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Model fit to experimental data for foam-assisted deep vadose zone remediation

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HIGHLIGHTS

- Presented detailed guidelines how to fit a foam model to experimental data.
- Investigated what kind of inputs needed/how they are interconnected.
- Showed how to interpret the outcome of model fit.
- Examined the effect of back pressure and gas compressibility.

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ABSTRACT

This study investigates how a foam model, developed in Roostapour and Kam [1], can be applied to make a fit to a set of existing laboratory flow experiments in an application relevant to deep vadose zone remediation.

This study reveals a few important insights regarding foam-assisted deep vadose zone remediation: (i) the mathematical framework established for foam modeling can fit typical flow experiments matching wave velocities, saturation history, and pressure responses; (ii) the set of input parameters may not be unique for the fit, and therefore conducting experiments to measure basic model parameters related to relative permeability, initial and residual saturations, surfactant adsorption and so on should not be overlooked; and (iii) gas compressibility plays an important role for data analysis, thus should be handled carefully in laboratory flow experiments. Foam kinetics, causing foam texture to reach its steady-state value slowly, may impose additional complications.

1. Introduction

The use of surface and subsurface storage tanks has been a common practice for waste management in order to keep liquid-based wastes. An example can be found at the U.S. DOE Hanford site at Washington State where fuels and nuclear products for the production of plutonium during the Cold War era were disposed into single and double shelled tanks over decades [2]. Over the years, some subsurface storage tanks experienced leak problems, causing subsurface contamination of unsaturated geological formations in the so-called vadose zone. The term deep vadose zone is used to refer these unsaturated geological layers, which are more than 100 ft below the ground surface and can go as deep as 500 ft, where open excavation remediation techniques are thought to be impractical both technically and economically.

There are mainly two major remediation processes considered for metal and radionuclide contaminants in the deep vadose zones [3,4]: (i) mobilization and recovery methods such as soil flushing, electro-kinetic mobilization, and vapor extraction which actively treat the affected areas by extracting the pollutants and (ii) sequestration and fixation methods such as precipitation, oxidation and reduction which treat the pollutants in place within the subsurface.

Foam injection in deep vadose zone remediation is somewhat different from other foam treatments demonstrated in oil recovery and NAPL remediation. First, surfactant preflush, much needed in typical foam processes in order to satisfy surfactant absorption and help propagation of stable foams, cannot be applied due to vertical migration of contaminants. Second, this application deals with a very dry initial condition (in fact, the entire Hanford site is located within a semi-desert area where the annual precipitation is less than several inches) with injection of foams at very high gas fraction. Third, foams are used as a delivery vehicle to transport chemical reagents in the aqueous phase so that they interact with the contaminants for immobilization and stabilization in place. These concepts are well described in Fig. 1.

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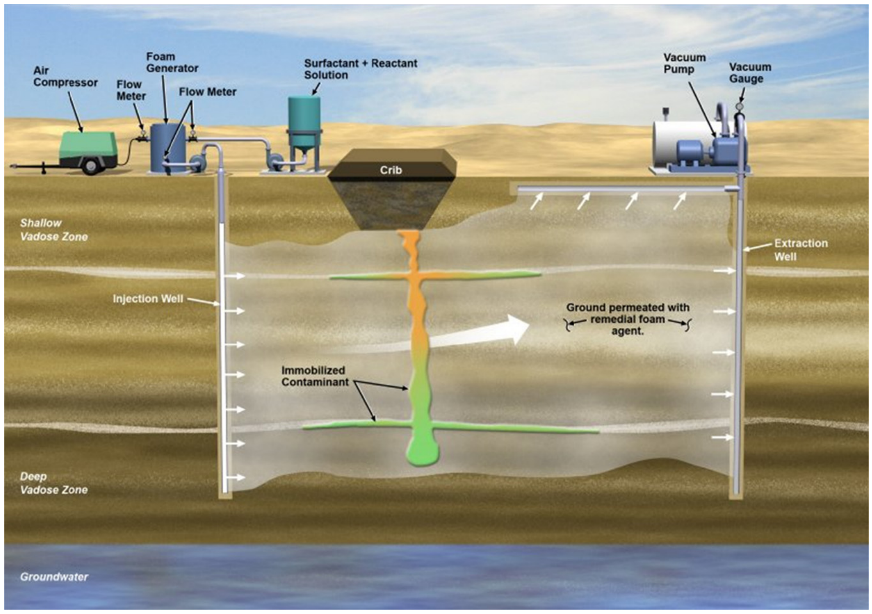

Fig. 1. A schematic of foam process to immobilize/stabilize subsurface contaminants in deep vadose-zone remediation (www.pnl.gov).

A series of recent experimental and modeling studies can be found for this particular foam application. Zhong et al. [5] conducted an experimental study consisting of 19 column tests to investigate foam transport in different sediment packs and injection foam qualities. Their study qualitatively identified three constant regions where water saturation did not change significantly. Zhong et al. [6] conducted another experimental study, focusing on how foam helps achieve better spatial distribution by amending flow characteristics within the contaminated zone in 1D and 2D flow experiments by using unsaturated porous media. Istok et al.'s study [7] presented a numerical method to formulate foams to deliver polyphosphate to the deep vadose zone contaminated with uranium, expecting the injected polyphosphate to react chemically with the pore water in vadose zone. Zhang et al. [8] showed an experimental study to look at how effective foam viscosity is affected by sediment properties and operating conditions, looking at the effect of different injection conditions. In addition, other types of studies can be found in related areas such as adsorption [9], visco-elastic polymer [10], vapor extraction [11], enhanced volatilization and enhanced sorption [12].

Among those earlier studies, the experimental study of Zhong et al. [13] is especially noteworthy because of detailed experimental data from laboratory flow tests during which foams at very dry conditions are injected into different soil columns. The displacement fronts for liquid bank and foams were monitored in conjunction with pressure measurement and average liquid saturation. Fig. 2 shows their flow apparatus in which air and 1 wt.% CS-330 (sodium lauryl ether sulfate) surfactant solutions were injected simultaneously into a foam generation column followed by a vertically mounted soil column through which the position of displacement fronts can be visualized as shown in Fig. 3.

In line with a wide range of those experimental studies, the study of Roostapour and Kam [1] investigated foam transport mechanism in a porous medium by using a mathematical technique called Method of Characteristics (MoC) where surfactant preflush was not allowed. Fig. 4 shows an example from Roostapour and Kam [1] where the initial water and gas saturations were 0.2 and 0.8 (i.e., $I:(S_w^I, S_g^I) = (0.2, 0.8)$), injection water and gas fractions were 0.2 and 0.8 (i.e., $J:(f_w^J, f_g^J) = (0.2, 0.8)$), gas-phase mobility reduction factor (MRF) was 100 (i.e., meaning that gas viscosity increases by a factor of 100 by foaming), level of surfactant adsorption (D_{sf}) was 0.2 (i.e., meaning that 0.2 pore volume of surfactant solution is required to satisfy surfactant adsorption), and limiting water saturation (S_w^*) was 0.2 (i.e., meaning that foam completely collapses if the media is too dry with $S_w < 0.2$). Solving two fractional flow curves (one with surfactant and the other with no surfactant in water) in the f_w vs. S_w domain simultaneously, the MoC-based fractional flow analysis produced effluent history, saturation profile, and time–distance diagram. The general output from the modeling study is consistent with that from experimental study of Zhong et al. [5] – the migration of three constant states such as initial condition, injection condition, and intermediate state (denoted by *I*, *J*, and *IJ* in Fig. 4 respectively) is governed by two shock fronts (denoted by slow-moving Buckley–Leverett shock, V_{sh1}, and fast-moving Buckley–Leverett shock, V_{sh2}), one surfactant chemical front (denoted by chemical shock, V_{sf}) and propagation of injected

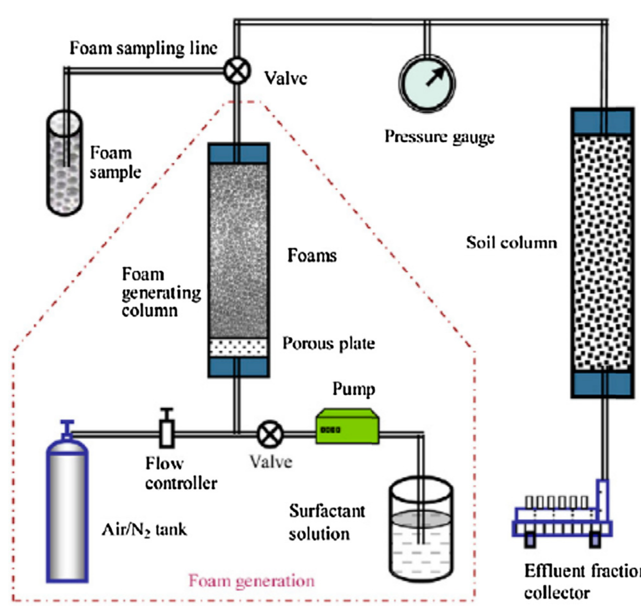

Fig. 2. A schematic of experimental set up in Zhong et al.'s study [13].