrayyan and Battikhi, 2005; Mater et al., 2006; Liu et al., 2009; Xu et al., 2009; da Rocha et al., 2010). Numerous technologies have been developed to treat waste oil sludge. However, due to the recalcitrant nature of many compounds within sludge, they are often difficult to treat in a way that is both environmentally sustainable and cost effective (Hu et al., 2013).

Recently, smouldering of liquids embedded in a porous medium was presented as a novel approach to soil remediation (Pironi et al., 2009; Switzer et al., 2009; Pironi et al., 2011). This technology, termed Self-sustaining Treatment for Active Remediation (STAR), uses the high energy content of recalcitrant contaminants (e.g., coal tar, crude oil) to fuel a smouldering combustion reaction, destroying the contaminant in the process. This technology has been proven effective in multiple laboratory (Pironi et al., 2009; Switzer et al., 2009) and field-scale studies (Scholes et al., 2015; Grant et al., 2016), including applications below the groundwater table. Although originally developed for in situ remediation, STAR is also being developed for ex situ
applications (STARx). STARx will be ideal for treating waste oil sludge that has been intentionally mixed with sand to create a porous matrix, or stockpiles of excavated contaminated soil.

A numerical model was developed to approximate the evolution of the smouldering front during STAR applications (MacPhee et al., 2012), and was shown to correctly predict the average rate and ultimate extent of treatment for two-dimensional (2-D) lab-scale experiments (Hasan et al., 2015). The model was proven to be numerically stable and can solve large, complex domains with heterogeneous saturation and permeability fields (MacPhee, 2010; MacPhee et al., 2012). However, the model has never been calibrated or validated against large-scale conditions. This chapter provides an overview of literature pertaining to smouldering, the development of STAR and the numerical model, and previous work with the model.

2.2 Smouldering Combustion

Relative to flaming combustion, smouldering combustion is a slow, low temperature, flameless, exothermic reaction where oxygen directly attacks the surface of a condensed phase fuel (Ohlemiller, 1985; Ohlemiller, 2002; Rein, 2009). This diffusion limited process includes chemical reactions, in addition to heat, mass, and momentum transport in the gas and solid phases (Ohlemiller, 1985). In contrast to flaming combustion where oxidation and heat release both occur in the gas phase, reactions occur on or within the fuel surface during smouldering combustion (Rein, 2009). Familiar examples of smouldering combustion include charcoal barbeques (Figure 2.1) and cigarettes. Smouldering combustion is much less studied, and thus less well understood than flaming combustion (Rein, 2009). Existing smouldering research has focused on the safety and environmental hazards associated with smouldering including residential fires (Hotta et al., 1987; Purser, 2002; Watanabe and Tanaka, 2004; Wakelyn et al., 2005), commercial and aerospace flights (Friedman, 1998; Fiorino, 2003), wild land fires (Page et al., 2002; Bertschi et al., 2003; Rein et al., 2009), and subsurface fires in peat, coal seams, or landfills (Renner, 1978; Nolter and Vice, 2004; Stracher and Taylor, 2004; Rein, 2009). Recently, a few beneficial applications of intentional smouldering have been published including coal seam gasification (Blinderman et al., 2013), biochar production (Lehmann, 2007), and soil remediation (Pironi et al., 2009; Pironi et al., 2011; Switzer et al., 2014; Scholes et al., 2015).
Both solid (e.g., coal, cotton, tobacco, saw dust, paper, peat, wood, organic fibers, synthetic foams, and charring polymers) and liquid fuels (e.g., soil remediation) can smoulder (Rein, 2009), however, smouldering of a liquid (e.g., waste oil sludge) requires the fuel to be embedded in a porous medium. Regardless of the fuel phase, similar conditions must be met for a material to sustain smouldering. The fuel, or material in which the fuel is embedded, must be permeable enough to allow sufficient oxygen delivery to the reaction zone, and must provide adequate thermal insulation such that the net energy released balances the energy required for the reaction to propagate (Ohlemiller, 1985; Ohlemiller, 2002; Rein, 2009). The fuel must also have a large surface area per unit volume to enhance oxidant attack (Ohlemiller, 1985; Rein, 2009). While the heat losses of the system are proportional to the sample surface area, the heat generated is proportional to volume (Rein, 2009) suggesting heat losses diminish with increased scale (Switzer et al., 2014).

Following ignition, a smouldering reaction is maintained by convective and diffusive oxygen transport to the reaction site, where convective transport can be enhanced by the buoyant motion of high temperature gases produced from the reaction (Torero and Fernandez-Pello, 1995). In contrast to unintentional applications of smouldering, where oxygen is delivered through natural convection, engineered applications apply a forced air supply to sustain the reaction. Heat evolved from the exothermic process is partially transferred ahead of the current reaction zone via conduction, convection, and radiation, and partially lost to the surrounding environment.
(Ohlemiller, 2002). When the heat generated, transferred, and stored in the system exceeds external heat losses, the reaction becomes “self-sustaining”, implying no additional external energy is required to maintain the reaction (Ohlemiller, 2002). If either the fuel or oxidant supply becomes insufficient, the reaction can no longer sustain itself and will quench.

As the fundamentals of smouldering combustion are not yet well understood by the scientific community, smouldering reactions are typically characterized based on the relation of the oxidant flow relative to the direction of smouldering (Rein, 2009). Idealized one-dimensional (1-D) cases of smouldering are termed “forward smouldering” when the reaction and oxidant move in the same direction, and “opposed smouldering” when the reaction propagates opposite to the oxidant flow (Ohlemiller and Lucca, 1983) as shown below in Figure 2.2.

![Figure 2.2. (a) Forward smouldering, where the reaction propagation and oxidant flow occur in the same direction. (b) Opposed smouldering, where the reaction propagation and oxidant flow occur in opposite directions from Hasan (2013).](image)

In forward smouldering, the oxidant flows through previously burned areas before reacting with the fuel (Ohlemiller and Lucca, 1983). The oxygen-depleted gas then transports heat evolved from the reaction to pre-heat and pyrolyze material directly ahead of the current reaction zone (Leach et al., 2000). This preheating phenomenon creates two distinct temperature fronts, and as such this mode of propagation is often characterized with a combination of pyrolysis and oxidation reactions. In opposed smouldering, the regions of preheating and oxidation are non-
distinct and overlap each other, and are summarized with a global oxidation reaction (Ohlemiller and Lucca, 1983). Intentional smouldering of liquid contaminants exclusively uses forward smouldering and all discussion hereafter will assume this mode. Smouldering can occur under oxidant or kinetically limited conditions (Ohlemiller, 2002). Kinetically limited conditions occur when the oxygen supplied to the reaction exceeds stoichiometric requirements; therefore the propagation rate is limited by reaction kinetics. Under oxygen limited conditions, all available oxygen is completely consumed and additional oxygen must be supplied to maintain propagation of the smouldering front (Pironi et al., 2009).

2.3 Self-sustaining Treatment for Active Remediation

2.3.1 Current Approaches for Waste Oil Sludge Treatment

Hu et al. (2013) provided a comprehensive review of existing technologies for treating waste oil sludge. As illustrated below in Figure 2.3, these technologies can be classified as either oil recovery or sludge disposal methods.

![Figure 2.3. Overview of current waste oil sludge treatment methods, including oil recovery and disposal, from Hu et al. (2013).](image)
Oil recovery technologies aim to recover valuable oil from the sludge and to reduce the volume of sludge for disposal. Common oil recovery methods include solvent extraction (Taiwo and Otolorin, 2009; El Naggar et al., 2010; Zubaidy and Abouelnasr, 2010), centrifugation (da Silva et al., 2012), surfactant enhanced oil recovery (EOR) (da Silva Lima, 2011; Yan et al., 2012), and pyrolysis (Chang et al., 2000; Schmidt and Kaminsky, 2001; Liu et al., 2009). While all four of these technologies are relatively fast, they also have high overall costs (due to capital, operating or maintenance costs) (Hu et al., 2013). Other limitations of these technologies include the large amounts of organic solvents required for solvent extraction, the high energy consumption associated with centrifugation and pyrolysis, and the need for secondary treatment to remove surfactant from the oil recovered in surfactant EOR (Hu et al., 2013). Each recovery method also creates a range of by-products that require additional treatment, including unrecoverable sludge slurry/solids, wastewater, volatile organic compounds (VOCs) or char (Hu et al., 2013). Common sludge disposal methods include incineration (Sankaran et al., 1998; Zhou et al., 2009), stabilization/solidification (Karamalidis and Voudrias, 2007a; Karamalidis and Voudrias, 2007b; Leonard and Stegemann, 2010), and landfilling (Bhattacharyya and Shekdar, 2003; Khan et al., 2004; Butt et al., 2008). While incineration is rapid and can achieve a drastic reduction in sludge volume, pre-treatment sludge dewatering and supplemental fuel required during treatment increase the overall cost. Stabilization is a low cost, efficient method to immobilize contaminants, however it also requires pre-treatment dewatering and post-treatment management of the stabilized products. Landfilling is an inexpensive method that can handle large sludge volumes; however it is a very slow process for contaminant degradation and requires a large area. None of these existing technologies are able to provide inexpensive and rapid sludge treatment with low energy consumption.

2.3.2 Chronological Development of STAR

Self-sustaining Treatment for Active Remediation (STAR) is an engineered smouldering combustion reaction that was originally developed for source zone remediation of contaminated soils (Pironi et al., 2009; Switzer et al., 2009; Pironi et al., 2011). This patented technology takes advantage of the high calorific value of many liquid hydrocarbon contaminants to ignite and sustain a smouldering combustion reaction. Liquid hydrocarbon contaminants embedded in porous media are particularly well suited for self-sustained smouldering combustion as the liquid
coated sand grains provide a high contaminant surface area and the soil porosity allows for adequate oxidant delivery to the contaminant (Pironi et al., 2009). Additionally, the porous media provides thermal insulation, mitigating heat losses, and the soil’s specific heat capacity enables recycling of heat evolved from the reaction (Pironi et al., 2009). During a typical STAR application, a localized section of contaminated material is heated to a pre-determined temperature (Figure 2.4a). A forced air supply is then provided to ignite the smouldering combustion reaction, which propagates away from the ignition source (Figure 2.4b). For self-sustained smouldering to be viable in any context, a minimum air flux and minimum contaminant concentration must be present, the values of which are dependent on the scale, contaminant, and porous medium. Once the reaction is deemed self-sustaining based on temperature or emissions data, the heater is turned off while the air source is maintained (Figure 2.4c). As the liquid contaminant is the fuel, the reaction is both self-tracking, and self-terminating when all contaminant has been destroyed (Figure 2.4d). The reaction can also be externally quenched by removing the air supply, making it a controllable, safe process.
Figure 2.4. Conceptual diagram of the (a) preheating, (b) ignition, (c) self-sustained smouldering, and (d) the end of treatment phases in a typical STAR application.
Pironi et al. (2009) presented the first experimental study exploring the viability of smouldering liquid contaminants embedded in porous media. The effects of air injection rate and initial contaminant concentration were explored with a series of beaker-scale experiments that employed upwards, forward smouldering of coal tar in sand. Pironi et al. (2009) observed a near linear increase in the rate the smouldering front propagates away from the ignition source (i.e., smouldering velocity) with increased injected air flux, as shown in Figure 2.5. The results also showed a linear decrease in smouldering velocity with increased initial contaminant concentration. This work established a standard experimental procedure that has since been applied in subsequent STAR studies. The methods of characterization applied by Pironi et al. (2009), including average smouldering velocity, peak temperature as a function of distance from ignition source, rate of forced air flux, and initial contaminant concentration, have since been applied to characterize other STAR studies.

**Figure 2.5.** Relationship between forward smouldering velocity and injected air flux from select STAR experimental studies, where injected air flux was the primary variable.
In a series of 1-D vertical column experiments, Switzer et al. (2009) identified a range of contaminant types and soil conditions that can achieve self-sustained smouldering. Sustained smouldering was achieved in medium and coarse sand, peat, and layered sand systems, with coal tar with and without water, mineral oil, crude oil, vegetable oil, dodecane, dichloroacetic acid (DCA)/grease, trichloroethylene (TCE)/oil, and a variety of field materials. Other key findings from Switzer et al. (2009) included that the smouldering behavior is a function of contaminant type and initial concentration, contaminant is completely destroyed after the smouldering front passes through a given region, and self-sustained propagation can be achieved with a one-time, short duration energy input supplied to ignite a single location.

A systematic evaluation of the effects of key parameters on liquid contaminant smouldering was completed by Pironi et al. (2011). Through a series of column-scale experiments, process sensitivity to contaminant concentration, water saturation, soil type, and air flow rate were examined using coal tar and crude oil samples. Self-sustained smouldering and complete treatment were achieved with a range of contaminant concentrations, soil types, and water saturations. The process was most sensitive to the injected air flux. For coal tar, the relationship between contaminant concentration, peak temperatures, and treatment velocities was concentration dependent, while crude oil experiments exhibited lesser increases in peak temperature and a relatively constant treatment velocity with increased contaminant concentration. Water acted as a heat sink in partially water saturated experiments, increasing ignition times, decreasing peak temperatures, and decreasing smouldering velocities in some instances. In addition to identifying a range of conditions that can achieve self-sustained smouldering, Pironi et al. (2011) provided additional confidence in the robustness of the STAR technology.

Switzer et al. (2014) conducted experiments at bench, intermediate, and pilot field-scales under similar operational conditions to explore the effects of experimental scale. Two contaminants, coal tar and mixed oil waste, were tested separately in a 0.003 m$^3$ column, 0.3 m$^3$ drum, and 3 m$^3$ bin. Peak temperatures, contaminant destruction efficiency, and treatment velocities were found to be independent of scale for a given contaminant. Particularly at the bin-scale, STAR was shown to handle heterogeneous distributions of airflow, material properties, and contaminant concentrations. Matching previous experimental studies, a linear correlation between injected air
flux and smouldering velocity was observed, as shown in Figure 2.5 for two porous media that were tested. Again, treatment velocity was found to depend on moisture content, with higher moisture contents achieving slower treatment rates. Switzer et al. (2014) also confirmed that as scale increases, the minimum contaminant concentration required for self-sustained smouldering decreases due to increasing surface area to volume ratios.

Scholes et al. (2015) presented the first in situ field test of STAR at a former industrial facility with coal tar contamination below the groundwater table. The field test successfully treated two distinct geological units; a shallow fill unit comprised of sand, brick, and other construction materials, and a deeper unit of coarse to medium sand. Based on temperature data and post treatment samples, total contaminant destruction was conservatively estimated at over 3700 kg in 12 days of treatment in the shallow unit, and over 860 kg in 11 days of treatment in the deep unit with respective destruction efficiencies of 99.3% and 97.3%. The rate and uniformity of the smouldering front expansion were observed to be strongly impacted by in situ heterogeneity, due to its influence on the injected air distribution. Grant et al. (2016) provided a summary of the successes and lessons learned from applications of STAR to date, including the impact of natural geologic heterogeneity on the spatial evolution of the smouldering front, as the contaminated soil must be permeable enough to deliver adequate oxygen to the reaction.

Salman et al. (2015) proved that TCE contaminated soils can be augmented with vegetable oil to achieve self-sustained smouldering otherwise not possible due to the volatile nature of TCE. Bench-scale experiments explored the effects of vegetable oil type, concentration, TCE to vegetable oil ratio, the use of an emulsified vegetable oil, and oil injection versus manual mixing of the oil and sand. Opposed to conventional STAR applications where treatment is achieved via mass destruction during combustion, in this study contaminant removal primarily occurred through volatilization of the TCE, allowing for subsequent vapor capture and treatment.

In addition to smouldering liquid contaminants to remediate soil, STAR has also been explored as a potential waste management approach by Yermán et al. (2015), and Rashwan et al. (2016), who studied the smouldering of human faeces mixed with sand, and wastewater biosolids mixed with sand, respectively. As shown in Figure 2.5, a linear relationship between injected air flux and average vertical smouldering velocity was also observed for smouldering biosolids with a
range of moisture contents (Rashwan et al., 2016). From Figure 2.5, which only includes data from literature discussed in this section, it can be seen that while a near linear relationship is observed across a range of studies, the slope of the relationship is not constant. This is because the average vertical smouldering velocity is expected to also be a function of the contaminant, soil, and system scale.

2.4 Modelling STAR

2.4.1 The Phenomenological Smouldering Model

MacPhee et al. (2012) presented the development and proof of concept of a numerical model that predicts the evolution of the leading edge of a smouldering reaction in contaminated soil. The “Phenomenological Smouldering Model” (PSM), is a phenomenological model that solves conditions of heterogeneous fuel, airflow, and soil permeability, and can simulate large-scale applications of STAR. Throughout this thesis, model calibration refers to adjusting model parameters to reproduce a known result, model validation refers to confirming the calibrated models ability to accurately reproduce results from a real system without further parameter adjustment, and verification refers to ensuring the governing equations have been correctly implemented in the model. Multi-physics modelling of smouldering combustion is often limited to small-scale, one-dimensional (1-D) systems due to the complexity of smouldering combustion and the need for a large number of kinetic parameters (Rein, 2005). The PSM couples a multi-phase flow model (Gerhard and Kueper, 2003c; Gerhard and Kueper, 2003a) with a calibrated analytical expression for the forward smouldering velocity (Pironi et al., 2009; Rein, 2009) and a front expansion model (Richards, 1990; Richards, 1995) to approximate the smouldering front expansion in a 2-D vertical cross-section. The model assumes that the rate of liquid smouldering in porous media is governed by oxygen availability at the reaction front and heat losses to the surrounding environment (MacPhee et al., 2012). While the multi-phase component of the PSM is rigorous and solves conservation equations, the front expansion component is practical and phenomenological (i.e., it takes into account the major effects and dependences in smouldering, but not the underlying processes), and is only an approximation for practical purposes. This approach was taken to have an efficient model that can solve large-scale systems, and can be applied as an engineering design tool. Limitations of the PSM include it must be calibrated to each soil/contaminant pair that is being modelled, and it neglects any temperature effects during
smouldering. The overall model process is summarized in Figure 2.6, and each component will be discussed in the following sections.

START TIME STEP

1. Multiphase Flow Model

\[ q_{i,j}^{\text{AIR}}(t) \]

\[ S_{i,j}^{\text{NAPL}}(t) \]

\[ \dot{m}_{i,j}^{\text{AIR}}(t) \]

2. Calibrated Forward Smouldering Velocity Expression

\[
V_{i,j}^{f}(t) = \frac{\dot{m}_{i,j}^{\text{AIR}}(t) c_{ps} (T_s - T_{\text{amb}}) + \frac{A}{V_o} \dot{m}_{i,j}^{\text{AIR}}(t) Y_{o,i}}{\rho_{bs} c_{ps} T_s - \left( \rho_{bs} c_{ps} + S_{i,j}^{\text{NAPL}}(t) \phi \rho_{f} c_{pf} \right) T_{\text{amb}}} 
\]

\[ a_{i,j}(t) = \alpha V_{i,j}^{f}(t) \]

\[ b_{i,j}(t) = \beta V_{i,j}^{f}(t) \]

\[ c_{i,j}(t) = \kappa V_{i,j}^{f}(t) \]

3. Front Expansion Model

4. Front Clipping and Re-gridding

5. NAPL Destruction

END TIME STEP

Figure 2.6. Process flow diagram for the PSM, adapted from MacPhee et al. (2012).
2.4.2 The Multiphase Flow Model

DNAPL3D is a three-dimensional (3-D) finite difference model that solves the flow of two immiscible fluid phases in porous media in space and time (Kueper and Frind, 1991; Gerhard et al., 1998; Gerhard and Kueper, 2003c; Gerhard and Kueper, 2003a; Grant et al., 2007). The model is typically applied to study groundwater contamination (Gerhard et al., 1998; Gerhard et al., 2001; Gerhard and Kueper, 2003b; Gerhard et al., 2007), where water and non-aqueous phase liquid (NAPL) are the wetting and non-wetting phases, respectively.

When a single fluid phase occupies a porous medium, the fluid flow per unit cross-sectional area is defined as the Darcy flux, $q$, and is given by:

$$ q = -k_i \left( \frac{\rho g}{\mu} \right) \left( \frac{dh}{dl} \right) $$

(1)

where $k_i$ is the intrinsic permeability of the porous medium, $\rho$ is the fluid density, $g$ is acceleration due to gravity, $\mu$ is the dynamic viscosity of the fluid, and $dh/dl$ is the hydraulic head gradient. $k_i$ is a soil property defined as the materials ability to transmit a fluid, and is related to hydraulic conductivity, $K$, for single phase flow by:

$$ K = \frac{k_i \rho g}{\mu} $$

(2)

where all variables were previously defined.

When two fluid phases occupy a porous medium, (e.g., waste oil sludge and air), the permeability to each phase are termed the wetting and non-wetting phase effective permeability, $k_{ew}$ and $k_{eN}$, respectively (Brooks and Corey, 1964). The effective permeability is typically a fraction of the intrinsic permeability, and is defined for each fluid phase by:

$$ k_{ew} = k_i k_{rw} $$

(3)

$$ k_{eN} = k_i k_{rN} $$

(4)

where $k_{rw}$ and $k_{rN}$ are the wetting and non-wetting phase relative permeability, respectively. The fraction of the pore space filled with the wetting and non-wetting phases are termed the wetting, $S_w$, and non-wetting, $S_N$, phase saturations, respectively. Effective permeability is then a function
of both intrinsic permeability (ranging orders of magnitude depending on soil properties), and relative permeability (ranging between 0 and 1.0, depending on the phase saturation). In most instances of dual-phase flow, the functional relationship of saturation-relative permeability is hysteretic and depends on whether the system is undergoing imbibition or drainage (Gerhard and Kueper, 2003c). In the PSM, the wetting phase is only ever removed from the system as the smouldering front advances, therefore only drainage conditions are considered. Similarly, as the wetting phase is assumed to be immobile in this work, relative permeability effects of the non-wetting phase govern. DNAPL3D employs the relative permeability-saturation constitutive relationship \((k_{rN} - S)\) of Gerhard and Kueper (2003c), which is defined for the non-wetting phase under drainage conditions by:

\[
k_{rN} = k_{rN}^{\text{max}} (1 - \bar{S}_d^{*})^{2\tau_d} \left(1 - \bar{S}_e^{*d} \frac{2 + \lambda_d}{\lambda_d}\right)
\]

where \(k_{rN}^{\text{max}}\) is the maximum relative permeability to the non-wetting phase, \(\tau_d\) is the drainage non-wetting phase relative tortuosity exponent, \(\lambda_d\) is the drainage pore size distribution index, and \(\Delta S_W^{*d}\) is a fitting parameter that determines the amount that \(k_{rN}\) abruptly jumps from zero to a positive finite value when \(S_w = S_w^M\). \(\bar{S}_e^{*d}\) is a scaled saturation variable for drainage that is defined as:

\[
\bar{S}_e^{*d} = \frac{S_W - S_r^k}{(S_W^M + \Delta S_W^{*d}) - S_r^k} \quad S_r^k \leq S_W \leq S_W^M
\]

\[
= 1 \quad S_W^M < S_W < 1
\]

where \(S_W^M\) is the saturation at which a nonzero relative permeability first appears (i.e., the emergence saturation), and \(S_r^k\) is a residual wetting phase parameter associated with \(k_{rN} - S\). These variables are illustrated in Figure 2.7, which gives examples of two hypothetical \(k_{rN} - S\) curves for drainage conditions from a typical rock core (blue), and a unconsolidated sand with a uniform grain size distribution (Gerhard and Kueper, 2003c).
Figure 2.7. Relative permeability-saturation curve for the non-wetting phase under drainage conditions where $S_r^k$ = residual wetting phase saturation, $S_w^M$ and $k_{re}$ = emergence wetting phase saturation and corresponding emergence non-wetting phase relative permeability, $k_{rN}^{max}$ = maximum relative permeability to the non wetting phase. Curves displayed are for a typical rock core (blue) and an unconsolidated sand with a uniform grain size distribution (red), modified from Gerhard and Kueper (2003c).

DNAPL3D solves the continuity equations for the mass balance of the wetting and non-wettings phases (Kueper and Frind, 1991):

\[
-\frac{\partial}{\partial x_i}[\rho_w q_{wi}] + Q_w = \frac{\partial}{\partial t} [\phi \rho_w S_w] \quad i = x, y, z \quad (7)
\]

\[
-\frac{\partial}{\partial x_i}[\rho_N q_{Ni}] + Q_N = \frac{\partial}{\partial t} [\phi \rho_N S_N] \quad i = x, y, z \quad (8)
\]

where $x, y, z$ are the spatial coordinates, $t$ is time, $\rho_w, \rho_N$ are the wetting and non-wetting phase densities, $q_{wi}, q_{Ni}$ are the wetting and non-wetting phase fluxes, $Q_w, Q_N$ are the wetting and non-wetting phase source/sink terms, and $\phi$ is the porosity of the porous medium. Equations 7 and 8 can be refined by employing the multiphase extension of Darcy’s law, assuming incompressible
fluids and porous media, laminar flow conditions, and ignoring source/sink terms. Coupling these equations with the capillary pressure relation \( P_c = P_{nw} - P_w \), where \( P_c \), \( P_{nw} \), and \( P_w \) are the capillary, non-wetting, and wetting phase pressures respectively, and assuming the condition \( S_w + S_N = 1 \), yields versions in which wetting phase pressure and wetting phase saturation are the primary variables to be solved:

\[
\begin{align*}
- \frac{\partial}{\partial x_i} \left[ k_{i,j} k_{r,W} \left( \frac{\partial P_w}{\partial x_j} + \rho_w g \frac{\partial z}{\partial x_j} \right) \right] - \phi \frac{\partial S_w}{\partial t} &= 0 \quad i = x, y, z \quad (9) \\
- \frac{\partial}{\partial x_i} \left[ k_{i,j} k_{r,N} \left( \frac{\partial (P_c + P_w)}{\partial x_j} + \rho_N g \frac{\partial z}{\partial x_j} \right) \right] + \phi \frac{\partial S_w}{\partial t} &= 0 \quad i = x, y, z \quad (10)
\end{align*}
\]

where \( k_{i,j} \) is the second order tensor defining the porous medium intrinsic permeability, \( k_{r,W}, k_{r,N} \) are the relative permeabilities to the wetting and non-wetting phases, \( \mu_w, \mu_N \) are the wetting and non-wetting phase viscosities, and the remaining variables have been previously defined.

Equations 9 and 10 are solved with a seven point, node centered, fully implicit, finite difference scheme, with second-order accurate spatial operators and a first-order accurate time derivative (Rosenberg, 1969). Absolute permeabilities are defined using harmonic means, and relative permeabilities are defined using saturations at the upstream node (Aziz and Settari, 1972). DNAPL3D also includes a capillary pressure-saturation (\( P_c-S \)) constitutive model (Gerhard and Kueper, 2003a). The non-linear nature of the equations is addressed with Newton-Raphson iteration and solved with a modified ORTHIM routine (Behie et al., 1984).

In the PSM, organic liquid and air are specified as the wetting and non-wetting phases, respectively. As shown in Figure 2.6, after solving the air pressure and organic liquid distribution throughout the initially conditioned system in Step 1, air pressure gradients are converted to Darcy air fluxes, and multiplied by the density of air to achieve local values of air mass flux, \( \dot{m}_{i,j}^{AIR}(t) \). Local values of air mass flux and organic liquid saturation are then relayed to the calibrated analytical expression for the forward smouldering velocity, Step 2 in Figure 2.6.
2.4.3 Front Expansion Model

The front expansion model (Step 3 in Figure 2.6) employs Richards’ equations (Richards, 1990; Richards, 1995), a set of geometrically based partial differential equations, which relate local forward smouldering velocities from Step 2 in Figure 2.6 to the expansion of the front as a whole. Richards’ equations are based on Huygens’ Principle, which assumes that for a given time step, each vertex on a fire front is an ignition point for a small fire that will burn in an elliptical region over that time step (Richards and Bryce, 1995; Finney, 1998). At the end of the time step, the new fire front is defined as the curve that envelopes all sub-ellipses. While Richards’ equations were originally applied as a predictive tool for forest fire modelling, both forest fire growth and smouldering expansion depend on air flow velocity and fuel concentration (Finney, 1998; Switzer et al., 2009; Pironi et al., 2011). Therefore MacPhee et al. (2012) deemed the equations appropriate for modelling STAR. The PSM is the first known application of Huygens’ Principle and Richards’ equations to model smouldering combustion (MacPhee et al., 2012). With Richards’ equations, the expansion rate of a sub-ellipse at time $t$ is defined by (Richards, 1990; Richards, 1995; Richards and Bryce, 1995):

$$\frac{dx}{dt} = \frac{a^2 \cos \theta \left( \frac{dy}{ds} \cos \theta - \frac{dx}{ds} \sin \theta \right) + b^2 \sin \theta \left( \frac{dx}{ds} \cos \theta + \frac{dy}{ds} \sin \theta \right)}{\sqrt{\left( a \left( \frac{dy}{ds} \cos \theta - \frac{dx}{ds} \sin \theta \right) \right)^2 + \left( b \left( \frac{dx}{ds} \cos \theta + \frac{dy}{ds} \sin \theta \right) \right)^2}} + c \cos \theta \tag{11}$$

$$\frac{dy}{dt} = \frac{-a^2 \sin \theta \left( \frac{dy}{ds} \cos \theta - \frac{dx}{ds} \sin \theta \right) + b^2 \cos \theta \left( \frac{dx}{ds} \cos \theta + \frac{dy}{ds} \sin \theta \right)}{\sqrt{\left( a \left( \frac{dy}{ds} \cos \theta - \frac{dx}{ds} \sin \theta \right) \right)^2 + \left( b \left( \frac{dx}{ds} \cos \theta + \frac{dy}{ds} \sin \theta \right) \right)^2}} + c \sin \theta \tag{12}$$

where $x, y$ are the Cartesian coordinates of the ellipse vertices, $s$ is the orientation of the sub-ellipse relative to the major axis of the main ellipse ($0 \leq s \leq 2\pi$), $\theta$ is the direction of the air supply relative to the x-axis, $a \, dt$ is half the major ellipse axis, $b \, dt$ is half the minor ellipse axis, and $c \, dt$ is the distance from the ellipse centre to the ignition point at the rear focus.

Equations 11 and 12 are solved fully explicitly with forward and central differences schemes for the temporal and spatial derivatives, respectively (Richards and Bryce, 1995). An example of a sub-ellipse that is generated using Richards’ equations is illustrated below in Figure 2.8. These equations assume a continuous 2-D plane, and their general form can be applied to conditions...
with variable fuel concentrations and air supplies at different scales (Richards, 1995; Richards and Bryce, 1995; Finney, 1998). The size and orientation of each sub-ellipse (x, y, a, b, c, and θ) depend on the local conditions at a particular node and are functions of s and t. The local forward smouldering velocity values, $V^f_{i,j}(t)$ (described below in Section 2.4.4), are related to the lateral, $V^l_{i,j}(t)$, and opposed, $V^o_{i,j}(t)$, rates of smouldering with equations 13-15, (Richards, 1990; Richards, 1995):

\begin{align*}
V^f_{i,j}(t) &= a_{i,j}(t) + c_{i,j}(t) \quad i, j = x, y \\
V^l_{i,j}(t) &= b_{i,j}(t) \quad i, j = x, y \\
V^o_{i,j}(t) &= a_{i,j}(t) - c_{i,j}(t) \quad i, j = x, y
\end{align*}

where $a$, $b$, and $c$ are the same as in Equations 11 and 12. Equations 13-15 can be rearranged using substitution of the constants $\alpha$, $\beta$, and $\kappa$ to yield:

\begin{align*}
a_{i,j}(t) &= \alpha V^f_{i,j}(t) \\
b_{i,j}(t) &= \beta V^f_{i,j}(t) \\
c_{i,j}(t) &= \kappa V^f_{i,j}(t)
\end{align*}
2.4.4 Calibrated Analytical Expression for Forward Smouldering Velocity

The multiphase flow and front expansion components of the PSM are linked at the local scale with Equation 19, the calibrated analytical expression for the forward smouldering velocity of liquid contaminants in porous media which was adapted from Pironi et al. (2009) and Rein (2009). Equation 19 uses the local air fluxes \( q_{i,j}^{AIR}(t) \) and saturations \( S_{NAPL,i,j}(t) \) from the multiphase flow equations to solve the local smouldering front velocities required in the front expansion model. This simplified analytical equation is based on global mass and energy balances across the reaction front assuming: constant gas mass flux, negligible smouldering velocity compared to the gas velocity, complete oxygen consumption at the reaction front, adiabatic and steady-state conditions (MacPhee et al., 2012). Compared to experimental data, the original analytical equation was shown to correctly predict the general data trends, but over predict the smouldering velocity magnitude (MacPhee et al., 2012). To correct for this, MacPhee et al. (2012) modified the expression to include a calibration parameter, \( A \), which must be uniquely calibrated to each soil/contaminant pair. The forward smouldering velocity, \( V_{i,j}(t) \), is

\[
V_{i,j}(t) = \frac{a + b + c - \sqrt{(a - b)^2 + 4ac}}{2}
\]

Figure 2.8. Schematic of a main and sub-ellipse generated with Richards’ equations to solve the new smouldering front at the end of a time step, from MacPhee (2010).
defined as:

$$V_{i,j}^f(t) = \frac{m_{i,j}^{AIR}(t)c_{PG}(T_s-T_{amb})+A^{AIR}_{i,j}(t)Y_{O,I}}{(\rho_{bs}c_{ps}T_s-(\rho_{bs}c_{ps}+S_{NAPL}(t)\phi\rho_{NAPL}c_{pNAPL})T_{amb})}$$

\(\theta_{i,j}(t)\) is orientation of the local air vector, \(m_{i,j}^{AIR}(t)\) is the local air mass flux, \(c_{PG}\) is the specific heat constant for the gas phase, \(T_s\) is the peak smouldering temperature, \(T_{amb}\) is the ambient system temperature, \(A\) is a calibration parameter, \(\Delta H_r\) is the effective heat of smouldering, \(v_O\) is the oxygen to fuel overall stoichiometric coefficient, \(Y_{O,I}\) is the initial mass fraction of oxygen present in the gas phase, \(\rho_{bs}\) is the bulk density of the solid, \(c_{ps}\) is the specific heat constant for the solid, \(S_{NAPL}^{i,j}(t)\) is the local contaminant saturation, \(\phi\) is the solid porosity, \(\rho_{NAPL}\) is density of the NAPL, and \(c_{pNAPL}\) is the specific heat constant for the NAPL.

In the front expansion component of the PSM, the ignition source is defined with an initial ellipse whose vertices are mapped to node centres. Equation 19 is solved at each vertex on the current ellipse, and the resulting velocities are passed to the front expansion model. In order for the smouldering front to advance at any vertex, conditions of minimum local contaminant concentration and minimum local air flux must be met. The minimum air flux, \(\lambda\), is a calibrated parameter and provides a crude approximation of the complex processes that are actually involved in extinction.

After solving the new smouldering front position, the vertices defining the new front undergoing clipping to remove any loops that formed by the front overlapping itself (Finney, 1998), and re-gridding to ensure the spatial definition of the front vertices is equivalent to the grid spacing of the multiphase flow model (Richards, 1995), Step 5 in Figure 2.6. Simple examples of front clipping and re-gridding are shown below in Figure 2.9. The PSM assumes any nodes behind the front have been completely treated, and all NAPL is removed from these nodes, leaving only a residual amount for model convergence (Step 5 in Figure 2.4).
Figure 2.9. Examples of pre and post (a) clipping, and (b) re-gridding, where the squares, dots, and closed curve represent the model nodes, smouldering front vertices, and smouldering front, respectively.

2.4.5 Previous Work with the PSM

MacPhee et al. (2012) originally calibrated the model to minimize the root mean square error between the predicted and experimental forward smouldering velocities of four column-scale experiments from Pironi et al. (2011) with different air fluxes but a constant contaminant saturation. Model validation confirmed the global behaviour of the front propagation, including the final extent of treatment, was correctly predicted (MacPhee et al., 2012). Figure 2.10a shows the model domain used during calibration and validation, while Figure 2.10b and c demonstrate the initial air flux vector distribution and position of the front at progressive times predicted by the calibrated model.
Additional simulations were performed confirming the models ability to handle heterogeneous contaminant saturation fields, heterogeneous soil permeability fields, point and line ignition sources, and multiple ignition sources. MacPhee et al. (2012) also investigated model sensitivity to nodal discretization and the front re-gridding scheme, confirming that the PSM is a numerically stable and computationally efficient tool that can approximate global smouldering front behavior, where permeability to the air phase plays a dominant role in predicting the smouldering velocity. In simulations where the smouldering front was anticipated to evolve as a smooth line, some small irregularities were observed on the predicted front (Figure 2.10c), which were explained as by-products of coupling the node based multi-phase flow model with the Cartesian-coordinate based front expansion model (MacPhee et al., 2012).

In the absence of experimental data, MacPhee et al. (2012) assumed values for calibration constants $\alpha$, $\beta$, and $\kappa$ from Equations 16-17, and the local air flux extinction threshold, $\lambda$ (Table 2-1). Hasan et al. (2015) conducted the first series of 2-D STAR experiments, smouldering coal tar in sand. These experiments quantified the vertical, horizontal, and downward smouldering propagation rates and the final extent of treatment. These experimental values were then used to calibrate the forward, opposed, and lateral rates and extent of treatment in the PSM. From these
experiments, Hasan et al. (2015) observed a positive linear relationship between injected air flux and average forward smouldering velocity, a non-linear positive relationship between injected air flux and lateral propagation of the front, and no opposed smouldering. The model calibration results from Hasan et al. (2015) are summarized below in Table 2-1, and the calibrated model was proven to well predict the experimental results.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>α (⁻)</td>
<td>0.875, assumed</td>
<td>0.50, fit</td>
</tr>
<tr>
<td>β (⁻)</td>
<td>0.875, assumed</td>
<td>0.150, fit</td>
</tr>
<tr>
<td>κ (⁻)</td>
<td>0.125, assumed</td>
<td>0.50, fit</td>
</tr>
<tr>
<td>λ (cm/s)</td>
<td>0.5, assumed</td>
<td>5.6, fit</td>
</tr>
<tr>
<td>A (⁻)</td>
<td>0.10, fit</td>
<td>0.10, from MacPhee et al. (2012)</td>
</tr>
</tbody>
</table>

An example of a 2-D simulation using the PSM is shown below in Figure 2.11, which includes the model domain, predicted initial air flux distribution, and predicted smouldering front evolution. In their modelling study, Hasan et al. (2015) found that the predicted air flux distribution was dependent on the predicted front propagation, and thus changed over time.
Figure 2.11. (a) model set up for calibration and validation simulations, examples of (b) the predicted initial air flux vector distribution, and (c) the predicted smouldering front position from time $t=0$ (ignition) to 55.83 min (end of treatment) at 2.5 minute intervals for 2-D smouldering, from Hasan (2013).
The model employs numerous assumptions to permit rapid, large scale engineering simulations that are not possible with detailed, thermodynamic models. Therefore, this model is suitable for simulations exploring the effects of parameters affecting air flux distribution, including injected air flux, contaminant saturation, and heterogeneity. The PSM is not suitable for simulations exploring situations where temperature effects are dominant, such as ignition or extinction of self-sustained smouldering, or fuel mobility. Other limitations of the model include a unique calibration is required for each soil/contaminant pair, and as it is only a dual-phase flow model, it does not consider the effects of water present as a third phase, and cannot currently be applied to predict smouldering behaviour below the groundwater table.

2.5 Summary

There is a pressing need for innovation in treating waste oil sludge, as volumes of this hazardous material continue to grow worldwide (da Silva et al., 2012; Hu et al., 2013). STAR is a thermal treatment technology that utilizes smouldering combustion to destroy liquid contaminants. STAR is an oxygen limited process, with multiple studies displaying a near linear relationship between injected air flux and the average vertical smouldering velocity. The robustness of STAR has been proven in a number of studies that investigated the impact of contaminant type, contaminant saturation, soil type, injected air flux, water saturation, heterogeneity, and scale (Switzer et al., 2009; Pironi et al., 2011; Switzer et al., 2014; Scholes et al., 2015; Grant et al., 2016).

Due to the complexity of smouldering combustion and the need for a large number of kinetic parameters, multi-physics modelling of smouldering combustion is often limited to small-scale, one-dimensional (1-D) systems (Rein, 2005). Therefore, in order to have a computational efficient engineering design tool that can handle large-scale and complex domains, MacPhee et al. (2012) developed a phenomenological smouldering model. The model approximates the evolution of the leading edge of the smouldering front in a 2-D vertical cross section, based on air and contaminant distributions throughout the system, while considering relative permeability effects. This approach to modelling smouldering combustion is valid for engineered smouldering applications, where air flux distribution is a key parameter. The model is useful for estimating the global behaviour of the smouldering front, including the average smouldering velocity and the final extent of treatment. However, it must be uniquely calibrated to each soil/contaminant pair, and does not consider temperature effects or thermodynamics. While the model has the
potential to be applied as an informative design tool, to date it has only been calibrated and validated against small scale 1-D and 2-D experiments, and has yet to be applied for engineering purposes.

2.6 References


Chapter 3

3 Numerical Modelling of the STARx Hotpad for Waste Oil Sludge Treatment

3.1 Introduction

Treatment of waste oil sludge is a worldwide problem (Hu et al., 2013). A by-product of the petroleum hydrocarbon industry, waste oil sludge was historically stored in unlined lagoons, and is often classified as a hazardous waste due to high concentrations of toxic substances, including polycyclic aromatic hydrocarbons (PAHs) and heavy metals (da Silva et al., 2012). The current global generation rate of waste oil sludge is estimated to be 60 million tonnes per year, which is in addition to the estimated 1 billion of waste oil sludge that was historically generated (da Silva et al., 2012). The physical and chemical properties of waste oil sludge depend on the crude oil source and how it was processed, but it is typically an emulsion of petroleum hydrocarbons, water, solids, and metals (Mazlova and Meshcheryakov, 1999). Numerous technologies have been developed to treat waste oil sludge, and thus reduce health risks for human and environmental receptors (Mrayyan and Battikhi, 2005; Mater et al., 2006; Liu et al., 2009; Xu et al., 2009; da Rocha et al., 2010). Existing treatment technologies include methods for sludge oil recovery (e.g., solvent extraction, centrifugation, surfactant enhanced oil recovery, and pyrolysis) and methods for sludge disposal (e.g., incineration, stabilization/solidification, and landfilling). However, all of the existing methods require large financial, land, and/or energy resources (Hu et al., 2013).

Recently, Self-sustaining Treatment for Active Remediation (STAR) was developed as a thermal remediation technology for contaminated soils (Pironi et al., 2009; Switzer et al., 2009; Pironi et al., 2011; Switzer et al., 2014). STAR is based on the principles of smouldering combustion, a flameless and exothermic oxidation reaction that can be self-sustaining under appropriate conditions (Ohlemiller, 2002). STAR utilizes the high calorific value of many recalcitrant liquid contaminants, such as creosote and coal tar, to sustain a smouldering reaction in porous media, destroying the contaminant in the process (Pironi et al., 2009; Switzer et al., 2009). Liquid contaminants embedded in inert soils grains are well suited for self-sustained smouldering
combustion as the liquid coated soil grains provide a high contaminant surface area, while the soil porosity allows for adequate oxidant delivery to the contaminant (Pironi et al., 2009). Additionally, the porous medium provides thermal insulation, mitigating heat losses, and the soil’s specific heat capacity enables recycling of heat evolved from the reaction (Pironi et al., 2009). This technology has multiple advantages and may be more sustainable than existing treatment technologies as it performs better with high contaminant concentrations, only requires a short, one time input of energy to ignite the reaction, and does not require an external fuel source to maintain the reaction (Switzer et al., 2009). STAR has been proven effective in treating a variety of contaminants at multiple field sites (Scholes et al., 2015; Grant et al., 2016), and is now being adapted for ex situ applications (STARx).

One STARx configuration under consideration is the “hotpad”, in which large batches of contaminated soil are treated in a pile placed upon an engineered base that includes co-located heating and air injection (Figure 3.1).

![Conceptual drawing of a full-scale hotpad implementation](Savron, 2016)

Hotpads may be a low cost, energy efficient method for treating liquid industrial waste (e.g., waste oil sludge) that has been intentionally mixed with sand, or stockpiles of excavated contaminated soils. The objective of the hotpad design process is to maximize batch treatment contaminant mass, while minimizing batch treatment time. Pilot-scale hotpad tests were
developed in order to inform the design and operation of the full-scale system. However, since these experiments are time and resource intensive, a limited number can be completed. Numerical simulations are a complementary means of gaining valuable insight into the anticipated system performance under various conditions.

Multi-physics modelling of smouldering combustion is often limited to small-scale, one-dimensional (1-D) systems due to the complexity of smouldering combustion and the need for a large number of kinetic parameters (Rein, 2005). MacPhee et al. (2012) developed a phenomenological model that simulates the propagation of a smouldering front in a two-dimensional (2-D) vertical cross-section in contaminated soil. The model has the ability to predict STAR propagation in large-scale, complex domains but requires calibration for each soil/contaminant pair. After original calibration and validation against 1-D column experiments (MacPhee et al., 2012), the model was subsequently calibrated and validated against bench-scale 2-D STAR experiments and was shown to correctly predict the time and extent of treatment in a 2-D vertical slice (Hasan et al., 2015). The model has never been applied to evaluate STARx, or as an engineering tool for STARx implementation.

This chapter presents the results of two pilot-scale hotpad experiments and the accompanying numerical modelling study that was completed to inform the design and operation of STARx hotpads. In this work, “pilot-scale” refers to approximately 1.4 m$^3$ of contaminated soil, containing 175 kg of organic liquid. Similarly, “full-scale” refers to approximately 156 m$^3$ of contaminated soil, representing roughly 20 000 kg of organic liquid. For the first time, the model was calibrated and validated against pilot-scale data and a measured relative permeability-saturation ($k_r$-$S$) constitutive function was utilized in the model. Sensitivity studies were conducted to infer the impacts of injected air flux rate, contaminant saturation, heterogeneity in permeability and saturation, and hotpad configuration at the pilot-scale. Additional full-scale hotpad simulations were also completed. This study provides predicted total treatment masses, times, and overall treatment rates that can be expected for full-scale, three-dimensional (3-D) systems.
3.2 Methods

3.2.1 Model Formulation

This work employed a phenomenological numerical model that can approximate the propagation of the leading edge of a smouldering reaction (hereafter, the smouldering front) in large-scale STAR applications with heterogeneous contaminant, airflow, and soil permeability conditions (MacPhee et al., 2012). As the model was fully described and tested in previous publications in both one- (MacPhee et al., 2012) and two-dimensions (Hasan et al., 2015), only a summary is provided here. Additional details are provided in Section 2.4.

The model couples a multi-phase flow model, DNAPL3D (Gerhard and Kueper, 2003c; Gerhard and Kueper, 2003a), with a front expansion model (Richards, 1990; Richards, 1995). The former has been used extensively for simulating the movement of two immiscible liquids in heterogeneous porous media (Kueper and Frind, 1991; Gerhard et al., 1998; Gerhard and Kueper, 2003c; Gerhard and Kueper, 2003a; Grant et al., 2007), while the latter has been used for predicting the movement of forest fire fronts in complex wind and fuel load environments (Finney, 1998). Here, in a given time step, \(t\), DNAPL3D first solves the flow of two immiscible fluids in porous media via the continuity equations for the mass balance of the wetting and non-wetting phases, where wetting phase pressure and saturation are the primary variables (Bear, 1972). In this work, waste oil sludge (hereafter referred to more generally as “the organic liquid”) and air are the wetting and non-wetting phases, respectively. After applying Darcy’s Law to solve the local (i.e., at each node, \(i,j\)) air fluxes, values of local air mass flux, \(m_{i,j}^A(t)\), and organic liquid saturation, \(S_{i,j}^O(t)\), are provided to an analytical expression for the local forward smouldering velocity (MacPhee et al., 2012):

\[
V_{i,j}^f(t) = \frac{\eta_{i,j}^A(t) c_p g (T_e - T_{amb}) + A \frac{\Delta H_p}{\rho_p} m_{i,j}^A(t) Y_O I}{(\rho_{bs} c_{ps} T_e - (\rho_{bs} c_{ps} + S_{i,j}^O(t) \phi \rho_o c_{po}) T_{amb})} i, j = x, y
\]

where definition of remaining variables is provided in Table 3-1. Equation 1 must be calibrated to each soil/contaminant pair using the calibration coefficient, \(A\).
Table 3.1 Smouldering Velocity Parameters for Equation 1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_{pg}$ Specific heat of the gas</td>
<td>1100 (J/kg/K)$^a$</td>
</tr>
<tr>
<td>$T_s$ Smouldering temperature</td>
<td>1030 (K)$^b$</td>
</tr>
<tr>
<td>$T_{amb}$ Ambient Temperature</td>
<td>293 (K)$^b$</td>
</tr>
<tr>
<td>$A$ Forward smouldering velocity calibration parameter</td>
<td>calibrated</td>
</tr>
<tr>
<td>$\Delta H_r$ Effective heat of smouldering</td>
<td>39.4 (MJ/kg)$^b$</td>
</tr>
<tr>
<td>$v_o$ Overall stoichiometric coefficient</td>
<td>2.89$^b$</td>
</tr>
<tr>
<td>$Y_{O, I}$ Mass fraction of oxygen in the gas phase</td>
<td>0.235 (kg O$_2$/kg gas)$^c$</td>
</tr>
<tr>
<td>$\rho_{bs}$ Bulk density of the soil</td>
<td>1700 (kg/m$^3$)$^d$</td>
</tr>
<tr>
<td>$c_{ps}$ Specific heat of the porous media</td>
<td>1265 (J/kg/K)$^c$</td>
</tr>
<tr>
<td>$\phi$ Porosity</td>
<td>0.38$^e$</td>
</tr>
<tr>
<td>$\rho_{o}$ Density of the organic liquid</td>
<td>850 (kg/m$^3$)$^d$</td>
</tr>
<tr>
<td>$c_{po}$ Specific heat of the organic liquid</td>
<td>1880 (J/kg NAPL/K)$^c$</td>
</tr>
<tr>
<td>$\alpha + \kappa$ Local forward velocity constant</td>
<td>1.0$^f$</td>
</tr>
<tr>
<td>$\alpha - \kappa$ Local opposed velocity constant</td>
<td>0.0$^f$</td>
</tr>
<tr>
<td>$\beta$ Local lateral velocity constant</td>
<td>0.15$^f$</td>
</tr>
<tr>
<td>$\lambda$ Air Extinction threshold</td>
<td>calibrated (cm/s)</td>
</tr>
</tbody>
</table>

$^a$ Bergman et al. (2011)
$^b$ Pironi (2009)
$^c$ Perry and Green (2008)
$^d$ Savron (2016)
$^e$ Grant (2005)
$^f$ Hasan et al. (2015)

The semi-analytical front expansion model then uses the local smouldering velocities calculated for each node with Equation 1. For a given shape of the smouldering front at time $t$, a series of “sub-ellipses” are generated along the perimeter to approximate the smouldering front expansion over that time step. The unique size and orientation of each sub-ellipse is based on the local forward smouldering velocity calculated by Equation 1 (MacPhee et al., 2012). For any sub-ellipse to expand, the local air flux and organic liquid saturation at that node must exceed the calibrated air flux extinction threshold, $\lambda$, and the saturation extinction threshold, $S_{MIN}$. The dimensions of the local sub-ellipse are then determined by the empirical constants $\alpha$, $\beta$, and $\kappa$ in combination with Equation 1, representing local forward, lateral, and opposed rates of smouldering (Richards, 1990). The outer perimeter of all local sub-ellipses is then enclosed, creating a new global smouldering front. This front then undergoes clipping and re-gridding to ensure the predicted front is continuous with adequate spatial definition (see Section 2.4.3 for more details). Organic liquid is removed from any nodes that are behind the new smouldering
front, assuming these nodes have been completely treated; this approximates observed STAR behaviour (Hasan et al., 2015).

The net effect of this coupled modelling approach is the ability to predict the complex shape of a 2-D smouldering front over time, given spatial variability in intrinsic permeability and accounting for how the air mass flux and organic liquid saturations change in space and in time (MacPhee et al., 2012; Hasan et al., 2015). The main advantage of the model is its ability to solve complex smouldering conditions with computational efficiency. However, as the model does not consider temperature effects or explicitly solve the energy equation, it is most appropriate for engineering simulations that are consistent with the processes for which it is valid (e.g., front propagation sensitivity to air flux, permeability, liquid saturation).

3.2.2 Model Calibration

3.2.2.1 Hotpad Experiment A

The model was calibrated to the results of Hotpad Experiment A. The pilot-scale hotpad is a 3 m x 3 m metal base with 0.45 m high sidewalls designed to hold contaminated soils and treat them with STARx (Figure 3.2). The hotpad base includes a 1.5 m x 1.5 m central plenum that provides co-located heating and air injection (Figure 3.3a). In Experiment A, approximately 2041 kg of coarse (0.95 mm) silica clean sand was mixed with 154 kg of manufactured waste oil sludge surrogate (the organic liquid) in fifteen batches. Each batch had an expected organic liquid saturation, $S_O$, of 40% by volume (based on the volumes added), and was mechanically mixed until deemed homogeneous on the basis of visual inspection. Using this mixture, a 0.3 m high contaminant pack with sloped slides was constructed, which extended 0.6 m beyond the plenum on all sides (Figure 3.2a). Then, a 0.3 m high clean sand cap was constructed on top (Figure 3.2b). A clean sand cap is typically included in all STARx applications for several benefits (e.g., heat retention, reduced surface temperatures, surface flaming prevention, emissions filtering, air control). The entire sand pack was instrumented with nine thermocouple bundles in a 3 x 3 grid to record spatial and temporal temperature variations during testing. After 9 hrs of pre-heating, a smouldering reaction was ignited with an injected air flow rate of 33 L/s (a Darcy air flux of 1.5 cm/s, considering the cross-sectional area of the plenum).
Figure 3.2. Pre-treatment loading of (a) the contaminant pack and (b) the clean sand cap in Hotpad Experiment A. Post-treatment excavation revealed (c) complete treatment in the centre of the contaminant pack, where the reddish color is due to iron oxidation and (d) an untreated, black crust on the edges of the contaminant pack base.

3.2.2.2 Model Set-Up

As shown in Figure 3.3a, a 3.00 m wide x 0.72 m tall model domain was designed to approximate a 2-D vertical cross-section of Hotpad Experiment A.
A maximum time step of 5 seconds was selected as this value was previously demonstrated to retain accuracy while preventing excessive run times (MacPhee et al., 2012). A nodal discretization of 0.015 m × 0.015 m was selected, for a total of 9600 nodes in the domain, which maximized resolution of the Intel Core processor with 64 GB RAM (typical run time was 30 hrs). Model testing revealed that further decreases in grid size produced no change in the predicted result (Appendix D). No-flow conditions were applied to the left and right boundaries to simulate the impermeable metal hotpad walls. The 0.15 m deep plenum was approximated with a constant air flux of 1.5 cm/s applied across a single row of nodes along the centre 1.5 m of the bottom boundary. The top row of nodes was specified as a free-exit boundary with a constant air pressure of 0 Pa and constant organic liquid saturation of 1%. Nodes located inside the contaminant pack were assigned an initial organic liquid saturation of 40% and nodes in the
clean sand cap were assigned a residual (i.e., immobile) organic liquid saturation of 1%. Note that this negligible wetting phase saturation is assigned to all uncontaminated nodes to maintain continuity of the wetting phase throughout the domain, as required by the model’s formulation. Any nodes located inside the contaminant pack are initially referred to as “contaminated”, and after the simulated smouldering front passes through a node, it is then referred to as ‘treated’. The remaining input parameters used during model calibration and all predictive simulations are summarized above in Table 3-1 and below in Table 3-2.

Table 3-2 Additional Fluid and Porous Media Parameters Used in Simulations

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\sigma)</td>
<td>Surface tension 0.033 (N/m)(^{a,b})</td>
</tr>
<tr>
<td>(\rho_{\text{air}})</td>
<td>Density of air 1.204 (kg/m(^3))(^{a,c})</td>
</tr>
<tr>
<td>(\mu_{\text{air}})</td>
<td>Air viscosity 1.81 E-05 (Pa s)(^{a,c})</td>
</tr>
<tr>
<td>(\mu_{\text{O}})</td>
<td>Organic liquid viscosity 51.108 (Pa s)(^{d,e})</td>
</tr>
<tr>
<td>(k_i)</td>
<td>Mean permeability Tested</td>
</tr>
<tr>
<td>(P_D)</td>
<td>Displacement pressure 258.0(^f)</td>
</tr>
</tbody>
</table>

\(^{a}\) At temperature of 20 °C
\(^{b}\) Pendent Drop Shape Method with an Axisymmetric Drop Shape Analyser (ADSA), Lord et al. (2000)
\(^{c}\) Potter (2002)
\(^{d}\) At temperature of 24 °C
\(^{e}\) Kinsman (2015)
\(^{f}\) Grant (2005)

Preliminary simulations revealed that predicted smouldering behavior in multi-dimensional scenarios is highly sensitive to the air relative permeability-saturation constitutive relationship in the model. Therefore, this relationship was measured for the specific soil/organic liquid pair being simulated. First, the intrinsic permeability, \(k_i\), of the 0.95 silica sand was measured (ASTM D6539). The organic liquid was then mechanically mixed with clean 0.95 silica sand to produce seven organic liquid saturations ranging from 10% to 95%, and the effective permeability, \(k_{\text{eff}}\), of each sample was determined (ASTM D6539). Only tests with a best-fit linear relationship between air flow rate and pressure drop exhibiting an \(R^2 > 0.95\) were retained. The non-wetting phase drainage relative permeability function (Gerhard and Kueper 2003c) was then fit to the data. As shown in Table 3-3, values of \(S_{O}^M\), \(S_{r}^k\), \(\Delta S_{O}^{\ast d}\), and \(\lambda_d\) were assumed (Grant, 2005) as they exert limited influence on the shape of the curve and are not easily quantified using the apparatus available. The dominant variables in this function, \(k_{rN}^{\text{max}}\) and \(\tau_d\), were used as fitting
parameters to minimize the root mean square error (RMSE) between the experimental data and the function.

The measured $k_i$ was applied to the contaminant pack and clean sand cap in the model domain, as well as the plenum (see Figure 3.3). Within each region, the permeability was assumed to be homogeneous and isotropic. The ignition source was specified as a 0.015 m high x 1.515 m long initial ellipse (i.e., time zero smouldering front) centered on the middle of the plenum. The measured liquid viscosity employed (Table 3-2) corresponds to 24 °C; temperature effects on liquid viscosity were not explored in this work. A minimum organic liquid saturation for smouldering, $S_{\text{MIN}}$, of 7% was assumed based on previous modelling studies (MacPhee et al., 2012; Hasan et al., 2015), and is not anticipated to impact the results of this work.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_r N_{\text{max}}$</td>
<td>Maximum relative permeability to the non-wetting phase</td>
</tr>
<tr>
<td>$\tau_d$</td>
<td>Drainage non-wetting phase relative tortuosity exponent</td>
</tr>
<tr>
<td>$\lambda_d$</td>
<td>Pore size distribution index</td>
</tr>
<tr>
<td>$S_{O M}$</td>
<td>Emergence saturation</td>
</tr>
<tr>
<td>$S_r N^k$</td>
<td>Residual wetting phase parameter associated with $k_r N$</td>
</tr>
<tr>
<td>$\Delta S_O$</td>
<td>Fitting parameter that determines $k_r N$ when $S_O = S_{O M}$</td>
</tr>
</tbody>
</table>

$^a$ Grant (2005)

3.2.2.3 Model Calibration

The model was calibrated to reproduce three metrics from Hotpad Experiment A: (i) average vertical smouldering velocity, (ii) treatment time, and (iii) the extent of treatment. The calibration coefficient, $A$, in the forward smouldering velocity expression (Equation 1) was systematically adjusted so that the model reproduced (i), then the air flux extinction threshold, $\lambda$, was adjusted so that the model reproduced (ii) and (iii).

The experimental average vertical smouldering velocity was calculated using temperature data averaged from all nine thermocouple bundles (Appendix A). The experimental treatment time corresponds to the time when smouldering ceases. For this work, only the period of self-sustained combustion was considered, which is defined as the time from when the heater is turned off until combustion finishes. Additional time required for preheating and cooling will increase total treatment times from those reported in this work. Carbon monoxide (CO)
emissions were measured throughout the hotpad experiment and used as an indication of combustion. It is typically assumed that combustion is essentially complete when CO emissions fall below 30 parts per million (ppm) (Savron, 2016). The post-treatment boundary between clean and contaminated material was measured to quantify the extent of treatment (see Figure 3.2).

The time when the predicted smouldering front first reaches the top of the contaminant pack is hereafter referred to as the “breakthrough time”. The predicted average vertical smouldering velocity was calculated as the vertical height at the centre of the contaminant pack divided by the breakthrough time. As the breakthrough time is simply the first arrival of the predicted smouldering front, it is only used to compare simulations and does not provide an absolute time. In reality there will likely be a range of breakthrough times. The predicted treatment time was defined as either the time when no contaminated nodes remained (i.e., complete treatment), or when the number of contaminated nodes did not change for at least 2 hrs, whichever occurred first. The predicted extent of treatment was taken as the predicted position of the smouldering front at the predicted treatment time.

3.2.3 Model Validation

The model was validated against Hotpad Experiment B, which used the same organic liquid and sand as Hotpad Experiment A, but a different contaminant pack configuration and injected air flux (1.3 cm/s). The validation simulation applied the same input parameters and boundary conditions as the calibration simulation, while the domain configuration and injected air flux reflected the different experimental conditions, as shown in Figure 3.3b. No calibration or parameter adjustment was conducted. Performance of the validation simulation was evaluated against the same metrics that were used for model calibration. However, due to thermocouple placement in Hotpad Experiment B, temperature data was only available from a single thermocouple at the top of the 0.6 m contaminant pack to calculate the average vertical smouldering velocity (Figure 3.3b).

3.2.4 Predictive Simulations

A comprehensive suite of predictive simulations was completed to infer the effects of system design (i.e., hotpad dimensions, contaminant pack configuration), operational parameters (i.e.,
injected air flux, organic liquid saturation), and environmental factors (i.e., heterogeneity) on the overall rate and extent of treatment. The objective of these simulations was to identify conditions that would maximize hotpad batch treatment mass while minimizing batch treatment time. Note that all treatment rates and masses reported in this study are only representative of the 2-D model domain, which is a cross-sectional vertical slice of the actual 3-D hotpad system with an assumed depth of 1 meter into the page. It is expected that the treatment rate (mass per time) and total mass treated for a 3-D system can be approximately estimated by multiplying the simulated results by the actual contaminant pack depth, although some error will be introduced by neglecting corner effects in the third dimension. It is expected that temporal metrics like breakthrough time and total treatment time will be similar between 2-D and 3-D systems.

3.2.4.1 Sensitivity Study

A sensitivity study was performed to explore the effects of key parameters on predicted smouldering behavior. All of these simulations used contaminant pack configuration TRAP1 shown in Figure 3.4. The base case simulation (3a in Table 3-4) exhibited a homogenous contaminant pack saturation of 40%, homogeneous sand permeability, and an injected air flux of 1.5 cm/s. Seven simulations (3b through 3h in Table 3-4) were conducted to explore the effects of injected air flux (0.33 – 3.0 cm/s or 8 – 68 L/min), and contaminant pack saturation (20% – 80% or 37 400 – 149 600 mg/kg). As each parameter was varied, the others were kept fixed at the base case value.

Sensitivity to heterogeneity of both intrinsic permeability and saturation of the contaminant pack were explored in ten additional simulations (3i to 3r in Table 3-4). For treatment of organic liquid mixed with sand, heterogeneity may occur due to operational reasons (e.g., incomplete mechanical mixing of the sand and organic liquid) or environmental conditions (e.g., non-uniform soil sources, natural variation in organic liquid waste type). For treatment of excavated contaminated soils, heterogeneity is anticipated to occur primarily from environmental conditions (e.g., natural heterogeneity in soil type, spatial variation in contaminant type and concentration). A computer program, KGEN, was used to generate five realizations of a spatially correlated random intrinsic permeability field. KGEN employs the Turning Bands (Mantoglou and Wilson, 1982) method while assuming an exponential autocorrelation function (Kueper and Gerhard, 1995). The ratio of standard deviation to the mean, or coefficient of variation (COV),
was used to compare the degree of variance, and thus heterogeneity, between fields. Each permeability field was assigned the same mean natural logarithm of the hydraulic conductivity, \( \ln(K) \), (equal to the measured value), and exhibited COVs ranging from 0 (homogeneous base case) to 0.26; the latter representing a range of soil types from medium gravel to fine sand (Bear, 1972). These five random permeability fields were normalized to produce five random saturation fields with a mean saturation of 40\%, exhibiting COVs from 0 (homogeneous base case) to 0.29, the latter exhibiting 95\% of the nodes with organic liquid saturations between 17\% and 63\% of the pore space. The heterogeneous permeability and saturation fields that were generated for Simulations 3i-3r are summarized below in Table 3-5 and Table 3-6, respectively. All ten fields had horizontal and vertical correlation lengths of 8.17 cm and 8.13 cm, respectively, which is reasonable for a mechanically mixed contaminant pack. Areas of high permeability in the permeability fields correspond to areas of low saturation in the saturation fields, therefore such areas are expected to exhibit higher relative air fluxes in both sets of simulations.
<table>
<thead>
<tr>
<th>Simulation</th>
<th>Configuration</th>
<th>Plenum Width (m)</th>
<th>Injected Air Flux (cm/s)</th>
<th>Mean Saturation</th>
<th>Permeability Heterogeneity</th>
<th>Saturation Heterogeneity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Calibration</td>
<td>1.5</td>
<td>1.50</td>
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<td>Homogenous</td>
</tr>
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<td>2</td>
<td>Validation</td>
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<td>Homogenous</td>
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<td>3a (base case)</td>
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<td>Homogenous</td>
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<td>Homogenous</td>
</tr>
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<td>3d</td>
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<td>Homogenous</td>
</tr>
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<td>TRAP1</td>
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<td>0.40</td>
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<td>Homogenous</td>
</tr>
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<td>0.80</td>
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</tr>
<tr>
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</tr>
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<tr>
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</tr>
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<td>0.40</td>
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</tr>
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<td>1.50</td>
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<td>Medium</td>
</tr>
<tr>
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<td>1.50</td>
<td>0.40</td>
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<td>Medium High</td>
</tr>
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<td>TRAP1</td>
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<td>1.50</td>
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<td>High</td>
</tr>
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<td>Homogenous</td>
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<tr>
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<td>1.50</td>
<td>0.40</td>
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</tr>
<tr>
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</table>
Table 3-5 Summary of Heterogeneous Permeability Fields

<table>
<thead>
<tr>
<th>Field</th>
<th>Mean ln(K)</th>
<th>Variation, Normalized ln(K)</th>
<th>Mean $k_i$ (m$^2$)</th>
<th>Minimum $k_i$ (m$^2$)</th>
<th>Maximum $k_i$ (m$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>homogeneous</td>
<td>-0.51</td>
<td>0.00</td>
<td>6.12E-10</td>
<td>6.12E-10</td>
<td>6.12E-10</td>
</tr>
<tr>
<td>1P</td>
<td>-0.51</td>
<td>0.05</td>
<td>6.11E-10</td>
<td>2.25E-10</td>
<td>1.33E-09</td>
</tr>
<tr>
<td>2P</td>
<td>-0.51</td>
<td>0.07</td>
<td>6.10E-10</td>
<td>1.81E-10</td>
<td>1.77E-09</td>
</tr>
<tr>
<td>3P</td>
<td>-0.52</td>
<td>0.15</td>
<td>6.07E-10</td>
<td>4.05E-11</td>
<td>6.51E-09</td>
</tr>
<tr>
<td>4P</td>
<td>-0.52</td>
<td>0.21</td>
<td>6.05E-10</td>
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<td>1.96E-08</td>
</tr>
<tr>
<td>5P</td>
<td>-0.52</td>
<td>0.26</td>
<td>6.04E-10</td>
<td>5.18E-12</td>
<td>3.90E-08</td>
</tr>
</tbody>
</table>

*Note: All hydraulic conductivity (K) values reported in this work are given in units of cm/s, and all intrinsic permeability ($k_i$) values are given in units of m$^2$.

Table 3-6 Summary of Heterogeneous Saturation Fields

<table>
<thead>
<tr>
<th>Field</th>
<th>Mean Saturation</th>
<th>Variation, Normalized Saturation</th>
<th>Minimum Saturation</th>
<th>Maximum Saturation</th>
</tr>
</thead>
<tbody>
<tr>
<td>homogenous</td>
<td>0.40</td>
<td>0.00</td>
<td>0.40</td>
<td>0.40</td>
</tr>
<tr>
<td>1S</td>
<td>0.40</td>
<td>0.04</td>
<td>0.35</td>
<td>0.45</td>
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<tr>
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<td>0.40</td>
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<tr>
<td>3S</td>
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<td>0.62</td>
</tr>
<tr>
<td>4S</td>
<td>0.40</td>
<td>0.21</td>
<td>0.12</td>
<td>0.72</td>
</tr>
<tr>
<td>5S</td>
<td>0.40</td>
<td>0.29</td>
<td>0.01</td>
<td>0.85</td>
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</tbody>
</table>

3.2.4.2 Hotpad Configuration

The initial organic liquid mass, and thus the potential batch treatment mass, is dependent on the height, width, and shape of the contaminant pack. Different configurations are expected to alter the distribution of air throughout the system, affecting rates and extents of treatment. Simulations 4a through 4g in Table 3-4 explored the effects of trapezoidal, rectangular, and pyramid shaped contaminant packs (Figure 3.4), while maintaining a 1.5 m plenum width, 1.5 cm/s injected air flux, 40% homogeneous contaminant pack saturation, and homogeneous permeability fields. Trapezoidal configurations were used to explore the effects of the “plenum overlap” (i.e., the extent to which the contaminant pack base extends beyond the plenum’s edge), which is expected to influence air flow patterns and extent of treatment. For example, in contrast to the 0.6 m plenum overlap in TRAP1, TRAP2 has a 0.1 m plenum overlap. The pyramid configurations, which had no plenum overlap, were designed to isolate the effects of the
contaminant pack height to width ratio, which ranged from 0.2 (PYR1) to 1.0 (PYR4). The rectangular configurations have more simplified geometry but would be more difficult to erect in the field. REC1 is a rectangular contaminant pack, for example emplaced with temporary walls, surrounded by clean sand. REC2 has permanent side walls that ensure the width of the contaminant pack is equal to the plenum width. REC2 is a valuable reference case because, like laboratory column experiments, it provides homogenous and unidirectional air distribution throughout the contaminant pack.

Figure 3.4. Trapezoidal (TRAP), rectangular (REC), and pyramid (PYR) contaminant pack configurations for Simulations 4a through 4g. The contaminant pack, clean sand cap, open air, and plenum are shaded pink, brown, white, and red, respectively.
3.2.4.3 Field-scale Design

When full-scale hotpads are implemented in the field, a network of adjacent hotpad units will be constructed to maximize the plenum footprint and potential treatment mass. The effective size of a hotpad system for a proposed field trial is 9.3 m wide x 8.4 m long x 2 m high at the centre, thereby treating approximately 20 tonnes of organic liquid in one batch, assuming a 40% organic liquid saturation. Two field-scale hotpad configurations, FIELD1 and FIELD2 in Figure 3.5, were tested in Simulations 5a and 5b in Table 3-4. Both configurations had a maximum contaminant pack height of 2 m, a 0.5 m tall clean sand cap, and a 9.3 m plenum width. The primary difference between these designs is that the wider contaminant pack in FIELD1 contains a higher initial organic liquid mass. Two sides of the hotpad are bordered with a soil berm, reproducing conditions at the proposed field test site. To isolate the effects of scale, the organic liquid saturation, sand permeability, and injected air flux values were identical to Simulation 3a. To accommodate this larger domain size, node discretization was increased to 0.05 m x 0.05 m for these simulations.

**FIELD1**

**FIELD2**

Figure 3.5. Full-scale hotpad configurations used in Simulations 5a and 5b, where the contaminant pack, clean sand cap, open air, plenum, and berms are shaded pink, brown, white, red, and black, respectively.
3.3 Results & Discussion

3.3.1 Model Calibration

In Hotpad Experiment A, the heater was turned off at 620 min, and self-sustained smouldering continued until 1602 min (Appendix A), yielding an experimental treatment time of 982 min. Thermocouple data revealed an average upwards vertical smouldering velocity of 0.11 cm/min. The post-treatment excavation confirmed that all organic liquid was destroyed, excluding a thin crust around the edges of the contaminant pack (Figure 3.2c and d). This crust of pyrolized contaminated soil exhibited the outline shown in Figure 3.6. The majority of the crust occurs in regions outside of the plenum’s direct influence, corresponding to air flux too low to support smouldering (further discussed in Section 3.3.3.1). Figure 3.6 shows that the final crust outline may have extended slightly outside the initial contaminant pack outline; this can occur due to upward (air-induced) mobilization of heated organic liquid and/or the re-condensation of volatilized compounds (Kinsman, 2015). The exploration of such secondary effects associated with STAR is beyond the scope of this work.

![Initial contaminant pack and clean sand cap outlines compared to the post-treatment crust from Hotpad Experiment A.](image)

Figure 3.6. Initial contaminant pack and clean sand cap outlines compared to the post-treatment crust from Hotpad Experiment A. Domain width and height are given in meters.

The intrinsic permeability of the sand was determined (geometric mean of seven tests) to be 6.12 x 10^{-10} m^2. Figure 3.7 presents the relative permeability-saturation measurements and the best-fit relative permeability function, employing \( k_{rN,max} = 0.90 \) and \( \tau_d = 0.12 \) (RMSE = 0.04), that was implemented for model calibration and all subsequent predictive simulations. Further details on relative permeability testing are available in Appendix B. It is noted that this \( k_{rN}-S \) function does not exhibit the curvature typically shown in textbooks (based upon rock cores), but is consistent
with those measured for unconsolidated sands with a uniform grain size distribution (Gerhard and Kueper, 2003c).

Figure 3.7. Measured relative permeability-saturation data and the best-fit function employed in all predictive simulations in this work, where effective saturation is \( \frac{S_o - S_r^k}{1 - S_r^k} \).

From a series of eight simulations that systematically altered the calibration parameters, the values \( A = 0.25 \) and \( \lambda = 0.5 \) cm/s were determined to minimize the two objective functions that quantified the difference between experimental and model-predicted calibration metrics (Appendix C). Figure 3.8a shows the predicted initial air flux distribution for the model calibration run (Simulation 1 in Table 3-4). The arrow size indicates that the air flux magnitude is highest in the centre of the contaminant pack, nearest to the plenum. The air flux magnitude decreases and its orientation shifts towards the horizontal with increasing lateral distance from the centerline. Figure 3.8b, providing the predicted position of the smouldering front at various times, reveals that the smouldering front first reaches the top of the 0.3 m contaminant pack (i.e., breakthrough) after 283 min (4.7 hrs). This corresponds to an average vertical smouldering velocity of 0.11 cm/min, which matches the 0.11 cm/min observed experimentally. The final
position of the simulated front was reached at 1016 min (~17 hrs), which compares well to the experimentally determined time of 982 min (~16 hrs). Moreover, the predicted shape of the untreated material closely matches that observed after Experiment A (Figure 3.8b). The relatively uniform manner in which the predicted smouldering front evolved is not surprising given the homogenous nature of the permeability and saturation fields. It is noted that the predicted front is similar but not perfectly symmetrical across the vertical centreline of the domain. This is due to small numerical differences between corresponding nodes on the left and right, and those differences occasionally result in +/- 1 node advance in the smouldering front. Moreover, this process results in a smouldering front with small (+/- 1 node) perturbations, which correctly represents a real (non-smooth) smouldering front. In Figure 3.8, it is shown that in this case these micro-perturbations do not grow with time, resulting in a relatively smooth front (at the macro scale) at all times. However, this is not always the case and this topic will be further explored in subsequent sections.

![Figure 3.8](image.png)

**Figure 3.8.** (a) Initial contaminant pack and clean sand cap outline with initial (i.e., t=0 at onset of smouldering) air flux vector distribution. (b) The predicted smouldering front position at 100, 283 (breakthrough), and 1016 min (end of treatment) for Simulation 1 (black) compared to the experimental extent of treatment (red). Note: \( \uparrow = 1.5 \text{ cm/s} \)

Figure 3.9 shows the predicted total organic liquid mass versus time, or treatment curve, for Simulation 1. It reveals that the predicted breakthrough time of 283 min separates the treatment
curve into an initial period of linear mass destruction (302 kg/day), followed by a non-linear tailing of the treatment rate (223 kg/day to 0.25 kg/day, per meter depth into the page) as the smouldering front approaches the end of treatment. The linear treatment rate in Figure 3.9 corresponds to when the smouldering front is travelling primarily upwards through the central area above the plenum dominated by high air flux (see Figure 3.8a).

**Figure 3.9. Predicted treatment curve (total organic liquid mass versus time) and predicted average velocity of the entire smouldering front versus time for Simulation 1 (calibration).**

Over this period, the average front velocity slightly decreases from 0.11 to 0.08 cm/min (Figure 3.9) as the local air fluxes slightly decrease with contaminant pack height (see Section 3.3.3.1 for additional details). Over the same period, the length of the smouldering front increases from 1.6 to 2.3 m (i.e., the front is slowing and growing). These two processes essentially offset each other, resulting in a relatively constant treatment rate. However, after breakthrough, the front primarily propagates laterally through areas on the edges of the contaminant pack dominated by lower air flux; this transition corresponds to the significant decrease in the average smouldering front velocity and the corresponding tailing mass destruction rate. The linear segment of the mass destruction curve accounts for 80% of the total mass destroyed but only 28% of the treatment time. In contrast, the non-linear segment accounts for 20% of the total mass destroyed.
but 72% of the treatment time. Note that the untreated crust at the end of treatment accounts for 12% of the initial organic liquid mass.

3.3.2 Model Validation

In Experiment B, thermocouple data yielded an average vertical smouldering velocity of 0.06 cm/min (Appendix A). The heater was turned off after 227 min of preheating and self-sustained smouldering continued until 1333 min, yielding a treatment time of 1106 min (Appendix A). The post-treatment excavation revealed treatment of the entire contaminant pack (i.e., no crust remained). Simulating Experiment B without any model adjustment provided results that matched well with the experiment, including predicting treatment of the entire contaminant pack (Appendix F, Figure A.14). The predicted average vertical smouldering velocity and treatment time were within 19% and 24% of the experimental values, respectively. Table 3-7 summarizes the main experimental and predicted metrics for the calibration and validation simulations.

<table>
<thead>
<tr>
<th>Table 3-7 Summary of Model Calibration and Validation Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calibration</td>
</tr>
<tr>
<td>---------------</td>
</tr>
<tr>
<td>Average Smouldering Velocity (cm/min)</td>
</tr>
<tr>
<td>Treatment Time (min)</td>
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<tr>
<td>Model Matches Experimental Extent of Treatment?</td>
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</table>

The discrepancy in velocities in the validation exercise is partially due to the low spatial resolution of thermocouple data in Hotpad Experiment B. Also, while Equation 1 predicts a uniform front propagation and linear velocity in homogeneous conditions, thermocouple data from lower contaminant pack heights in Experiment B revealed non-linear experimental velocities, suggesting minor heterogeneity was present in either organic liquid concentration or soil properties (Appendix A, Figure A.2). The discrepancy in treatment times may be explained by the fact that some organic liquid was relocated into the clean sand cap, either by mobilization or volatilization/recondensation, and then treated by smouldering, as revealed by the post-treatment excavation. Therefore the experimental treatment time likely over predicts the duration of smouldering strictly in the contaminant pack, which is all that is considered by the model.
3.3.3 Sensitivity Study

3.3.3.1 Injected Air Flux

Simulations 3b to 3e investigated the effects of the injected air flux. Figure 3.10 illustrates that as the injected air flux was increased from 0.75 to 3.00 cm/s, the predicted initial distribution and magnitude of the air vectors changed as expected. The initial air flux distribution was contoured to delineate the air flux extinction threshold (below which smouldering cannot be sustained), as shown below in Figure 3.10 (blue line). Increasing the injected air flux shifted the air flux extinction contour laterally outwards, thus increasing the extent of the treated region. The air flux distributions in these simulations changed little with time, revealing that the air flux distribution was not strongly coupled to evolution of the saturation field. As seen in Figure 3.10, the final extent of treatment (red line) closely matches the initial air flux extinction contour in all cases. This suggests that the final extent of treatment can be approximated from the initial air flux distribution under these conditions.
Figure 3.10. Initial air flux distribution for Simulations 3d (top), 3a (middle), and 3e (bottom), with outlines of the initial contaminant pack (black dashed), clean sand cap (black solid), plenum (black solid), and predicted final extent of treatment (red). The air flux extinction contour of 0.5 cm/s is shown in blue. Air flux inside the contour nearest the plenum exceeds the extinction threshold, while the areas outside the contour fall below the threshold at t=0. Note: $\downarrow = 1.5$ cm/s.

The injected air flux magnitude significantly affected the predicted rate and extent of treatment. The red curve in Figure 3.11 illustrates the positive, non-linear relationship between injected air flux and predicted extent of treatment. The 0% treatment case corresponds to an injected air flux of 0.33 cm/s (Simulation 3b in Table 3-4); a value lower than the air flux extinction threshold of 0.5 cm/s to ensure no smouldering occurred. When the injected flux equaled 0.5 cm/s (Simulation 3c in Table 3-4), the air flux threshold was exceeded in small areas directly above the left and right edges of the plenum, ultimately treating 1.3% of the contaminant pack.
(Appendix D). With further, small increases in injected air flux, the predicted treatment volume rapidly increased. Beyond an injected air flux of 1.5 cm/s, diminishing increases in predicted treatment volume occur. This relationship is a direct result of the shifting smouldering extinction contour explained above.

$$\text{Average Vertical Smouldering Velocity (cm/min)}$$

**Figure 3.11.** Final percent of the contaminant pack treated versus plenum injected air flux for Simulations 3b to 3e (red), average vertical smouldering velocity versus plenum injected air flux (blue), smouldering velocity predicted by Equation 1 versus injected air (black), and average vertical smouldering velocity versus average vertical air flux along the contaminant pack centerline (green).

Figure 3.11 also reveals the predicted linear increase in average vertical smouldering velocity with increasing injected air flux (blue line and markers). This underscores that the injected air flux dictates the rate of mass destruction in the critical period when it is highest, prior to breakthrough (as seen in Figure 3.9). The average vertical smouldering velocity is a global average over all nodes along the contaminant pack centerline, incorporating flux vectors that can vary in space and time. As a result, its dependence on air flux is not equal to how the local smouldering velocity depends on the local air flux (Equation 1), as shown in Figure 3.11 (black
dashed line). For Simulations 3a, d, and e, the model predicted global vertical smouldering velocities were consistently 20% less than the local velocity predicted by Equation 1. This reflects the 2-D nature of the air flux distribution in this domain, such that a fraction of the injected air results in horizontal flux components (see Figure 3.10). These centerline averages are plotted as green circles in Figure 3.11, and better match the values predicted by Equation 1. How much the injected air flux decreases over the contaminant pack height depends on the magnitude of the injected air flux, hotpad configuration, and scale of application (Appendix G). Figure 3.12 illustrates how injected air flux affects overall treatment rate, which is defined as the total amount of organic liquid destroyed over the total treatment time. Injected air fluxes of 0.50, 1.50, and 3.00 cm/s achieved overall treatment rates of 90, 121, and 247 kg/day (per m depth into the page), respectively.

![Overall Treatment Rate vs. Simulation](image)

**Figure 3.12.** Overall treatment rates for Simulations 3a through 4g at the pilot-scale. Note that Simulation 3b and 3c are not included as they did not achieve significant treatment of the contaminant pack.
3.3.3.2 Contaminant Pack Saturation

Sensitivity to contaminant pack saturation was investigated in Simulations 3f through 3h (Table 3-4). Increasing the contaminant pack saturation had noticeable effects on the smoothness of the predicted front, and the predicted overall rate and extent of treatment, but negligible effect on the predicted average vertical smouldering velocity. Figure 3.13 illustrates the predicted average vertical smouldering velocity’s insensitivity to contaminant pack saturation. This global behaviour occurs because the local smouldering front velocity is only weakly dependent on the local organic liquid saturation (MacPhee et al., 2012). Examination of the initial and final air flux extinction contours for Simulations 3f-3h confirmed that the air flow patterns changed little over time. Therefore the initial air flux contours can also be applied to predict the final extents of treatment for these simulations; however the approximation worsened as saturation increased (Appendix F, Figure A.18 to Figure A.20).

![Average Vertical Smouldering Velocity versus Organic Liquid Saturation](image)

**Figure 3.13.** Predicted average vertical smouldering velocity versus contaminant pack saturation for Simulations 3a, f, g, and h.

Figure 3.14 compares the predicted smouldering front position at two times for Simulations 3f and 3h, corresponding to contaminant pack saturations of 20% and 80%, respectively. Both predicted fronts have similar general positions at 333 min; however the 80% saturation case exhibits significantly more local channelling. As mentioned earlier, small perturbations along the
fronts occur in the model and correspond to real smouldering fronts (e.g., due to minor spatial variations in physical and thermal properties). These small perturbations grow over time in some cases and not in other cases, as shown by comparing the predicted fronts at their respective breakthrough times in Figure 3.14.

![Diagram showing predicted smouldering front positions](image)

**Figure 3.14.** Comparison of the predicted smouldering front position for 20% (red, Simulation 3f) and 80% (blue, Simulation 3h) contaminant pack saturations, at 333 min (a) and breakthrough (b).

Figure 3.15 compares the smouldering front position at the end of treatment for the four homogeneous saturations simulated. At 80% saturation, the channeling effects seen in Figure 3.14 were so severe that the predicted front by-passed large portions of the contaminant pack that were treated at lower saturations.
When multiple fluid phases occupy a pore space (e.g., air and organic liquid), the material’s effective permeability to each phase, $k_e$, is reduced relative to single phase flow (Brooks and Corey, 1964). Effective permeability is a function of both the intrinsic permeability and the fluid saturation (see Section 2.4.2 for further details). The decreased extent of treatment and increased local channeling in Figure 3.15 are due to higher effective permeability contrasts between
untreated and treated sections of the contaminant pack that occur with higher contaminant pack saturations. Figure 3.16 illustrates how the effective permeability ratio of untreated to treated areas of the contaminant pack linearly decreases with higher contaminant pack saturations. As the effective permeability ratio decreases, preferential air flow in small, treated channels (like those shown in Figure 3.14a) becomes more pronounced, acting as a positive feedback loop to further increase local air fluxes, velocities, and channelling in these areas. The final percent of the contaminant pack treated is fairly constant until an effective permeability ratio of approximately 0.5, below which the extent of treatment significantly decreases (Figure 3.15 and Figure 3.16). These results suggest that for this soil/organic liquid pair, a critical threshold is passed when the effective permeability ratio falls below 0.5, resulting in front irregularities and air by-passing that produce untreated lobes. The practical significance of these by-passing effects is realized in the predicted overall treatment rates of Figure 3.12. The overall treatment rate increased between 20% and 60% liquid sand pack saturations (97 to 188 kg/day), due to higher initial organic liquid mass in the sand pore space. However, no additional increase in the overall treatment rate is observed by increasing the saturation from 60% to 80%, as the large by-passed sections offset the higher initial mass in the contaminant pack.

Figure 3.16. Effective permeability ratios and predicted final percent treated versus contaminant pack saturation for Simulations 3f, 3a, 3g, and 3h.
Additional simulations were conducted to confirm that effective permeability effects were responsible for this channelling behaviour. First, Simulation 3a was re-run with air relative permeability independent of organic liquid saturation: no channelling effects were observed and the predicted front was more symmetrical (Appendix I). Then, the value of $\tau_d$ in the $k_{rN}$-$S$ function was adjusted between 0.5 and 1.5 to create five relative permeability curves with unique relative permeability contrasts between untreated and treated material. Less channelling was observed at higher effective permeability ratios, further confirming the relationship between channeling and effective permeability contrasts (Appendix I).

### 3.3.3.3 Heterogeneity

Figure 3.17 presents the permeability and saturation distributions of the homogeneous base case compared to heterogeneous fields 1P/S, 3P/S, and 5P/S (Table 3-5 and 3-6), corresponding to the lowest, middle, and highest variances simulated for permeability and saturation, respectively. The right column of Figure 3.18 compares the predicted time and position of the front at breakthrough for the heterogeneous saturation simulations (3n to 3r in Table 3-4, corresponding to saturation fields 1S to 5S in Table 3-6). Variance in saturation had a minimal effect on the predicted vertical smouldering velocity, with all five cases achieving breakthrough within 1.1 hrs of the homogeneous base case. Figure 3.18 also shows that front irregularity due to local channeling increases with increased saturation variance. As the variance, and thus the maximum saturations in the contaminant pack increase, so do effective permeability contrasts and channelling effects. These results are similar to those previously presented in Section 3.3.3.2, however they are now due to saturation heterogeneity. The right column of Figure 3.19, presenting each case at the end of treatment, shows no distinct relationship between the degree of heterogeneity (i.e., COV) of the saturation field and the extent of treatment, ranging from 1 to 6% less than the homogenous base case. Similarly, no correlation between COV and overall treatment rate was observed, ranging from 89 to 146 kg/day (Figure 3.12), and total treatment times varied from 22% below to 29% above the base case treatment time of 32 hrs (Figure 3.19). Overall, the effect of saturation heterogeneity was relatively minor on predicted treatment outcomes.

Heterogeneity of permeability had a much larger impact on predicted treatment outcomes. The left column of Figure 3.18 compares the predicted time and position of the front at breakthrough
for the heterogeneous permeability simulations (3i to 3m in Table 3-4, corresponding to heterogeneous permeability fields 1P to 5P in Table 3-5). In these simulations, increased heterogeneity resulted in earlier breakthrough (Figure 3.18) with a linear relationship between breakthrough time and COV ($R^2 = 0.97$), as shown in Figure 3.20. This is due to enhanced channeling of air with increased permeability variance. Figure 3.18 reveals that breakthrough is dominated by a high permeability region on the left side of the plenum. Recall that treatment rates significantly decrease after breakthrough as mass destruction shifts from upwards to lateral treatment (Section 3.3.1). The left column of Figure 3.19 suggests that increased variance in permeability decreases the extent of treatment. Figure 3.20 quantifies this, showing a linear relationship between percent of the contaminant pack treated and COV ($R^2 = 0.99$). As a result, the overall treatment rate also decreases with increasing variance (Figure 3.12), from 126 to 61 kg/day (per meter depth into the page). However, similar to the heterogeneous saturation simulations, no clear relationship between total treatment time and variance was observed. This may be due to the increased presence of both high and low air flux zones, and thus simultaneous rapid and slow treatment sub-regions, that occurs when variance is increased.

As previously discussed (Section 3.3.3.2), effective permeability can play a dominant role in influencing the predicted extent of treatment, and is a function of both intrinsic permeability and organic liquid saturation. However, because intrinsic permeability can vary up to six orders of magnitude in these simulations, while contaminant saturation can only vary within one, effective permeability is more sensitive to intrinsic permeability. For example, the saturations of the most heterogeneous saturation field (5S) vary between 0.01 and 0.85, resulting in a range of effective permeabilities between $1.1 \times 10^{-10}$ m$^2$ to $5.5 \times 10^{-10}$ m$^2$. Similarly, the intrinsic permeabilities of the most heterogeneous permeability field (5P) vary between $5.2 \times 10^{-12}$ m$^2$ to $3.9 \times 10^{-8}$ m$^2$, resulting in effective permeabilities between $3.3 \times 10^{-12}$ m$^2$ to $2.5 \times 10^{-8}$ m$^2$. Therefore, heterogeneous domains with similar COVs predict higher sensitivity to $k_i$ versus $S_o$. 

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Figure 3.17. Homogeneous, low, medium and high variance permeability (left) and saturation fields (right). Permeability fields are given in ln(K) where K is in cm/s, and saturations are the fraction of the pore space filled with organic liquid. Light shading indicates high permeability or low saturation, while dark shading indicates low permeability or high saturation.
Figure 3.18. Smouldering front position at time of first breakthrough for Configuration TRAP 1 with homogeneous saturation and permeability fields (Simulation 1, top centre), heterogeneous permeabilities (Simulations 3i-3m, bottom left column) and heterogeneous saturations (Simulation 3n-3r, bottom right column).
Figure 3.19. Smouldering front position at the end of treatment for Configuration TRAP1 with homogeneous saturation and permeability fields (Simulation 3a, top centre), heterogeneous permeabilities (Simulations 3i-3m, bottom left column) and heterogeneous saturations (Simulations 3n-3r, bottom right column).
3.3.4 Hotpad Configuration

Simulations 4a-4g investigated the influence of hotpad design, including trapezoidal, pyramid, and rectangular configurations (Table 3-4 and Figure 3.4). Overall, the simulations revealed that a trade-off exists between the total treated mass and the overall treatment rate. The treatment curves in Figure 3.21 illustrates this, where the slope of each curve corresponds to the treatment rate and the difference between the initial and final organic liquid mass corresponds to the total mass treated. For figures that depict the initial air flux distributions for each configuration, see Appendix F.

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**Figure 3.20.** Predicted breakthrough times and final percent of contaminant pack treated versus coefficient of variation for heterogeneous permeability Simulations 3i through 3m.
Figure 3.21. Organic liquid mass versus time for simulations testing hotpad configuration. For simulations that achieved breakthrough, the breakthrough time is noted with black diamonds.

The highest initial organic liquid mass (210 kg) and highest total mass treated (161 kg) was achieved by configuration TRAP1 (Figure 3.4). By widening the contaminant pack base beyond the plenum, the outermost portions extended into areas of increasingly lower air flux (see Figure 3.10c). These low air flux zones are responsible for the tailing of the treatment rate after breakthrough that is seen in Figure 3.21 (similar to the calibration simulation). The end result is a high total treatment mass, and an overall treatment rate of 121 kg/day that is lower than other configurations due to the tailing (Figure 3.12). This tailing was eliminated in TRAP2 by decreasing the base width, thus removing the contaminant pack from these low air flux zones, achieving a higher overall treatment rate of 167 kg/day (Figure 3.12) at the expense of total treatment mass (87 kg).

Compared to rectangular or trapezoidal shapes, pyramid configurations PYR1-PYR4 contained lower initial organic liquid masses and achieved lower treatment rates; moreover, configurations PYR3 and PYR4 had higher fractions of untreated material at the end of treatment (Figure 3.21). As the contaminant pack height was increased in configurations PYR1 through PYR4, the initial air flux distributions altered accordingly (Appendix F). In PYR3 and PYR4, the high air pressure loss across the height, and availability of shorter flow paths laterally resulted in air fluxes too
low for smouldering in the pyramid’s peak (Figure A.59 and Figure A.60 in Appendix F). This resulted in untreated mass at the top of the pyramid which, as shown above, can be avoided by selecting a trapezoidal configuration.

REC2, with vertical walls constraining the contaminant pack, achieved the highest treatment rate (263 kg/day) in this suite of simulations (treatment curve in Figure 3.21, overall treatment rate in Figure 3.12). The vertical walls on either side of the plenum forced the air distribution to approximate 1-D conditions, with all injected air traveling vertically upwards. As the air flux magnitude was constant with contaminant pack height, REC2 predicted a constant, high rate of upwards smouldering throughout. REC2 also achieved complete treatment since the reaction was forced throughout the entire contaminant pack. The slightly wider contaminant pack base in REC1 achieved a higher total treatment mass (132 kg) than REC2 (114 kg). However, due to the lack of walls, the 2-D air distribution in REC1 caused the air flux magnitude to decrease with contaminant pack height, thus achieving a lower treatment rate (188 kg/day) than REC2. It is noted that implementing REC2 in the field would required the addition of walls to the hotpad base, a constraint not shared by the other designs.

An additional simulation was run with configuration TRAP2 to determine the influence of the clean sand cap on the predicted treatment extent and time. Removing the clean sand cap had negligible impact on the air flux distribution within the domain, and thus the time and extent of treatment were only altered minimally (Figure A.75 and Figure A.76). This result makes sense as the effective permeability ratio between the contaminant pack and clean sand cap was 0.71 in these simulations, exceeding the critical threshold of 0.5 that was proposed in Section 3.3.3.2.

3.3.5 Full-scale Configurations

Full-scale configurations, FIELD1 and FIELD2 in Figure 3.5 (Simulations 5a and 5b in Table 3-4) investigated the effects of scale on the time and extent of treatment. The predicted results are summarized in Table 3-8.
Table 3-8 Summary of Field-scale Simulations 5a and 5b

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Average Vertical Smouldering Velocity (cm/min)</th>
<th>Break-through Time (hrs)</th>
<th>Total Treatment Time (hrs)</th>
<th>Total Mass Destroyed, per m into the page (kg)</th>
<th>Overall Treatment Rate (kg/day)</th>
<th>Extent of Treatment (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5a</td>
<td>0.11</td>
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<td>52.5</td>
<td>2721</td>
<td>1244</td>
<td>98</td>
</tr>
<tr>
<td>5b</td>
<td>0.11</td>
<td>31.1</td>
<td>38.1</td>
<td>2043</td>
<td>1288</td>
<td>100</td>
</tr>
</tbody>
</table>

Both configurations achieved average vertical smouldering velocities of 0.11 cm/min, which is at the upper end of the range of velocities predicted at the pilot-scale under homogeneous saturation and permeability conditions, with the same injected air flux. This is due to the increased plenum width, from 1.5 m at the pilot-scale to 9.3 m at the full-scale. A wider plenum enables the inner portions of the contaminant pack to better approximate 1-D flow conditions, with the vertical components of the air flux vectors remaining closer to the plenum injected value (air flux distribution figures available in Appendix E). Compared to Simulation 3a where the average vertical flux components decreased by 20% along the centerline of the 0.6 m liquid sand pack (as discussed in Section 3.3.3.1), the centerline averages only decreased by 4% and 7% over the 2 m tall contaminant pack in Simulations 5a and 5b, respectively.

The predicted overall treatment rates achieved in full-scale simulations were roughly an order of magnitude higher than the pilot-scale. This increase is primarily due to a comparable increase in the plenum surface area between scales, enabling the system to hold a higher initial organic liquid mass over the plenum footprint for a given contaminant pack height. As a result, as the smouldering front propagates upwards, it destroys a greater organic liquid mass at any height in the contaminant pack. The taller field-scale contaminant pack delayed the time of breakthrough, thus extending the linear portion of the predicted treatment curve, which indirectly increased the overall treatment rate. For pilot-scale configuration TRAP1 with a 0.6 m contaminant pack height, the linear and tailing portions of the treatment curve accounted for 35% and 65% of the total treatment time, respectively. In contrast, delayed breakthrough in the 2 m contaminant pack of FIELD1 extended the linear portion of the predicted treatment curve to 57% of the total treatment time, while the tailing period was reduced to 43%.

If implemented at an actual field site, based on a contaminant pack that is approximately 9.3 m wide x 8.4 m long x 2.0 m high with a 40% contaminant saturation, configurations FIELD1 and
FIELD2 are predicted to treat 20 186 kg of organic liquid in 2.2 and 1.6 days, respectively. These mass estimates are conservative as they only consider mass destroyed directly over the plenum footprint, neglecting material in the plenum overlap. Note that actual field batch treatment times will be larger than those estimated in this work, due to additional time required for pre-heating prior to ignition, and cooling at the end of treatment.

### 3.4 Conclusions and Implications

This chapter presented results from pilot-scale experiments and a numerical modelling study that was conducted to explore the effects of system design, operational parameters, and environmental factors on the performance of STARx hotpad systems. The model can be used to predict the average vertical smouldering velocity, extent of treatment, total treatment masses and times, and overall treatment rates. Using a measured relative permeability-saturation constitutive function, the model was calibrated and validated against pilot test STARx experimental data. Subsequently, the model was applied as an engineering tool to evaluate STARx hotpad design and operation. A sensitivity study was completed at the pilot-scale to investigate the impact of injected air flux, contaminant pack saturation, and heterogeneity. This study demonstrated the importance of configuration design and effective permeability ratios within the pack on air flow patterns, and the subsequent influence on the fraction of mass treated rapidly versus the fraction associated with tailing destruction rates. This study also demonstrated how injected air flux can be manipulated to dictate destruction rates and extents in STARx systems. The overall treatment rate is predicted to increase by roughly an order of magnitude between pilot and field-scale systems, primarily due to a comparable increase in the plenum footprint. The findings from this study provide additional confidence in the robustness of the model and can be applied to inform future STARx designs.

A field test of the full scale hotpad system is scheduled for Fall 2016, using a configuration similar to FIELD1 or FIELD2. The modelling results can be applied to infer optimal conditions for hotpad treatment. Firstly, this study suggests that the highest practical injected air flux should be applied to maximize the rate and extent of treatment. A trapezoidal contaminant pack with a 60% organic liquid saturation should be selected to maximize the total treatment mass and overall treatment rate, while avoiding the channelling (and the associated decreased performance) expected to occur at higher saturations. While the critical threshold for the
effective permeability ratio was identified as 0.5 in this study, it may change for other soil/organic liquid pairs, likely with shifts in the air relative permeability-organic liquid saturation curve.

The results suggest that the extent of treatment is more sensitive to heterogeneity in intrinsic permeability than heterogeneity in saturation. Therefore, sourcing a relatively uniform sand with which to mix the organic liquid is more important than achieving a homogeneous mixture. Although this study focused on organic liquid waste mixed with sand, these results are also expected to apply to treating excavated contaminated soils, where heterogeneity may play an even larger role due to natural variability in the environment.

It is acknowledged that this study employed several approximations and assumptions for practical purposes. For example, the model only approximates the leading edge of the smouldering reaction, neglecting the trailing edge and smouldering front thickness. Smouldering fronts are expected to be thin relative to the scale of these systems, so it is expected this is a reasonable assumption. Also, the model neglects temperature effects, and energy generation, transfer, and loss. As a result, it does not account for potential organic liquid migration due to temperature-induced viscosity reductions as fuel mobility was not considered in this study. While this is known to occur in some cases (Kinsman, 2015), it is expected to be a minor factor in these scenarios. Furthermore, the multiphase flow code only considers two phases, air and organic liquid, neglecting any moisture content that may be present. Moisture is expected to be minimal in the intentionally mixed packs considered here. The model validation provides confidence that indeed these assumptions are reasonable in this context. Therefore, these assumptions are not expected to significantly impact the conclusions presented in this study.

3.5 References


Chapter 4

4 Summary and Recommendations

4.1 Summary

This thesis used numerical modelling to infer the predicted effects of system operation, design parameters, and environmental factors on the performance of STARx hotpad systems. While all experiments and simulations presented in this work were based on STARx hotpads, it is expected that the findings also apply to other STAR and STARx systems. After successful model calibration and validation against unique pilot-scale hotpad experiments, a comprehensive sensitivity study was conducted to explore the effects of the injected air flux rate, contaminant saturation, heterogeneity within soil permeability and contaminant saturation, and hotpad configuration. Simulations were also conducted at the full-scale to infer the effects of system scale. The modelling results provide predictions of the average vertical smouldering velocity, total treatment time, and extent of treatment. When the simulated scale was increased from pilot to full-scale, the predicted average vertical velocities were similar, while predicted overall treatment rates increased by roughly an order of magnitude for the same injected air flux and contaminant pack saturation, primarily due to the increased plenum footprint. A proportional increase in treatment time was not observed, suggesting the full-scale is more efficient than the pilot-scale hotpad system.

4.2 Key Findings

The major findings of this work are summarized as the importance of effective permeability contrasts, and recommendations for optimized hotpad design:

4.2.1 The importance of Effective Permeability Effects

- This was the first study to investigate the influence of effective permeability on predicted smouldering behaviour in STAR applications, and the measured relative permeability-saturation function employed in this work was significantly different than the curve used in previous STAR modelling studies.
• When the effective permeability ratio between untreated and treated materials fell below a critical threshold of 0.5, the predicted overall rate and extent of treatment significantly decreased due to severe local channelling along the front that ultimately left large untreated lobes.

• Sensitivity to the effective permeability ratio may have positive implications for design purposes. For this pairing of soil and organic liquid, the results suggest that the extent of treatment can be approximated from the initial air flux extinction contour when the effective permeability ratio exceeds 0.5. Using the model to predict the location of the extinction threshold contour for a given hotpad configuration enables the contaminant pack design to take advantage of high air flux areas, while avoiding low air flux areas to maximize the overall treatment rate and minimize the formation of an untreated crust. However, when the effective permeability ratio falls below 0.5, then the air distribution may be time dependent and the same approximation is not valid. Regardless of the effective permeability ratio, there is still value in running the model as it provides insight into time dependent variables such as the predicted smouldering velocity, the treatment time, and treatment rate.

• Due to the high effective permeability ratio of the contaminant pack to clean sand cap, inclusion of the clean sand cap did not influence the predicted results. Therefore, it was concluded that additional simulations altering the clean cap design were not warranted. However, the clean sand cap may have a more dominant role in controlling air flow patterns for other soil/organic liquid pairs with lower effective permeability ratios.

• For the simulated soil/organic liquid pair, the hotpad was predicted to be more robust with respect to heterogeneity in organic liquid saturations, achieving extents of treatment similar to a perfectly mixed (homogeneous) contaminant pack; however the treatment time may be affected. For other soil/organic liquid pairs with lower effective permeability ratios, it is anticipated that the model will show more sensitivity to variance in saturation. The hotpad was predicted to be less robust in response to variance in soil permeability, which significantly decreased the extent of treatment. This is because altering intrinsic permeability has a much larger impact on the effective permeability. These results
suggest that when implemented in the field, overly thorough mixing of the organic liquid and sand prior to placement of the contaminant pack is not warranted. However, emphasis on obtaining a homogenous source material for the sand pack is important, as a heterogeneous soil is predicted to significantly degrade system performance.

4.2.2 Recommendations for Optimized Design

- Adjusting the injected air flux was shown to have the greatest impact on the predicted rate and extent of remediation. Higher air fluxes move the air flux extinction contour laterally outwards, thereby increasing the fraction of the contaminant pack where air fluxes are high enough to sustain smouldering. The modelling results suggest that the highest feasible injected air flux should be used, within the practical limitations of the air pump, and considering the effects of sand bed fluidization and reaction front cooling that occur at high air fluxes.

- Contaminant pack saturation negligibly affected the predicted average vertical smouldering velocity. However, local channeling along the front was predicted to increase with saturation, becoming so pronounced at 80% saturation that lobes of material in the central upper portions of the contaminant pack were left untreated. This saturation corresponds to the critical effective permeability ratio. Therefore to maximize the initial organic liquid mass in the sand pack, and minimize untreated lobes due to channeling, a 60% contaminant pack saturation is recommended.

- The various configurations tested revealed a trade-off exists between total treated mass and overall treatment rate. To optimize both treatment rates and masses while considering design practicality, a trapezoidal configuration extending beyond the plenum is recommended. As mentioned above the model could be used to inform the design of the contaminant pack base, thus limiting the amount of untreated material at the end of each batch. This plenum overlap may provide additional benefits when the effective permeability ratio between the contaminant pack and clean cap decreases, as it may prevent injected air from bypassing directly from the plenum to the clean sand cap until breakthrough occurs.
• Examination of the air flux fields in the trapezoidal configurations tested suggests that the contaminant pack height was not optimized, as the air flux magnitude at the top of the contaminant pack exceeded the air flux extinction threshold. Increasing the vertical height of the contaminant pack, while maintaining the current base width, would increase the total initial organic liquid mass and delay the time of breakthrough. Therefore, this would decrease the tailing portion of the predicted treatment curve and increase the overall treatment rate, making this configuration even more appealing.

Overall, the model was shown to perform well at the pilot and full-scales, and the above mentioned key findings are expected to be valuable when designing future STARx systems.

4.3 Recommendations

This thesis presented a numerical modelling study that investigated the performance of STARx hotpad systems.

For future work, the following is recommended:

• Currently, the model is calibrated and validated against the only two hotpad experiments conducted with the same contaminant and soil type. While each experiment used a unique sand pack configuration, both used the same contaminant pack saturation, and similar injected air fluxes. To provide additional confidence in the model performance and confirm assumptions about smouldering behaviour outside of the range of conditions that were tested in Hotpad Experiments A and B, additional experiments could be conducted at the pilot-scale (e.g., high/low air injected air fluxes, high/low organic liquid saturations). Similarly, additional hotpad experiments with different soils and contaminant types would also be informative as they would allow new model calibrations, and comparison between calibrations. Once implemented in the field, collection of hotpad temperature and emissions data will allow for comparison of the predicted and actual full-scale results, further enhancing confidence in the model or identifying additional limitations that were not identified earlier.

• Given the prevailing effects of effective permeability ratios in this work, and the sensitivity of model performance to the relative permeability-saturation function
employed, it is highly recommended that relative permeability testing should be a component of all subsequent STAR modelling studies. If this is not feasible, then a variety of relative permeability curves should be simulated to define the upper and lower bounds of the effects of each parameter, based on the unknown, actual effective permeability ratio.

- To expand the potential applications of the model, a third phase could be added to the multiphase flow code to be able to predict smouldering behaviour below the groundwater table for in situ STAR applications.

- Once a multi-physics smouldering combustion model is published, predicted results in simple domains could be compared between models to possibly identify limitations of the phenomenological model and further improve its formulation.

- Additional experiments could be conducted to better define the relationship between injected air flux and smouldering velocity at different scales in both 1-D and 2-D systems.

- As the modelling results were shown to be most sensitive to the magnitude of injected air flux, additional simulations exploring the effects of increasing the injected air flux during the simulation (i.e., stepping up the air flow rate during treatment) could be conducted.
Appendices

Appendix A: Supporting Information for Hotpad Experimental Values

In Hotpad Experiment A, in each thermocouple bundle A through I (Figure A.1), individual thermocouples were instrumented at progressive heights of 0, 2.5, 5, 10, 15, 20, and 30 cm above the plenum. For each bundle, the time for the 0 cm (contaminant pack base) and 30 cm (contaminant pack top) thermocouples to reach 300 °C was determined, and a local vertical smouldering velocity was then calculated as shown below. The local vertical smouldering velocities from all bundles were then average and used as the model calibration velocity:

\[
\frac{30 \text{ cm} - 0 \text{ cm}}{\text{time 30 cm TC reaches 300 °C (min)} - \text{time 0 cm TC reaches 300 °C(min)}}
\]

In Hotpad Experiment B, in each thermocouple bundle A through I, individual thermocouples were instrumented at progressive heights of 0, 2.5, 5, 10, 15, 20, 30, 40, 50, and 60 cm above the plenum. However, thermocouple data was only available at the top of the 60 cm contaminant pack for thermocouple bundle E, therefore the local velocity of this bundle was calculated as shown below and used as the model validation velocity.

\[
\frac{60 \text{ cm} - 0 \text{ cm}}{\text{time 60 cm TC reaches 300 °C (min)} - \text{time 0 cm TC reaches 300 °C(min)}}
\]

For both hotpad experiments, the time a given height reached 300 °C was averaged for all thermocouple bundles. The average smouldering velocities were then calculated between successive thermocouple heights. Figure A.2 compares these average velocities to the velocities that were calculated above, illustrating that while the model is calibrated to reproduce a single global average smouldering velocity, there is actually variation in the experimental velocity with contaminant pack height.
<table>
<thead>
<tr>
<th>Thermocouple Bundle</th>
<th>0 cm</th>
<th>2.5 cm</th>
<th>5 cm</th>
<th>10 cm</th>
<th>15 cm</th>
<th>20 cm</th>
<th>30 cm</th>
<th>Local Velocity for Each TC Bundle 0 cm – 30 cm (cm/min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>475.25</td>
<td>482.75</td>
<td>509.25</td>
<td>624.25</td>
<td>669.00</td>
<td>726.00</td>
<td>808.75</td>
<td>0.0900</td>
</tr>
<tr>
<td>B</td>
<td>410.25</td>
<td>440.25</td>
<td>485.00</td>
<td>597.00</td>
<td>678.75</td>
<td>706.75</td>
<td>753.50</td>
<td>0.0874</td>
</tr>
<tr>
<td>C</td>
<td>512.75</td>
<td>522.00</td>
<td>539.50</td>
<td>639.25</td>
<td>678.00</td>
<td>724.50</td>
<td>856.50</td>
<td>0.0873</td>
</tr>
<tr>
<td>D</td>
<td>584.50</td>
<td>606.00</td>
<td>633.50</td>
<td>669.75</td>
<td>709.00</td>
<td>768.25</td>
<td>833.00</td>
<td>0.1207</td>
</tr>
<tr>
<td>E</td>
<td>542.00</td>
<td>601.00</td>
<td>645.75</td>
<td>682.50</td>
<td>722.00</td>
<td>749.00</td>
<td>821.00</td>
<td>0.1075</td>
</tr>
<tr>
<td>F</td>
<td>492.50</td>
<td>511.25</td>
<td>556.75</td>
<td>663.00</td>
<td>696.50</td>
<td>724.25</td>
<td>784.00</td>
<td>0.1029</td>
</tr>
<tr>
<td>G</td>
<td>638.75</td>
<td>665.75</td>
<td>690.75</td>
<td>736.50</td>
<td>786.50</td>
<td>817.25</td>
<td>898.75</td>
<td>0.1154</td>
</tr>
<tr>
<td>H</td>
<td>553.50</td>
<td>589.75</td>
<td>642.50</td>
<td>671.25</td>
<td>691.00</td>
<td>742.75</td>
<td>837.25</td>
<td>0.1057</td>
</tr>
<tr>
<td>I</td>
<td>574.00</td>
<td>595.25</td>
<td>639.00</td>
<td>686.00</td>
<td>705.50</td>
<td>736.00</td>
<td>801.25</td>
<td>0.1320</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td><strong>531.50</strong></td>
<td><strong>557.11</strong></td>
<td><strong>593.56</strong></td>
<td><strong>663.28</strong></td>
<td><strong>704.03</strong></td>
<td><strong>743.86</strong></td>
<td><strong>821.56</strong></td>
<td><strong>0.1054</strong></td>
</tr>
</tbody>
</table>

Average Time TC Height Reaches 300° C (min) 531.50 557.11 593.56 663.28 704.03 743.86 821.56

Average Velocity Between Successive Thermocouple Heights (cm/min) 0.0976 0.0686 0.0717 0.1227 0.1255 0.1287
Table A-2 Thermocouple Data and Calculations for Hotpad Experiment B

<table>
<thead>
<tr>
<th>Thermocouple Bundle</th>
<th>0 cm</th>
<th>2.5 cm</th>
<th>5 cm</th>
<th>10 cm</th>
<th>15 cm</th>
<th>20 cm</th>
<th>30 cm</th>
<th>40 cm</th>
<th>50 cm</th>
<th>60 cm</th>
<th>Local Velocity for Each TC Bundle 0 cm – 60 cm (cm/min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>181.00</td>
<td>201.75</td>
<td>225.25</td>
<td>289.75</td>
<td>330.75</td>
<td>385.50</td>
<td>465.50</td>
<td>566.25</td>
<td>852.25</td>
<td>-</td>
<td>0.0584</td>
</tr>
<tr>
<td>B</td>
<td>185.50</td>
<td>207.00</td>
<td>236.00</td>
<td>294.75</td>
<td>334.75</td>
<td>371.25</td>
<td>451.25</td>
<td>550.25</td>
<td>664.50</td>
<td>-</td>
<td>0.0584</td>
</tr>
<tr>
<td>C</td>
<td>173.75</td>
<td>193.00</td>
<td>211.50</td>
<td>274.00</td>
<td>309.00</td>
<td>349.00</td>
<td>464.25</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.0584</td>
</tr>
<tr>
<td>D</td>
<td>194.25</td>
<td>217.00</td>
<td>248.50</td>
<td>287.50</td>
<td>331.50</td>
<td>374.25</td>
<td>422.00</td>
<td>499.00</td>
<td>596.25</td>
<td>-</td>
<td>0.0584</td>
</tr>
<tr>
<td>E</td>
<td>161.50</td>
<td>190.00</td>
<td>231.75</td>
<td>316.50</td>
<td>375.00</td>
<td>406.00</td>
<td>467.75</td>
<td>548.75</td>
<td>broken</td>
<td>1189.75</td>
<td>0.0584</td>
</tr>
<tr>
<td>F</td>
<td>154.75</td>
<td>180.50</td>
<td>210.25</td>
<td>291.75</td>
<td>333.00</td>
<td>366.50</td>
<td>443.50</td>
<td>518.25</td>
<td>732.75</td>
<td>-</td>
<td>0.0584</td>
</tr>
<tr>
<td>G</td>
<td>181.00</td>
<td>201.50</td>
<td>222.00</td>
<td>290.00</td>
<td>322.50</td>
<td>356.25</td>
<td>484.25</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.0584</td>
</tr>
<tr>
<td>H</td>
<td>152.00</td>
<td>177.50</td>
<td>208.75</td>
<td>276.75</td>
<td>319.00</td>
<td>352.50</td>
<td>417.00</td>
<td>540.25</td>
<td>1267.50</td>
<td>-</td>
<td>0.0584</td>
</tr>
<tr>
<td>I</td>
<td>129.25</td>
<td>156.75</td>
<td>186.50</td>
<td>261.00</td>
<td>309.25</td>
<td>344.75</td>
<td>407.75</td>
<td>668.00</td>
<td>-</td>
<td>-</td>
<td>0.0584</td>
</tr>
</tbody>
</table>

|                      |       |       |       |       |       |       |       |       |       |       | Average 0.0584                                           |

| Average Time TC Height Reaches 300° C (min) | 168.11 | 191.67 | 220.06 | 286.89 | 329.42 | 367.33 | 447.03 | 555.82 | 822.65 | 1189.75 |
| Average Velocity Between Successive Thermocouple Heights (cm/min) | 0.1061 | 0.0881 | 0.0748 | 0.1176 | 0.1319 | 0.1255 | 0.0919 | 0.0375 | 0.0272 |          |
Figure A.1 Aerial view of thermocouple bundle layout in both hotpad experiments.
Figure A.2 Average vertical smouldering velocities between thermocouple heights for Hotpad Experiment A (blue diamonds) and B (red squares) compared to global averages over entire contaminant pack height for each experiment.
Figure A.3 Carbon monoxide (CO) emissions versus time for Hotpad Experiment A, where $t=0$ corresponds to time heater was turned off.

Figure A.4 Carbon monoxide (CO) emissions versus time for Hotpad Experiment B, where $t=0$ corresponds to time heater was turned off.
Appendix B: Supporting Information for Permeability Testing and Calculations

The results of the intrinsic sand permeability testing are summarized below in Table A-3. Only test numbers 1 through 7 were considered in the geometric average, based on their R-squared values.

<table>
<thead>
<tr>
<th>Test No.</th>
<th>Permeability (m^2)</th>
<th>R-squared</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>7.05E-10</td>
<td>0.9995</td>
</tr>
<tr>
<td>2</td>
<td>1.02E-09</td>
<td>0.9996</td>
</tr>
<tr>
<td>3</td>
<td>1.26E-10</td>
<td>0.9981</td>
</tr>
<tr>
<td>4</td>
<td>3.40E-09</td>
<td>0.9967</td>
</tr>
<tr>
<td>5</td>
<td>5.68E-10</td>
<td>0.9678</td>
</tr>
<tr>
<td>6</td>
<td>6.30E-10</td>
<td>0.9584</td>
</tr>
<tr>
<td>7</td>
<td>2.93E-10</td>
<td>0.9788</td>
</tr>
<tr>
<td>8</td>
<td>9.82E-10</td>
<td>0.3259</td>
</tr>
</tbody>
</table>

| Geometric Mean | 6.12E-10 |
| Standard Deviation | 1.11E-09 m^2 |
| 95% Confidence Interval | 8.24E-10 m^2 |

When mixing clean sand with organic liquid to achieve a specified saturation for the effective permeability testing, the below equation and the parameters in Table A-4 were assumed.

\[
saturation = \frac{NAPL \text{ mass} \times \text{sand density}}{(NAPL \text{ density} \times (\text{sand mass} - NAPL \text{ mass}) \times \text{porosity})} \times 100\%
\]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>NAPL Density (kg/m^3)</td>
<td>850</td>
</tr>
<tr>
<td>Sand Density (kg/m^3)</td>
<td>1600</td>
</tr>
<tr>
<td>Sand Porosity</td>
<td>0.33</td>
</tr>
</tbody>
</table>

For any saturation, only results with an R^2 > 0.995 were considered, and when a given saturation was tested multiple times, the arithmetic mean of all test results was taken. The relative permeability at each saturation was then calculated as \( k_{\text{effective}}/k_{\text{intrinsic}} \). The results of this process are summarized below in Table A-5.
The MATLAB Curve Fitting Tool was used to fit the relative-permeability constitutive function of Gerhard and Kueper (2003) to the experimental data such that the root mean square error (RMSE) between the function and experimental data was minimized. Two approaches were taken to minimize the RMSE; 1) fitting all six parameters in the function and 2) using a combination of fitted and assumed parameters. The upper and lower bounds assumed for each parameter are given below in Table A-6. The nine combinations of parameters and their respective RMSE’s are summarized in Table A-7, where a pink cell indicates the parameter value was assumed and a blue cell indicates the parameter value was fit. The values that were previously assumed by MacPhee et al., 2012 and Hasan et al., 2015 are listed in the first row. Combination 4 was selected as it produced the lowest RMSE and used a reasonable combination of assumed and fitted parameters.

### Table A-5 Summary of Relative Permeability Testing

<table>
<thead>
<tr>
<th>Test No.</th>
<th>Sw (%)</th>
<th>$k_{\text{effective}}$</th>
<th>$R^2$</th>
<th>Arithmetic Average of $k_{\text{effective}}$</th>
<th>$k_{\text{relative}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10</td>
<td>5.18E-10</td>
<td>0.9998</td>
<td>5.18E-10</td>
<td>0.85</td>
</tr>
<tr>
<td>2</td>
<td>20</td>
<td>5.08E-10</td>
<td>0.9998</td>
<td>5.08E-10</td>
<td>0.83</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>3.79E-10</td>
<td>0.9998</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>3.46E-10</td>
<td>0.9999</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>40</td>
<td>3.81E-10</td>
<td>0.9997</td>
<td>3.85E-10</td>
<td>0.63</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>4.51E-10</td>
<td>0.9995</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>3.67E-10</td>
<td>0.9999</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>60</td>
<td>3.16E-10</td>
<td>0.9999</td>
<td>2.93E-10</td>
<td>0.48</td>
</tr>
<tr>
<td></td>
<td>60</td>
<td>2.69E-10</td>
<td>0.9999</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>80</td>
<td>9.69E-11</td>
<td>0.9999</td>
<td>9.69E-11</td>
<td>0.16</td>
</tr>
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<td>0.9956</td>
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### Table A-6 Bounds Assumed for Curve Fitting

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<tr>
<th>Parameter $k_{\text{cr}}, \lambda_d, \tau_d, S^M_W, S^L_r, \Delta S^d_{sw}$</th>
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<th>Upper Bound</th>
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<td>$k_{\text{cr}}^\text{max}$</td>
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<td>10</td>
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<tr>
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</tr>
<tr>
<td>$S^L_r$</td>
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<tr>
<td>$\Delta S^d_{sw}$</td>
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<td>$k_{rN}^m$</td>
<td>$\lambda_d$</td>
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<td>---------------</td>
<td>------------</td>
<td>-------------</td>
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</tr>
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</tr>
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Appendix C: Selection of Model Calibration Parameters

First, the calibration coefficient, A, was altered to minimize the difference between the predicted and experimental average vertical smouldering velocity. For all simulations that modified A, a value of $\lambda = 0.5$ cm/s was assumed from MacPhee et al., 2012. In these simulations the average vertical smouldering velocity was independent of $\lambda$ because air fluxes less than $\lambda$ were not encountered in the area of the contaminant pack that dictated the average vertical smouldering velocity. Figure A.5 below shows that the objective function was minimized using a value of $A = 0.25$.

Figure A.5. Objective function (difference between model predicted and experimental average vertical smouldering velocity) versus calibration coefficient for the model calibration.

The predicted positions of the front directly before and after breakthrough are shown in Figure A.6 through Figure A.8.
Figure A.6. $A = 0.24, \lambda = 0.50 \text{ cm/s} – \text{Smouldering front position at } 17\,000 \text{ s (top) and } 17\,500 \text{ s (bottom).}$

Figure A.7. $A = 0.25, \lambda = 0.50 \text{ cm/s} – \text{Smouldering front position at } 17\,000 \text{ s (top) and } 17\,500 \text{ s (bottom).}$
Figure A.8. \( A = 0.26, \lambda = 0.50 \) cm/s – Smouldering front position at 16 500 s (top) and 17 000 s (bottom).
After selecting A, $\lambda$ was selected to minimize the difference between the experimental and simulated untreated crust in Hotpad Experiment A. The position of the three points along the experimental crust measured by Savron were compared to three similar points along the crust position at the predicted end of treatment. The position of the uppermost experimental point was compared to the peak point in the predicted crust, the lowermost experimental point was compared to the inner base point on the predicted crust, and the middle experimental point was compared to the predicted crust position at the same y-coordinate. For each value of $\lambda$ that was simulated, the distances between the experimental and simulated points for both the left and right crusts were summed. Figure A.9 below illustrates that the objective function was minimized using a value of $\lambda = 0.5$ cm/s. Comparison of the predicted and experimental crust is shown in Figure A.10.

![Graph](image)

**Figure A.9.** Objective function (total distance between simulated and experimental crust position) versus air flux extinction threshold for calibration simulation.
Figure A.10. For $A=0.25$, smouldering front position at the end of treatment for various values of $\lambda$ (black) compared to the experimental crust (red). Domain heights and widths are given in meters.
Appendix D: Model Sensitivity to Grid Size

An additional simulation was conducted with a grid resolution of 1.0 cm x 1.0 cm. The predicted position of the smouldering front from this simulation was similar to the calibration simulation (1.5 cm x 1.5 cm grid resolutions) as shown below in Figure A.11, which compares the predicted fronts at early time, breakthrough, and the ultimate extent of treatment. The predicted vertical smouldering velocity, total treatment time, and final mass treated from the 1.0 cm x 1.0 cm grid resolution were all within 10% of the values from the 1.5 cm x 1.5 cm grid resolution. Based on these results, and maximum array limitations of the computer processor employed in this work, a 1.5 cm x 1.5 cm grid resolution was deemed appropriate.

Figure A.11. Comparison of predicted smouldering front positions at 100 min (top), 283 min (middle), and 1016 min from calibration simulation using 1 cm x 1 cm (red) and 1.5 cm x 1.5 cm (blue) grid resolutions.
Appendix E: Simulations At and Below the Air Flux Extinction Threshold

Figure A.12. Predicted smouldering front position at the end of treatment for Simulation 3c, with an injected air flux of 0.50 cm/s (equal to the air flux extinction threshold), corresponding to 1.3% treatment of the contaminant pack.

Figure A.13. Predicted smouldering front position at the end of treatment for Simulation 3b, with an injected air flux of 0.33 cm/s (below the air flux extinction threshold), corresponding to 0% treatment of the contaminant pack.
Appendix F: Supporting Figures from All Simulations

This appendix includes figures from i) all simulations that were referenced in the text, and ii) figures from additional simulations that were not included in the text. For each simulation, the following figures are provided:

a. The predicted position of the smouldering front at initial, midway, breakthrough, and final (end of treatment) times

b. The initial air flux extinction contour compared to the predicted extent of treatment
Figure A.14. Predicted smouldering front position at 0, 167, 417, and 867 (end of treatment) min for Simulation 2 (validation).
Figure A.15. Predicted smouldering front position at 0, 333, 667 (breakthrough), and 1917 (end of treatment) min for Simulation 3a.
Figure A.16. Predicted smouldering front position at 0, 333, 667, and 1350 (end of treatment) min for Simulation 3d.
Figure A.17. Predicted smouldering front position at 0, 167, 333 (breakthrough), and 1133 (end of treatment) min for Simulation 3e.
Figure A.18. Predicted smouldering front position at 0, 333, 683 (breakthrough), and 1217 (end of treatment) min for Simulation 3f.
Figure A.19. Predicted smouldering front position at 0, 333, 667 (breakthrough), and 1817 (end of treatment) min for Simulation 3g.
Figure A.20. Predicted smouldering front position at 0, 333, 583 (breakthrough), and 1867 (end of treatment) min for Simulation 3h.
Figure A.21. Predicted smouldering front position at 0, 83, 583 (breakthrough), and 1650 (end of treatment) min for Simulation 3i.
Figure A.22. Predicted smouldering front position at 0, 83, 600 (breakthrough), and 1833 (end of treatment) min for Simulation 3j.
Figure A.23. Predicted smouldering front position at 0, 83, 350 (breakthrough), and 2567 (end of treatment) min for Simulation 3k.
Figure A.24. Predicted smouldering front position at 0, 83, 233 (breakthrough), and 2183 (end of treatment) min for Simulation 3l.
Figure A.25. Predicted smouldering front position at 0, 83, 200 (breakthrough), and 2300 (end of treatment) min for Simulation 3m.
Figure A.26. Predicted smouldering front position at 0, 333, 650 (breakthrough), and 1767 (end of treatment) min for Simulation 3n.
Figure A.27. Predicted smouldering front position at 0, 333, 650 (breakthrough), and 1500 (end of treatment) min for Simulation 3o.
Figure A.28. Predicted smouldering front position at 0, 333, 633 (breakthrough), and 1967 (end of treatment) min for Simulation 3p.
Figure A.29. Predicted smouldering front position at 0, 333, 617 (breakthrough), and 1917 (end of treatment) min for Simulation 3q.
Figure A.30. Predicted smouldering front position at 0, 333, 600 (breakthrough), and 1767 (end of treatment) min for Simulation 3r.
Figure A.31. Predicted smouldering front position at 0, 333, 717 (breakthrough), and 750 (end of treatment) min for Simulation 4a.
Figure A.32. Predicted smouldering front position at 0, 333, 683 (breakthrough), and 1017 (end of treatment) min for Simulation 4b.
Figure A.33. Predicted smouldering front position at 0, 333, 542 (breakthrough), 625 (end of treatment) min for Simulation 4c.
Figure A.34. Predicted smouldering front position at 0, 83, 167, and 333 (end of treatment) min for Simulation 4d.
Figure A.35. Predicted smouldering front position at 0, 333, and 700 (end of treatment) min for Simulation 4e.
Figure A.36. Predicted smouldering front position at 0, 333, and 1467 (end of treatment) min for Simulation 4f.
Figure A.37. Predicted smouldering front position at 0, 333, and 1350 (end of treatment) min for Simulation 4g.
Figure A.38. Predicted smouldering front position at 0, 833, 1800 (breakthrough), and 3150 (end of treatment) min for Simulation 5a.
Figure A.39. Predicted smouldering front position at 0, 833, 1867 (breakthrough), and 2283 (end of treatment) min for Simulation 5b.
Figure A.40. Initial air flux distribution in Simulation 2 with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (867 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.41. Initial air flux distribution in Simulation 3f with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (1217 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.42. Initial air flux distribution in Simulation 3g with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (1817 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.
Figure A.43. Initial air flux distribution in Simulation 3h with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (1867 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.44. Initial air flux distribution in Simulation 3i with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (1650 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.45. Initial air flux distribution in Simulation 3j with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (1833 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.
Figure A.46. Initial air flux distribution in Simulation 3k with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (2567 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.47. Initial air flux distribution in Simulation 3l with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (2183 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.48. Initial air flux distribution in Simulation 3m with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (2300 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.
Figure A.49. Initial air flux distribution in Simulation 3n with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (1767 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.50. Initial air flux distribution in Simulation 3o with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (1500 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.51. Initial air flux distribution in Simulation 3p with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (1967 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.
Figure A.52. Initial air flux distribution in Simulation 3q with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (1917 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.53. Initial air flux distribution in Simulation 3r with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (1767 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.54. Initial air flux distribution in Simulation 4a with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (750 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.
Figure A.55. Initial air flux distribution in Simulation 4b with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (1017 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.56. Initial air flux distribution in Simulation 4c with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (625 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.
Figure A.57. Initial air flux distribution in Simulation 4d with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (333 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.58. Initial air flux distribution in Simulation 4e with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (700 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.
Figure A.59. Initial air flux distribution in Simulation 4f with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (1467 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.60. Initial air flux distribution in Simulation 4g with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (1350 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.
Figure A.61. Initial air flux distribution in Simulation 5a with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (3150 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.62. Initial air flux distribution in Simulation 5b with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (2283 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.
Appendix G: Centerline Air Flux Values for Select Configurations

For the homogeneous domains tested the vertical components of the air flux vectors were always highest along the contaminant pack centerline; therefore this region governs the average vertical smouldering velocity. Figure A.63 below illustrates the decrease in vertical components of the local air fluxes along the contaminant pack centerline for Simulations 3a to 3h and 5a to 5b in Table 3-4.

![Figure A.63](image-url)

**Figure A.63.** Vertical component of local air fluxes along the contaminant pack centerline versus contaminant pack height for Simulations 3a-3f (pilot-scale) and 5a-5b (full-scale).
Appendix H: Model Sensitivity to $\tau_d$

To confirm the impact of effective permeability ratio between untreated and treated sections of the contaminant pack on local channeling and the predicted extent of treatment, values of $\tau_d = 0.5, 0.75, 1.0, 1.25, \text{ and } 1.5$ were simulated in the model. The resultant relative permeability-saturation curves for each value of $\tau_d$ are shown below in Figure A.64, illustrating that lower $\tau_d$ values result in higher relative permeabilities. For each simulated value of $\tau_d$, the predicted position of the front at various times is shown in Figure A.65 to Figure A.69, and the predicted initial air flux extinction contours are shown in Figure A.70 to Figure A.74.

![Relative permeability-saturation curves](image)

**Figure A.64.** Relative permeability-saturation curves for a range of $\tau_d$ values that were tested in the model to confirm the impact of effective permeability ratios.
Figure A.65. Predicted smouldering front position at 0, 100, 308 (breakthrough), and 758 (end of treatment) min for Simulation 1, for $\tau_a = 0.50$. 
Figure A.66. Predicted smouldering front position at 0, 100, 308 (breakthrough), and 758 (end of treatment) min for Simulation 1, for $\tau_d = 0.75$. 
Figure A.67. Predicted smouldering front position at 0, 100, 283 (breakthrough), and 675 (end of treatment) min for Simulation 1, for $\tau_d = 1.00$. 
Figure A.68. Predicted smouldering front position at 0, 100, 308 (breakthrough), and 758 (end of treatment) min for Simulation 1, for $\tau_d = 1.25$. 
Figure A.69. Predicted smouldering front position at 0, 100, 308 (breakthrough), and 758 (end of treatment) min for Simulation 1, for $\tau_0 = 1.50$. 
Figure A.70. Initial air flux distribution in Simulation 1, for $\tau_d = 0.50$, with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (758 min) in red.

Figure A.71. Initial air flux distribution in Simulation 1, for $\tau_d = 0.75$, with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (683 min) in red.

Figure A.72. Initial air flux distribution in Simulation 1, for $\tau_d = 1.00$, with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (675 min) in red.
Figure A.73. Initial air flux distribution in Simulation 1, for $\tau_d = 1.25$, with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (667 min) in red.

Figure A.74. Initial air flux distribution in Simulation 1, for $\tau_d = 1.50$, with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (575 min) in red.
Appendix I: Clean Sand Cap Effects

As shown below in Figure A.75 and Figure A.76, removing the clean sand cap in Configuration REC2 had minor impacts on the rate and extent of treatment.

Figure A.75. Initial air flux distribution in Configuration REC2 with no clean sand cap with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (950 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.
Figure A.76. Predicted smouldering front position at 0, 333, 867 (breakthrough), and 950 (end of treatment) min for Configuration REC2 with no clean sand cap.
Appendix J: Additional Full-scale Configurations

Two additional field-scale configurations were tested; FIELD1b and FIELD2b. FIELD1b is identical to FIELD1, except an impermeable crust was simulated on the outer lower edges of the contaminant pack. This is a hypothetical crust left from a previous hot pad treatment. FIELD2b is identical to FIELD2b, except the clean sand cap height was increased from 0.5 m to 1.0 m to confirm that the clean sand cap does not affect predicted results at the full-scale. The following figures show the predicted front at various times and the predicted initial air flux extinction contour.
Figure A.77. Predicted smouldering front position at 0, 833, 1783 (breakthrough), and 2533 (end of treatment) min for Configuration FIELD1b with an impermeable crust (shaded grey).
Figure A.78. Predicted smouldering front position at 0, 83, 1900 (breakthrough), and 2217 (end of treatment) min for Configuration FIELD2b with a 1 m clean sand cap.
Figure A.79. Initial air flux distribution for Configuration FIELD1b with an impermeable crust (shaded in grey), with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (2533 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.

Figure A.80. Initial air flux distribution for Configuration FIELD2b with a 1 m clean sand cap, with the extinction contour level of 0.5 cm/s shown in blue versus the final extent of treatment (2217 min) shown in red. The contaminant pack, clean sand cap, and plenum are outlined in black dashed, black solid, green lines, respectively.
Curriculum Vitae

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EDUCATION
M.E. Sc. with Collaborative Program in Environment and Sustainability, September 2014 – August 2016
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Western Scholarship of Distinction, 2009

Alexander Rutherford Scholarship, 2009

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Numerical Modelling for Environmental Engineers
Teaching Assistant
The University of Western Ontario: 2014, 2015

SCHOLARLY ACTIVITIES

STARx Thermal Treatment System: Optimizing Hotpad Systems with Two-Dimensional Numerical Modelling
Speaker Presentation
CSCE 2016 Environmental Specialty Conference, London, ON, June 4, 2016

STARx Thermal Treatment System: Optimizing Hotpad Systems with 2-D Numerical Modelling
Poster Presentation
10th International Conference on Remediation of Chlorinated and Recalcitrant Compounds, Palm Spring California, May 23, 2016

Numerical Modelling of STAR to Optimize the Design of Ex-Situ Soil Treatment Systems
Speaker Presentation
IAH-CNC 2015, Waterloo, ON, October 29, 2015

Numerical Modelling of STAR to Optimize the Design of Ex-Situ Soil Treatment Systems
Speaker Presentation
RENEW/INTEGRATE, London ON, October 2, 2015

Two-Dimensional Numerical Modelling of Smouldering Combustion for Field-scale Soil Remediation
Poster Presentation
SyNRGS. Toronto, ON, September 27, 2014