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STOMP Application To Represent Bioslurping Extraction Technique – Extraction Radius Analysis

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SUMMARY: Bioslurping technique is one possible operational configuration of Multiphase Extraction (MPE) to remediate porous media contaminated by Light Non Aqueous Phase Liquids (LNAPls) contaminants. The numerical simulator known as STOMP - Subsurface Transport Over Multiple Phases - was modified during Matos de Souza's DSc research to include bioslurping processes in 3-D domain assuming the presence of a fixed tube tip extraction position and using the well model concept. In this article, an extraction radius analysis is conducted using a base model built with data from a hypothetical LNAPL recovery case study presented in the literature. The determination of the extraction radius of an application of remediation technique based on flow is extremely important in the project and design of the technique. The extraction radius of influence was evaluated for different times of extraction. Besides that, an additional analysis was performed showing the relationship between applied vacuum pressure and the extraction radius of influence. The modeling results were found to be consistent with the expected physical behavior and the simulator adequately represented the multiphase extraction process intended with the bioslurping technique configuration and its radius of influence.

KEYWORDS: Bioslurping, STOMP, multiphase extraction, radius extraction analysis.

1 INTRODUCTION

Organic contamination has been the subject of numerous scientific studies regarding, among other things, environmental investigations and remediation of contaminated areas. Most of the oil contaminants consist of organic compounds that have a low solubility in water and show up as a separate liquid phase in soil or groundwater.

Various soil and groundwater remediation techniques involving a range of physical, chemical and/or biological processes have been used over the years. Multi-Phase Extraction (MPE) techniques have been widely used for petroleum contaminants, given their ability to remediate the vadose zone through gas extraction, and the saturated zone through the extraction of liquids, without the need of soil removal for ex-situ treatment.

MPE applications may follow different configurations, depending upon how the extraction is performed. The three main forms are generally known as Dual Phase Extraction (DPE), Total Phase Extraction (TPE), and Bioslurping. Of these, bioslurping is the technique discussed in the paper. Bioslurping combines elements from three different remediation techniques: vacuum-enhanced pumping, SVE – Soil Vapor Extraction - and bioventing. Bioslurping is a variation of the TPE configuration as it uses a single conduit for extracting the vapor and liquid phases, but with the ultimate goal of trying to maximize LNAPL recovery.

However, despite the extensive use of bioslurping remediation technique in the field, its application has relied on practical experience from previous projects, and hence is subject to much empiricism. A few numerical models have been developed with the purpose to simulate extraction processes promoted by the application of some kind of multiphase remediation technique. Examples are given by Li et al. (2003), Yen et al. (2003) and Huang et al. (2007). Most of these studies make use of two-dimensional (2-D) vertically averaged models. The complexity of the many processes involved in multiphase flow makes it difficult to derive and use relatively simple analytical models for predicting the extraction and removal rates of contaminants from porous media. The applicability of analytical models is limited by the many assumptions generally needed to derive them.

According to Kaluarachchi (1996), Miller *et al*. (1998) and US Army (1999), among others, the mathematical description of three-phase flow is complex and has been the subject of intense debate in the specialized technical literature. Despite these difficulties and some non-consensus situation, there is a need for some type of predictive three-dimensional (3-D) MPE model, including the bioslurping configuration, which are now increasingly used for remediation of LNAPL contaminated porous media.

Matos de Souza (2015) adapted the Subsurface Transport Over Multiple Phases (STOMP) simulator to represent bioslurping remediation. The numerical simulator was modified to include bioslurping processes in 3-D assuming the presence of a fixed tube tip extraction position and using the well model concept. Matos de Souza et al. (2016) presented the well model approach used in STOMP and a number of bioslurping scenarios tested using porous medium and fluid property data presented in US Army (1999). Subsequently, the model was applied to a field case in Brazil allowing for a direct comparison of field extraction data and numerical predictions. The results of the model test and field site simulations suggest that the new module may be used in the design of field applications and in the analysis of production data.

This paper presents an additional assessment to the work done in Matos de Souza (2015) related to the analysis of the extraction radius of influence. The influence of the extraction was tested for different scenarios, i.e., time of remediation and vacuum applied. This analysis was performed using the Bioslurping module developed to represent Bioslurping extraction in STOMP simulator, using a hypothetical LNAPL recovery case study presented in US Army (1999).

2 METHODOLOGY

2.1 STOMP Simulator

The STOMP simulator was developed by the Hydrology Group of PNNL-Pacific Northwest National Laboratory, located in Richland, WA, USA. STOMP is a scientific tool designed to produce numerical predictions of thermal and hydrogeologic flow and transport phenomena in variably saturated subsurface environments contaminated with volatile or nonvolatile organic compounds (WHITE & OOSTROM, 2000). This fully implicit integrated finite difference mode of the simulator has been used to simulate a variety of 3-phase systems (e.g., Oostrom and Lenhard, 2003; Oostrom et al., 2007; Yoon et al., 2009).

The multifluid extraction simulations were conducted with the water-air-oil mode of the STOMP simulator (White and Oostrom, 2006). The applicable governing equations are the component mass conservation equations for water, air, and oil:

$$\frac{\partial}{\partial t}\left[\sum_{\gamma=l,g}\left(n\omega_\gamma^w\rho_\gamma S_\gamma\right)\right] = -\sum_{\gamma=l,g}\left\{\nabla F_\gamma^w + \nabla J_\gamma^w\right\} + \dot{m}^w$$

(1a)

$$\frac{\partial}{\partial t}\left[\sum_{\gamma=l,g}\left(n\omega_\gamma^a\rho_\gamma S_\gamma\right)\right]=-\sum_{\gamma=l,g}\left\{\nabla F_\gamma^a+\nabla J_\gamma^a\right\}+\dot{m}^a$$

(1b)

$$\frac{\partial}{\partial t}\left[\sum_{\gamma=l,g,n}\left(n\omega_\gamma^o\rho_\gamma S_\gamma\right)+(1-n)\omega_s^o\rho_s\right]= -\sum_{\gamma=l,g,n}\left\{\nabla F_\gamma^o+\nabla J_\gamma^o\right\}+\dot{m}^o \quad (1c)$$

where the subscripts *l*, *g*, *n*, and *s* denote the aqueous, gas, NAPL, and solid phases, respectively; the superscripts *w*, *a*, and *o* indicate the water, air, and oil components, respectively; *t* is time [T]; n is the porosity; ω is the component mass fraction; ρ is the density [M/L^3]; S is the actual liquid saturation; F is the advective mass flux [M/L^{2}T]; J is the diffusive-dispersive mass flux [M/L^{2}T]; and $\dot{m}$ is the component mass source rate [M/T]. The reader is referred to White and Oostrom (2006) for details on the flux formulations.

STOMP simulator has a modular code architecture and is controlled through a text file, which must be named "input" for proper execution. This input file has a structured format composed of cards, which contain associated groups of input data (White & Oostrom, 2006). The group of necessary input data to run a specific simulation case is dependent upon the operational mode.

2.2 Bioslurping Well Module

The bioslurping process in STOMP is modeled using the well model concept and is specified using the source card. This card allows a user to control sources and/or sinks of mass, energy and solutes by defining time-varying sources. The card also offers several possibilities for entering sources, sinks or well source models. By definition, sinks are negative sources, while sources refer to an influx of mass, energy or solute into a node. Matos de Souza (2015) and Matos de Souza et al. (2016) present a detailed description about Bioslurping well module implementation in STOMP.

For the multiphase mass removal of oil, water, and air components using the bioslurping remediation option, the following multiphase mass extraction was implemented into the STOMP simulator:

$$m^i=-WI\sum_{\gamma=l,g,n}\left(\frac{\rho_\gamma\omega_\gamma^i k_{r\gamma}}{\mu_\gamma}\left[P_\gamma^{fbs}-P_\gamma^{well}\right]\right) \quad (2)$$

where the superscript *i* and the subscript γ denote the components (*w*, *a*, and *o*) and the phases (*l*, *g*, *n*, and *s*), respectively; $k_{r\gamma}$ is the relative permeability of fluid phase γ; μ_γ viscosity of phase γ [M/(LT)]; *WI* is the modified Peaceman well index [L^3]; P_γ^{well} is the user-imposed well phase pressure [M/LT^2]. The phase pressure at the bioslurping tip (P_γ^{fbs}) is computed from the grid block field pressure (P_γ^f) as follows:

$$P_\gamma^{fbs}=P_\gamma^f+\Delta l_z g_z\rho_\gamma \quad (3)$$

where Δl_z is the distance from the slurp tube tip to the grid cell center [L], and g_z is the gravitational acceleration [L/T^2]. The bioslurping well model in STOMP is specified by declaring six entries: 1) a well trajectory, 2) position of the slurp tube tip, 3) well characteristics (i.e., well casing radius, skin factor), 4) well bore pressure, 5) time operations and 6) maximum volumetric production rate.

The well direction is not restricted to a vertical orientation, despite bioslurping technique application has the purpose to maximize oil recovery and, as the LNAPL is lighter than water, the oil is on top of water. For this reason, vertical wells are the best condition to apply the bioslurping technique and so far, just vertical wells have been used. The Peaceman Well Index (*WI*) in (2) for 3D well systems is given by (Shu et al., 2005):

$$WI = \sqrt{(WI_x)^2 + (WI_y)^2 + (WI_z)^2} \tag{4}$$

Where

$$WI_x = \left[\frac{2\pi\sqrt{k_y k_z} L_x}{\ln\left(\frac{r_{o,x}}{r_w}\right) + s_k} \right] \tag{5a}$$

$$WI_y = \left[\frac{2\pi\sqrt{k_x k_z} L_y}{\ln\left(\frac{r_{o,y}}{r_w}\right) + s_k} \right] \tag{5b}$$

$$WI_z = \left[\frac{2\pi\sqrt{k_y k_x} L_z}{\ln\left(\frac{r_{o,z}}{r_w}\right) + s_k} \right] \tag{5c}$$

In (5), L_j is the length of the projected screened interval [L] in the *j*-direction, s_k is the skin factor, r_w is the well radius [L], k_j is the intrinsic permeability in the *j*-direction [L^2], and $r_{o,j}$ is the equivalent well block radius [L]. The skin factor (s_k) is a dimensionless number and accounts for hydraulic property changes adjacent to a well. A positive value indicates damage resulting in a reduction of well productivity, whereas a negative value indicates an enhanced productivity as a result of well stimulation (Furui et al., 2002). The equivalent well block radius ($r_{o,j}$) in (5) was defined by Peaceman (1983) as the radius at which the steady-state flow pressure in the aquifer (or reservoir) is equal to the numerically calculated pressure of the grid block containing the well. He derived the following expressions for the three principal directions:

$$r_{o,x} = 0.28 \left[\frac{\left(\left\{\frac{k_y}{k_z}\right\}^{1/2} \Delta z^2 + \left\{\frac{k_z}{k_y}\right\}^{1/2} \Delta y^2 \right)^{1/2}}{\left(\left\{\frac{k_y}{k_z}\right\}^{1/4} + \left\{\frac{k_z}{k_y}\right\}^{1/4} \right)} \right] \tag{6a}$$

$$r_{o,y} = 0.28 \left[\frac{\left(\left\{\frac{k_x}{k_z}\right\}^{1/2} \Delta z^2 + \left\{\frac{k_z}{k_x}\right\}^{1/2} \Delta x^2 \right)^{1/2}}{\left(\left\{\frac{k_x}{k_z}\right\}^{1/4} + \left\{\frac{k_z}{k_x}\right\}^{1/4} \right)} \right] \tag{6b}$$

$$r_{o,z} = 0.28 \left[\frac{\left(\left\{\frac{k_x}{k_y}\right\}^{1/2} \Delta y^2 + \left\{\frac{k_y}{k_x}\right\}^{1/2} \Delta x^2 \right)^{1/2}}{\left(\left\{\frac{k_x}{k_y}\right\}^{1/4} + \left\{\frac{k_y}{k_x}\right\}^{1/4} \right)} \right] \tag{6c}$$

where Δj is the *j*-direction grid cell dimension. The reader is referred to Matos de Souza (2015) for details about Bioslurping well model implementation in STOMP.

2.3 Extraction Radius of Influence

A conceptual model of contamination and extraction was developed using data from a LNAPL recovery simulation documented in US Army (1999). This same conceptual model of contamination and extraction was used for model test simulations presented by Matos de Souza et al. (2016) where a number of extraction parameters was evaluated.

The simulations were performed for a hypothetical case with an initial apparent LNAPL thickness of 1.5 m in the extraction well, as depicted in Figure 1. The schematic presents the fluid levels in a well containing NAPL and the corresponding fluid distribution in an adjacent porous medium under equilibrium conditions before fluid extraction with the well model.

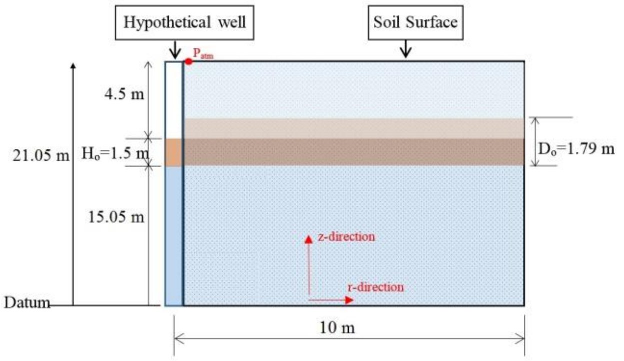

Figure 1. Schematic of a subsurface well system for the extraction radius of influence analysis.

The objective is to identify the distance in the *r*-direction from the tube location where the effects of extraction are no longer observed, i.e., the oil, water and air vertical profiles are the same as in the initial condition. This location could be indicated by the levels of the LNAPL and water in the porous medium, for example. In terms of LNAPL saturations in a porous medium, the radius of influence could be represented by the first position in the horizontal direction where *Do*, i.e., the soil hydrocarbon thickness defined by Lenhard & Parker (1990) - see Fig. 1, has the same value as before the vacuum application.

Table 1 provides a summary of the characteristics of the simulations performed in this work. Tests 1 and 2 were conducted to check the extraction radius of influence for two different extraction times, but applying the same vacuum pressure (11.325 kPa). Tests 3 and 4 were simulated applying the limits of vacuum range defined in US Army (1990) during the same extraction time (100 days).

Table 1. Summary of simulations performed.

Simulation name	Extraction time (days)	Applied vacuum (kPa)*
Test 1	100	11.325
Test 2	500	11.325
Test 3	100	1.33
Test 4	100	66.26

* Range reported in US Army (1990).

The well, hydraulic, and fluid properties assumed in all simulations are shown in Table 2.

Table 2. Hydraulic properties, fluid properties, and well/operational characteristics used in the simulations.

Parameter	Value
Hydraulic properties	
Hydraulic conductivity (m/s)*	1.27 x 10^{-6}
Porosity*	0.35
Van Genuchten α (1/cm)*	0.0067
Van Genuchten n_v *	1.7
Irreducible saturation	0.10
Fluid properties	
Gas-NAPL scaling factor*	3.3
NAPL-aqueous phase scaling factor*	1.4
NAPL density (kg/m^3)*	730
NAPL viscosity (Pa s)*	0.62
Well/operational characteristics	
Radius (m)	0.1016
Screen length (m)	1.0
Slurp tube tip elevation (m)	16.05

*US Army (1999).

All simulations were performed using a three-dimensional (3-D) domain using a cylindrical coordinate system. The domain included a hypothetical extraction well (at the first node of the domain in the radial direction), with its surroundings extending 10 m into the radial direction (r-direction). Along the vertical direction (z-direction), aligned with the negative gravitational vector, the domain had a length of 21 m. A regular grid block of 10 cm was used to discretize in r-direction and a variable grid was used in z-direction to allow a more detailed description of the region where the free phase was assumed (grid block size of 50 cm for 0 m $< z <$ 10 m and a grid block of 10 cm for 10 m $< z <$ 21 m).

Boundary conditions were set up to represent the hypothetical field condition of having one well extraction in a multi-well extraction system. Therefore, a no-flow NAPL boundary condition was imposed at the site boundary. The bottom of the domain was closed for all three phases. No-flow boundary conditions were also applied to all phases along the top of the domain with the purpose to represent a sealed surface. This scenario is the best condition to apply the MPE technique because it enhances horizontal airflow and increases the radius of influence (US Army, 2002). Regional groundwater flow in the aquifer was not considered in the simulations. The prescribed initial (hydrostatic) conditions of the aqueous and gaseous phases were assumed to be maintained along the outer boundary. The initial oil and water vertical distributions were obtained by specifying fluid pressures at known fluid-fluid interfaces in combination with fluid pressure gradients. The vacuum pressure used in the simulations (Table 1) was in the range of pressures given by US Army (1999).

3 RESULTS AND DISCUSSION

The total quantity of oil in the domain, before applying the extraction, was equal to 1012.89 kg. This quantity was calculated by the code at t = 0 for the imposed 10-m long domain. The total quantity of oil slurped during 100 days of extraction was equal to 42.90 kg in test 1 simulation.

Figure 2 shows plots of the soil hydrocarbon thickness (D_o) along the r-direction of the porous medium at time t = 0 (before extraction) and at two different times of continuous extraction (50 days and 100 days) for test 1.

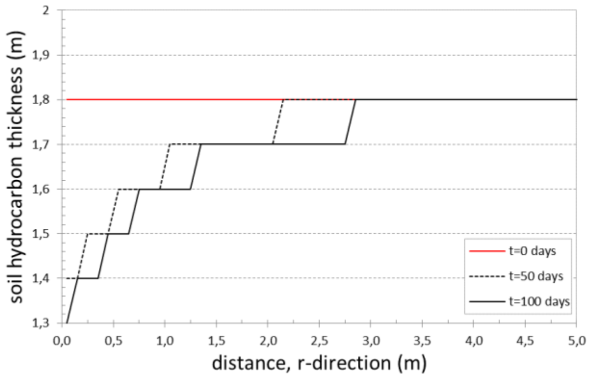

Figure 2. Plots of D_o in the r-direction obtained with simulation Test 1.

The results in Fig. 2 show that the extraction has an effect up to around 3 m from the well (in the r-direction) when the system is operated for 100 days. However, when the extraction took place for only 50 days, the influence radius was much smaller, approximately 2.2 m. This difference can be explained by the boundary conditions that were set up for this test: a no flow condition for NAPL phase at the outer boundary. The idea was to estimate the performance and influence of one well, while assuming that no additional LNAPL could flow into the domain from outside the domain, as in a multi-well field with 20 m spacing between each pair of wells. With this condition, the amount of oil in the domain is finite and, disregarding groundwater recharge, an increase in the radius of influence of the extraction can be expected as the vacuum is continuously applied over time.

Test 2, for which the results are shown in Fig. 3, used the same input data as test 1, except for the total extraction time, which was extended to 500 days, in order to certify the increase of extraction influence over time.

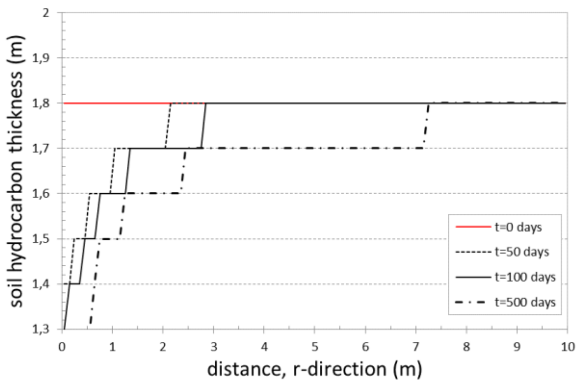

Figure 3. D_o along the r-direction of the porous medium for simulation Test 2.

Typically, in Brazil, MPE remediation systems operate on average between 1 and 2 years. Hence the 500 days of extraction time should be representative of a usual field test. The radius of influence of the extraction was found to be 7.25 m for a 500 day period of extraction, as shown in Fig. 3.

Fig.4 shows the relationship between soil hydrocarbon thicknesses (D_o) and the extraction radius of influence when different pressures are applied. In all simulations, the D_o remained 1.8 m at the time before starting the extraction, as expected to occur since there is still no flow. The results obtained show a reduction in soil hydrocarbon thickness when the vacuum applied is increased. Furthermore, it is also observed an increase in the extraction radius of influence as the vacuum pressure is increased. These two tendencies are expected to occur in field applications. The vacuum pressure range simulated was the same reported in US Army (1990), who reported a relationship between the flow rate and the applied vacuum for their particular conditions. However, as reported in Matos de Souza (2015) and Matos de Souza et al. (2016), high vacuum pressures do not necessarily lead to a higher volume of oil extracted from the porous medium, and a more complete analysis have to be performed when the purpose is to design a Bioslurping system application.

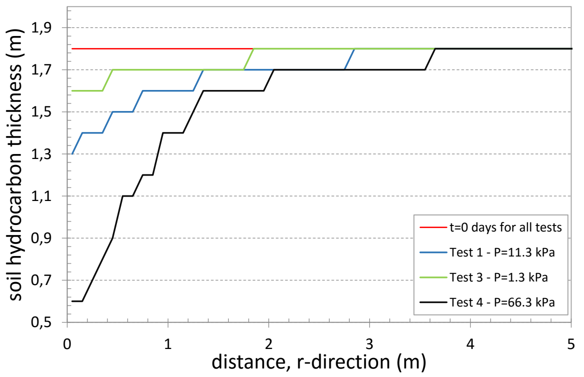

Figure 4. D_o along the r-direction of the porous medium for simulations with different vacuum pressure of extraction: Test 1, Test 3 and Test 4.

The step-like representation, instead of smooth lines, of the graphs of Figures 2, 3 and 4, are caused by the discretization of the domain, since the STOMP model performs calculations for the central position of each element of the grid. In practice, it is important to combine the discretization of the mesh that produces results with an acceptable level of accuracy and a good computational performance.

4 CONCLUSION

The Bioslurping module developed to represent Bioslurping extraction in STOMP simulator was applied to analyze some results of extraction radius of influence of a hypothetical LNAPL recovery case study.

The analysis developed in this article had the purpose to relate the extraction radius of influence over remediation time and with the vacuum pressure in the extraction system. The results obtained show a positive relationship between extraction time, applied vacuum and extraction radius of influence, according to what was expected to happen as the boundaries were closed and the oil mass was finite in the domain.

The simulations performed showed that the model can be successfully employed on simulating the multiphase extraction process intended with the bioslurping technique configuration and its radius of influence.

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