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### ► To cite this version:

Nicolas Philippe, Hossein Davarzani, Manuel Marcoux, Stéfan Colombano, Delphine Kaifas, et al.. Modeling of non-isothermal DNAPL/water flow in porous media: application to coal tar soil remediation. Computational Methods in Water Resources, Jun 2018, Saint-Malo, France. hal-01735196

**HAL Id: hal-01735196**

**<https://hal.science/hal-01735196>**

Submitted on 15 Mar 2018

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# Modeling of non-isothermal DNAPL/water flow in porous media: application to coal tar soil remediation

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**Key words:** porous media, two-phase flow, non-isothermal flow, and coal tar remediation

## Introduction

Polycyclic Aromatic Hydrocarbons (PAHs) are main constituents of coal tar, which are found on coking plant wastelands. Coal tar is classified as a Dense Non-Aqueous Phase Liquid (DNAPL), meaning its density is superior to water. This property implies that coal tar is generally found in depth of saturated zones, and coupled with its high viscosity, coal tar is a complex liquid to recover. The pumping rate of coal tar is generally low due to its viscous nature and possible capillary effect. A thermal enhancement, up to 70 °C, coupled with pumping, has shown to be sufficient to improve the mobility of coal tar and , consequently, the recovery rate [1-3]. However, these studies do not propose laboratory-scale experiments and modeling in order to characterize the coupling between heat and mass transfers happening in the process. The main objective of this work is to study the impact of temperature on the DNAPL and water flow rates in porous media. This will help to gain better understanding on how a temperature increase in the soil effectively enhances the recovery rate of coal tar.

## Experimental setups

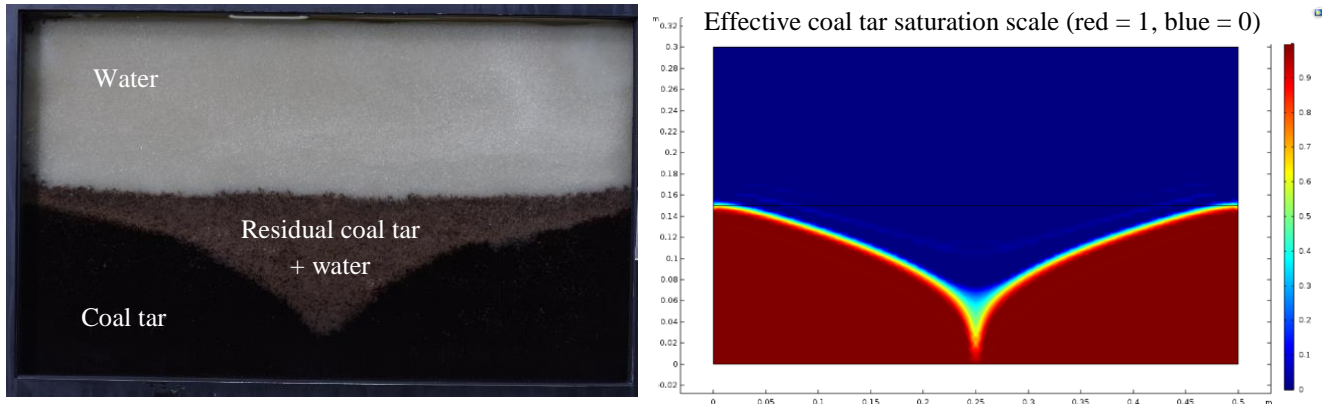
The two-phase flow of coal tar and water was reproduced in a porous medium consisting of homogenous glass beads. First, a Tempe cell (diameter 5.8 cm, height 5.5 cm) was used in order to obtain capillary pressure – saturation relationships between coal tar and water at 20 °C and at 50 °C with a thermal chamber. Then, we used 1D columns (diameter 5.8 cm, height 25.5 cm), to characterize the changes in coal tar migration rates at 20 °C and 50 °C. Finally, laboratory-scale recovery tests were conducted in a 2D tank (length 50 cm, height 30 cm, width 7 cm) under isothermal conditions. A 15 cm coal tar lens was injected below a 15 cm water layer, and we used injection and pumping systems in the tank right and left borders in order to keep the coal tar and water heights constant at all times during the experiments. The coal tar in the 2D tank was pumped between 10 mL/min and 250 mL/min from the bottom center of the tank. A heating rod will be used in order to study the two-phase flow under non-isothermal conditions. This setup will allow us to study both temperature and pumping effects on the water and DNAPL saturations fields, as well as the temperature field changes due to the two-phase flow and the well condition. In all the previous setups, the saturation and temperature fields were obtained through time-domain reflectometry (TDR) within an onboard thermistor. In addition, an imaging method was developed based on the relationship between optical density and DNAPL saturation to obtain the saturation fields for 2D tank case.

## Mathematical formulations and numerical simulations

In order to model the DNAPL and water flow in porous media, the Darcy's Law for multiphase flow was used. DNAPL and water were considered immiscible and the capillary pressure – saturation relationship was obtained through the Tempe cell experiments. The temperature effect on the physical properties of the DNAPL (here, coal tar), such as density, dynamic viscosity and wettability, were experimentally inquired. The results show that an increase in temperature between 10 °C and 50 °C only decreases dynamic viscosity of coal tar between  $8.5 \times 10^{-2}$  Pa.s and  $1.3 \times 10^{-2}$  Pa.s. For the model, we used a quadratic function to interpolate coal tar dynamic viscosity at all temperatures between 10 °C and 50 °C.

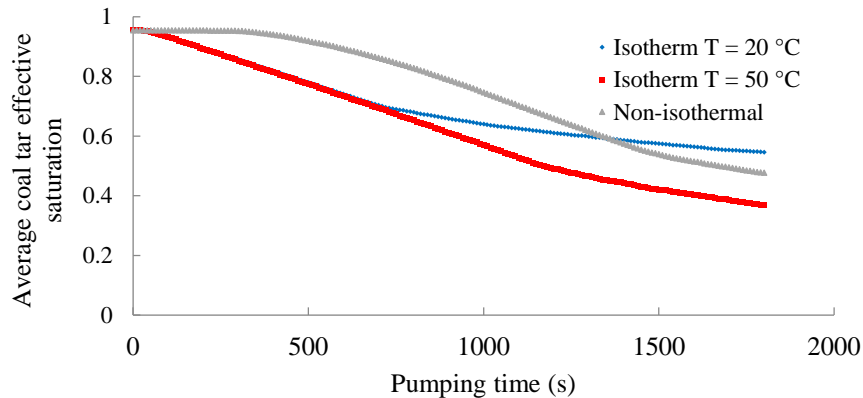
We considered heat transfers by conduction and forced convection due to the DNAPL-water pumping pressure. Both local thermal equilibrium (LTE) and local thermal non-equilibrium (LTNE) were considered. The obtained coupling equations were solved numerically using COMSOL Multiphysics® software in order to simulate coal tar migration fronts in 1D column, and coal tar pumping tests in 2D tank. Air-water two-phase flow was reproduced in the 2D tank in homogeneous glass beads in order to calibrate and validate the numerical models with experimental data. The simulations with coal tar and water were initially run in isothermal conditions, thus ignoring energy balance equation. We worked in the same conditions as in the 2D

tank experiments: the bottom part (15cm) of the tank is initially saturated with DNAPL, while the rest of the tank is saturated with water. As mentioned, the DNAPL and water height were kept constant by setting hydrostatic pressures to the sides of the tank. Finally, a production well boundary condition was used at the bottom center part of the tank to reproduce the experimental pumping rate. In the experiments, we generally stop before water enters into the producing well, whereas in the simulations, we consider that coal tar can no longer be produced as soon as its effective saturation near the well is zero and in place, only water is produced afterwards. The results from both experimental and numerical cases at 20 °C (isothermal case) are shown on *Figure 1* for the same initial conditions and at the same pumping time. We found a good agreement between numerical and experimental results.



*Figure 1:* An example of the comparison between 2D tank experimental and numerical pumping tests at the same time.

Then, non-isothermal pumping models were run by coupling both fluid dynamics viscosities with temperature and considering the local thermal equilibrium hypothesis valid. A hot plate (50 °C) was added to the left part of the tank while the right part was supposed to be constant at 20 °C. The top and bottom part of the tank were supposed insulated, and we let the tank heat for 300 seconds before starting the pumping process. The results show first, that after 1800 seconds of pumping time, only water is produced from the tank, as the average effective coal tar saturation is constant afterwards. In addition, the average effective saturation of DNAPL in the tank is lower at high temperature, which indicates a higher recovery rate of coal tar pure phase when the system is heated (*Figure 2*).



*Figure 2:* Averaged coal tar saturation in the tank during pumping for isothermal cases (20 °C, 50 °C) and non-isothermal case

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