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Numerical Modelling of Smouldering Combustion as a Remediation Technology for NAPL Source Zones

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1. Introduction

Non-Aqueous Phase Liquids (NAPLs) represent some of the most prevalent, most harmful and most recalcitrant contaminants in the environment. Existing technologies are often expensive and results in incomplete remediation of NAPL source zones. Smouldering combustion is a novel concept that has significant potential for the remediation of NAPLs. Many common NAPLs are combustible and capable of generating substantial amounts of heat when burned. Smouldering is a flameless form of combustion in which a condensed phase fuel undergoes surface oxidation reactions within a porous matrix. The exothermic nature of the technique generates a self-sustaining combustion reaction (illustrated in Figure 1) that represents a highly efficient and inexpensive remediation option.

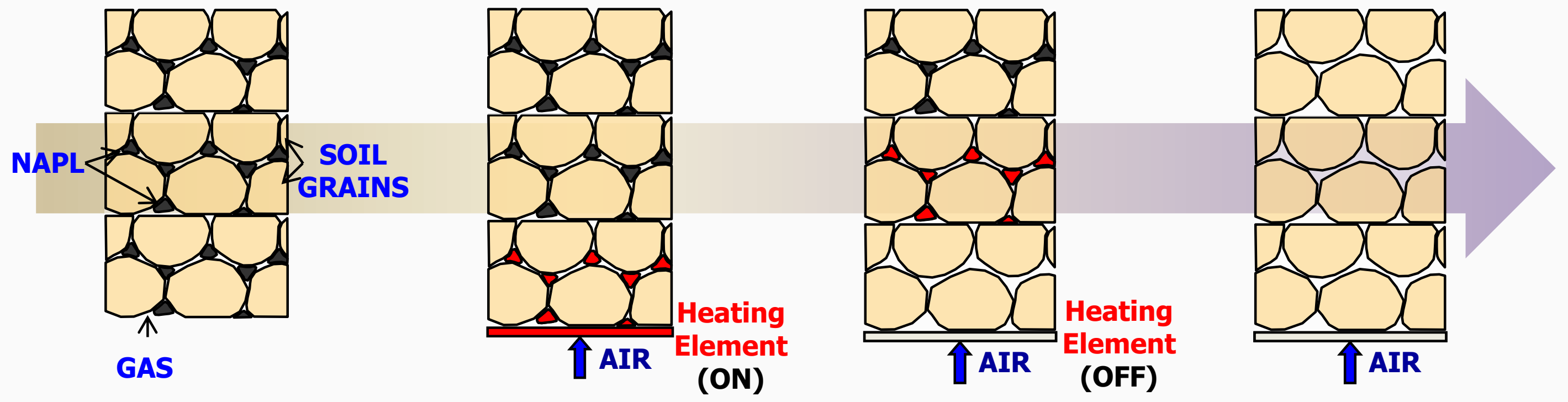
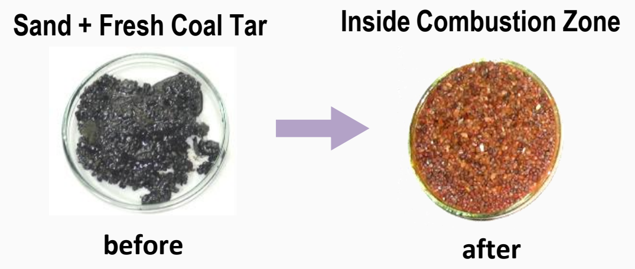


Figure 1: Conceptual model of self-sustained smouldering combustion of NAPL in porous matrix



	Amount Removed
Total Petroleum Hydrocarbons (TPH)	99.9+%
Polycyclic Aromatic Hydrocarbons (PAH)	99.9+%
Volatile (BTEX)	100%

The objective of this work is to develop a numerical model capable of simulating the propagation of a smouldering front in NAPL-contaminated porous media.

2. Model Development

A phenomenological approach was used in the development of a numerical model capable of simulating a propagating smouldering front. A general mathematical framework for fire spread modelling is presented in Richards (1995) in which the growth of the fire perimeter is approximated by a set of partial differential equations (Eq. 1a & 1b). The rate of growth is a function of key model parameters a, b and c which are dependant on fuel type, weather conditions, wind direction and speed (see Figure 2).

$$\frac{\partial x}{\partial t}=\frac{a^2\cos(\phi-\theta)\cos\theta-b^2\sin(\phi-\theta)\sin\theta}{\sqrt{(a\cos(\phi-\theta))^2+(b\sin(\phi-\theta))^2}}+c\cos\theta \quad \text{(1a)}$$

$$\frac{\partial y}{\partial t}=\frac{a^2\cos(\phi-\theta)\sin\theta+b^2\sin(\phi-\theta)\cos\theta}{\sqrt{(a\cos(\phi-\theta))^2+(b\sin(\phi-\theta))^2}}+c\sin\theta \quad \text{(1b)}$$

Forward spread rate: U=a+c
Lateral spread rate: V=b
Backward spread rate: W=a-c
Wind direction relative to x-axis=θ
(Richards, 1995)

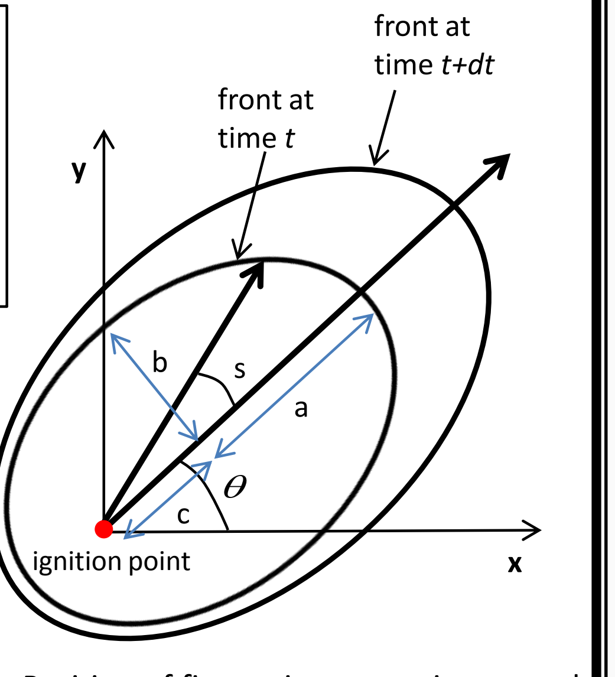
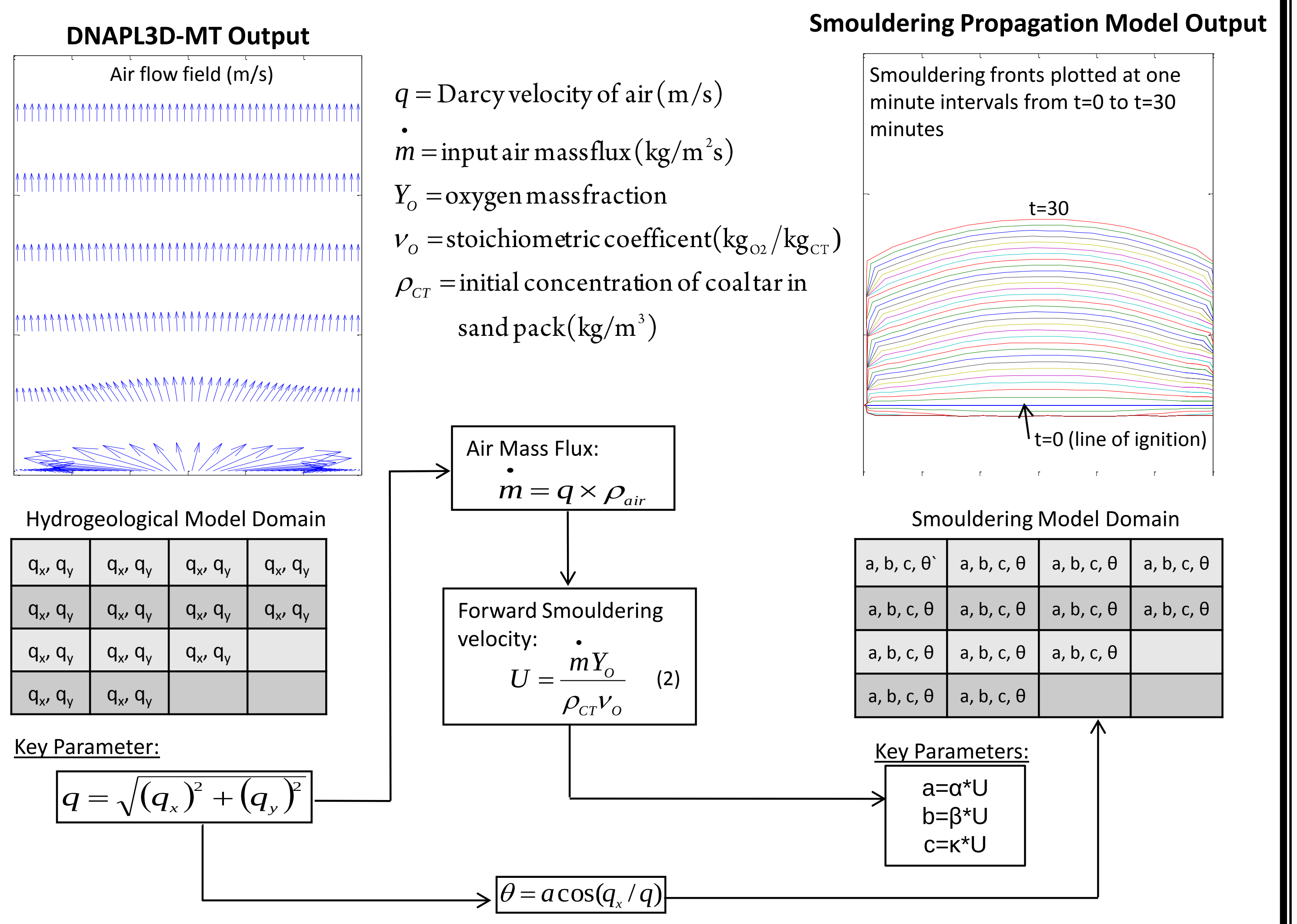


Figure 2: Position of fire perimeter at times t and t+dt and its relation to key model parameters

The fire model is modified in this work for smouldering behaviour; in particular, incorporating a correlation of the velocity of the smouldering front to key parameters such as contaminant type, NAPL saturation, and air mass flux developed from the column experiments. The model couples the multiphase flow code DNAPL3D-MT (Gerhard and Grant, 2007) with the Fire Model (Richards, 1995). Experiments conducted by Pironi et al. (2009) have demonstrated that the propagation rate of the smouldering front is highly dependant on the air mass flux. This is the basis for the analytical expression (Eq. 2) that is used to link the two models as illustrated by Figure 3:



q = Darcy velocity of air (m/s)
$\dot{m}$ = input air mass flux (kg/m^{2}s)
Y_O = oxygen mass fraction
ν_O = stoichiometric coefficent (kg$_{O2}$/kg$_{CT}$)
ρ_{CT} = initial concentration of coal tar in sand pack (kg/m^3)

Air Mass Flux:
$$\dot{m}=q\times\rho_{air}$$

Forward Smouldering velocity:
$$U=\frac{\dot{m}Y_O}{\rho_{CT}\nu_O} \quad (2)$$

Hydrogeological Model Domain

q_x, q_y	q_x, q_y	q_x, q_y	q_x, q_y
q_x, q_y	q_x, q_y	q_x, q_y	q_x, q_y
q_x, q_y	q_x, q_y	q_x, q_y	
q_x, q_y	q_x, q_y		

Key Parameter:
$$q=\sqrt{(q_x)^2+(q_y)^2}$$

Smouldering Model Domain

a, b, c, θ`	a, b, c, θ	a, b, c, θ	a, b, c, θ
a, b, c, θ	a, b, c, θ	a, b, c, θ	a, b, c, θ
a, b, c, θ	a, b, c, θ	a, b, c, θ	
a, b, c, θ	a, b, c, θ		

Key Parameters:
a=α*U
b=β*U
c=κ*U

$$\theta=a\cos(q_x/q)$$

Figure 3: Process by which the 2-D Darcy velocity air flow field produced by the multiphase flow model DNAPL3D-MT is linked to Fire Spread Model resulting in Smouldering Propagation Model Coefficients α, β and κ were set to 0.875, 0.875 and 0.125 respectively (Rein et al., 2007). A point source air diffuser and line ignition is simulated.

3. Simulations

DNAPL3D-MT and the Smouldering Propagation Model are employed to conducted three sets of simulations:
1. Validation of simulated air injection into water saturated porous media (data not shown)
2. Model comparison against column experiments of smouldering combustion propagation for coal tar in coarse sand (see Figure 5)
3. Sensitivity simulations to experimental set-up (see Figure 6)

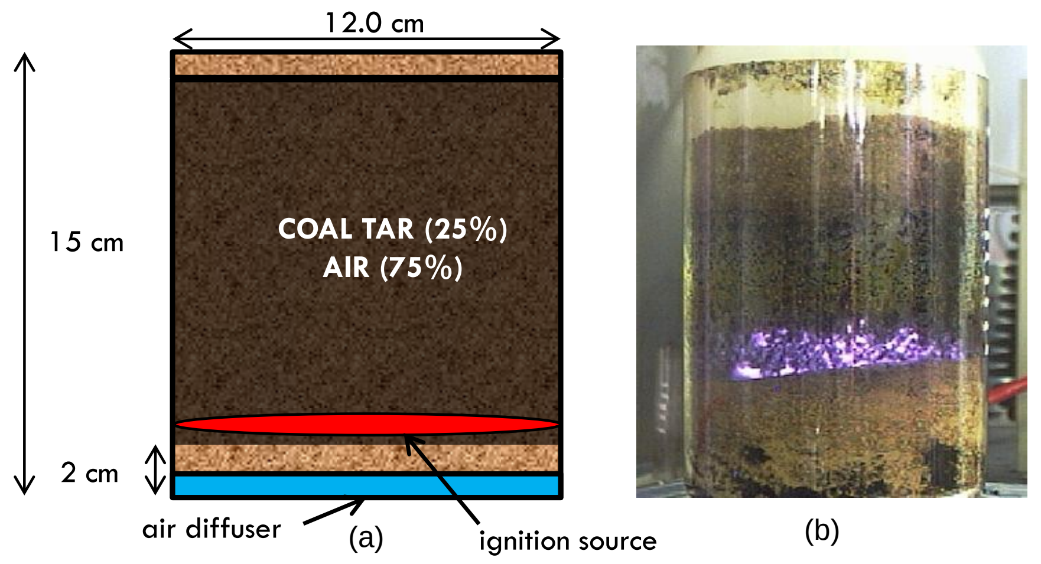


Figure 4: (a) Experimental set-up for column experiments (Pironi et al.,2009). (b) Photo of smouldering experiment in progress.

4. Results and Analysis

The simulated results of smouldering front propagation for various air mass fluxes is illustrated in Figure 5. Smouldering fronts are plotted at 1 minutes intervals from zero to thirty minutes. The forward velocity of the smouldering front (U) is shown to increase as air mass flux increases (see Figures 5a, 5b and 5c).

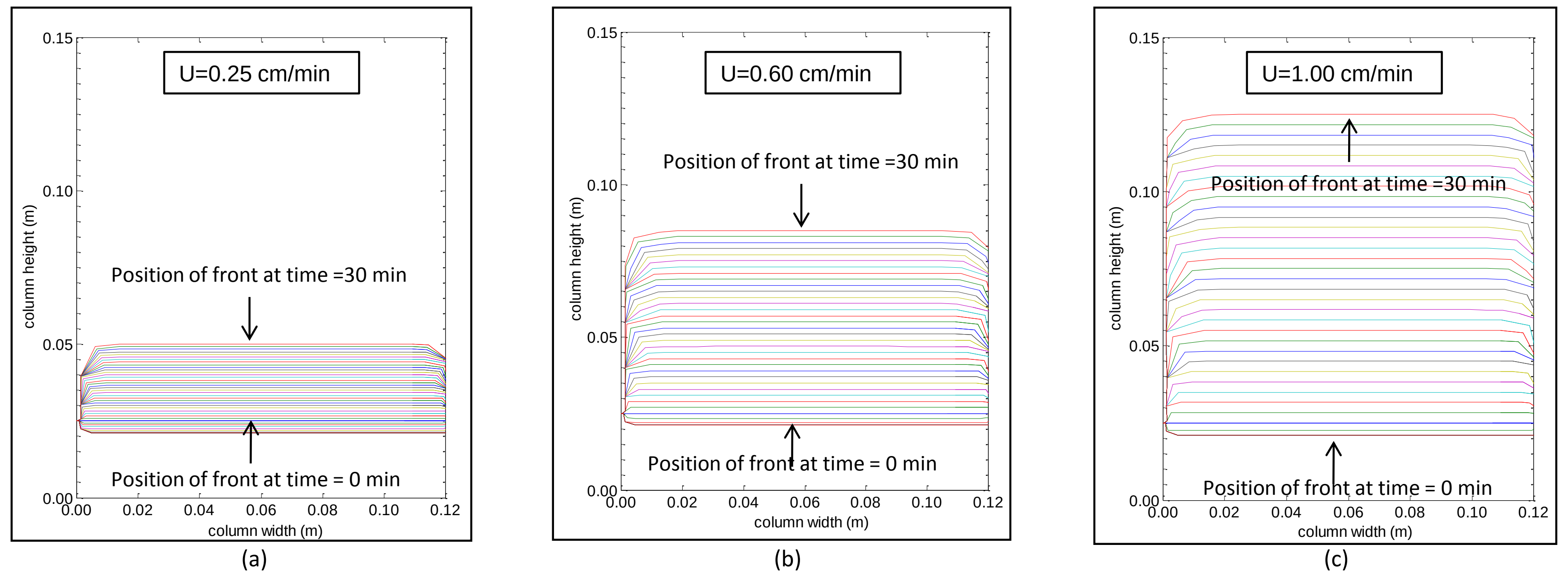
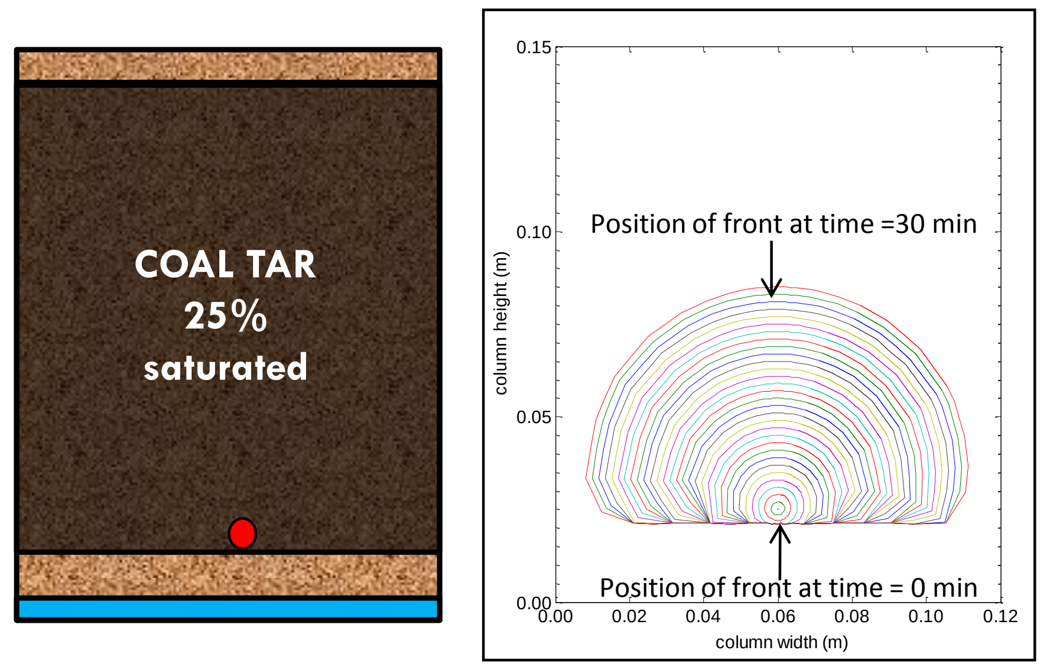


Figure 5: Simulated results of smouldering propagation for various air mass fluxes: (a) 0.047 kg/m^2/s (b) 0.113 kg/m^2/s (c) 0.189 kg/m^2/s.



Simulations were conducted to examine the effect of the experimental set-up on the shape and velocity of the smouldering front. In Figure 6, a point source ignition is simulated with the same air mass flux as that used in Figure 5b. The forward rate of smouldering (U) along the line of ignition remains the same but the front has a more circular shape. Figures 3, 5, 6 allow for comparison between different experimental configurations for point and line source ignitions and air diffusers.

Figure 6: Point source ignition experimental set-up and simulated result. An air mass flux of 0.113 kg/m^2/s was employed.

5. Conclusions and Future Work

- Adaption of a Fire Spread Model for simulation of smouldering of NAPLs in porous media by creating a link with multiphase flow code DNAPL3D-MT is successful.
- Ongoing work includes validation of Smouldering Propagation Model against experiments.
- Future work will include application of the model at more realistic scales to simulate smouldering of NAPLs in pilot studies and to explore and optimize model parameters and experimental set-ups.

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