

Using T2VOC to Model Kinetic Interphase Mass Transfer During Air Sparging

Ronald W. Falta¹, John S. Gierke², and Gretchen L. Hein²

¹Departments of Geological Sciences and Environmental Engineering and Science,
Clemson University, Clemson, SC

²Departments of Geological Engineering and Sciences and Civil and Environmental
Engineering, Michigan Technological University, Houghton, MI

ABSTRACT

The unstable nature of air sparging gas flow below the water table causes injected gas to flow locally through small channels, which are separated by a distance of one or several millimeters. Although it is possible to model the average air sparging darcy flux using a conventional multiphase flow approach, this type of model does not resolve local mass transfer effects which arise due to the millimeter scale gas channels. For this reason, compositional multiphase flow simulators such as T2VOC which assume local chemical equilibrium between the phases overestimate the rate of contaminant mass transfer to the gas phase during air sparging.

An alternative method is proposed for modeling the local mass transfer during air sparging. The method is based on the existing dual media formulation which is commonly used for modeling flow and transport processes in fractured media [see Pruess and Narasimhan, 1985]. Instead of considering fractures and matrix blocks, the method is applied to porous media to simulate the local gas channels which form during air sparging. This allows resolution of the local diffusive mass transfer between the flowing gas phase, and nearby stagnant water filled zones. Because each media is modeled with a single node separated by some local average distance, the diffusive mass transfer is mathematically analogous to a first order interphase mass transfer reaction.

INTRODUCTION

Recent studies have demonstrated that VOC removal during air sparging is limited by mass transfer into the flowing gas phase. Mass transfer limitations occur at several scales due to the heterogeneous nature of gas distributions during air sparging. At a large scale, the air sparging zone is very strongly influenced by heterogeneities which form capillary and permeability barriers to the gas flow. If the geometry and locations of these heterogeneities are well known, or if the media is homogeneous, it is possible to accurately model the sparge gas flow field using a conventional multiphase flow numerical approach [Hein et al., 1997; McCray and Falta, 1997]. This type of simulator, however, cannot resolve local (subgridblock) mass transfer effects which arise due to the millimeter scale gas channels which form during sparging. For this reason, compositional multiphase flow simulators which assume local chemical equilibrium between the phases overestimate the rate of interphase mass transfer during air sparging.

Figure 1 shows the effluent concentration measured during a recent air sparging experiment conducted at Michigan Tech. In this experiment, a clean, initially water-filled vertical column was sparged with gas containing 1000 ppmv trichloroethylene vapor. The water saturation in the column during sparging was about 75 percent, so significant TCE

retardation would be expected due to partitioning into the stagnant water phase (TCE has a dimensionless Henry's constant of 0.35). However, the experimental column effluent concentration, (solid line), exhibits a rapid breakthrough, followed by a very gradual increase up to the injected composition. An attempt to model this experiment with a conventional local equilibrium approach (solid triangles) results in a poor match of the data. The local equilibrium model predicts a strongly retarded breakthrough, followed by little tailing of the concentration profile. This poor match is largely a result of over predicting the rate of local interphase mass transfer.

TCE Breakthrough and Elution

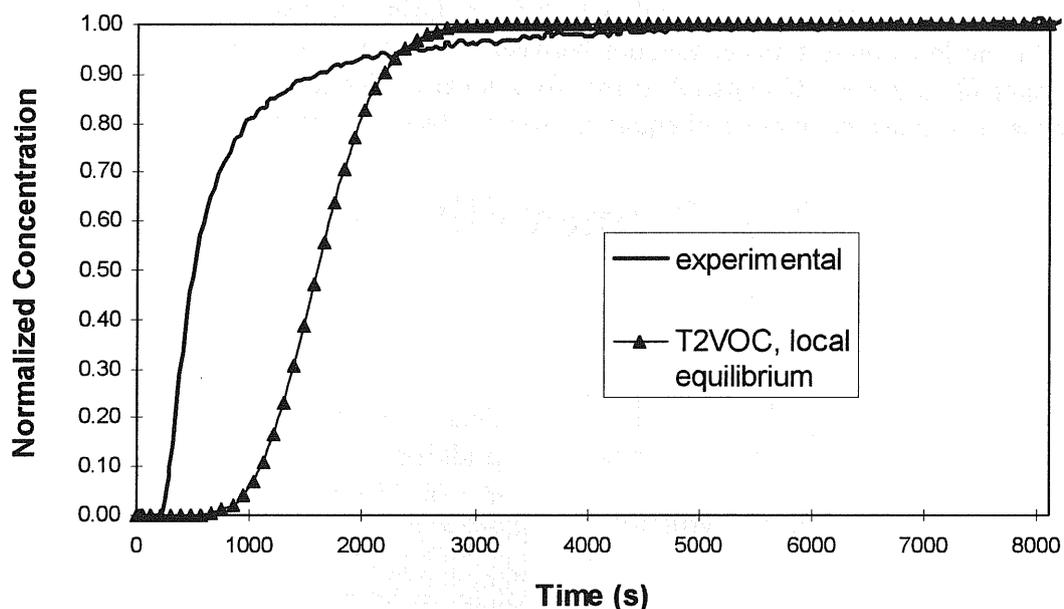


Figure 1. Comparison of experimental and simulated column effluent concentrations during a sparging experiment.

While most of the current 3-D compositional multiphase flow simulators assume local equilibrium between phases, there have been some efforts to model kinetic interphase mass transfer in multiphase contaminant transport [Sleep and Sykes, 1989]. The most widely used formulation assumes that the kinetic interphase mass transfer can be modeled as a heterogeneous first order reaction in each gridblock:

$$Q_{imt}^c = k_{imt} a (C_w^c / H - C_g^c)$$

where Q_{imt}^c is the rate of chemical mass transfer from the water to the gas phase per unit volume of porous media, C_w^c is the aqueous phase chemical concentration, C_g^c is the gas phase chemical concentration, and $k_{imt} a$ is the mass transfer coefficient-interfacial area

product. Implementing this type of mass transfer formulation in a compositional multiphase flow code is not trivial because the aqueous phase and gas phase forms of the chemical must be treated as separate components, with separate mass balance equations.

MODELING INTERPHASE MASS TRANSFER WITH A DUAL MEDIA APPROACH

We propose an alternative method for modeling the local mass transfer during air sparging. This technique is fairly straightforward, and can be easily implemented in existing compositional multiphase flow simulators which assume local phase equilibrium. The method is based on a dual media formulation which is commonly used for modeling flow and transport processes in fractured media [see Pruess and Narasimhan, 1985]. Instead of considering fractures and matrix blocks, the method is applied to porous media to simulate the effect of local gas channels which form during air sparging. This allows resolution of the local mass transfer kinetics between the flowing gas phase, and nearby stagnant water filled zones. Compared to the usual local equilibrium approach, the dual media approach doubles the number of equations to be solved at each time-step.

Dual Permeability Grid

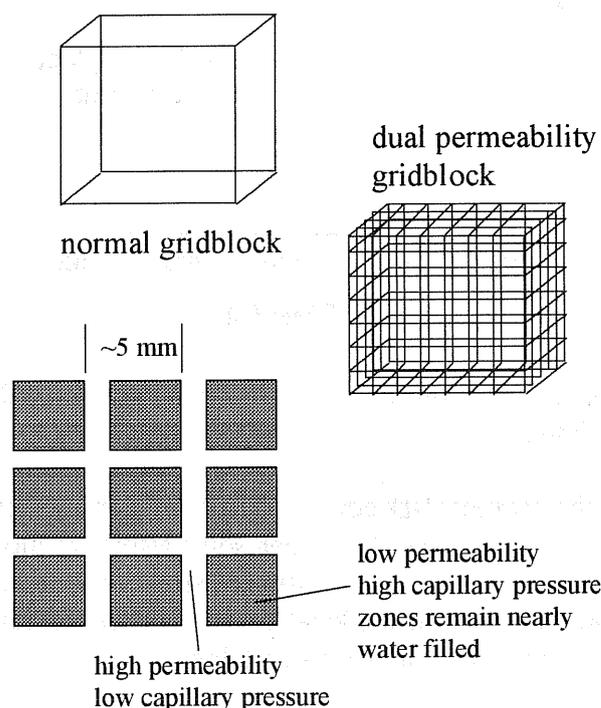


Figure 2. Schematic representation of a dual media gridblock.

Figure 2 shows a schematic diagram of the dual media formulation. Each "normal" gridblock is subdivided into two media. In the classical application of this method, these media would be fractures and matrix, and the fracture spacing would

typically be on the order of one to several meters. The two media are connected inside the gridblock by a single one-dimensional connection, with a single average interfacial area between the two media in the gridblock. The average distance between the two media, and the average interfacial area are computed based on the distributions of the two media within the gridblock (the three-dimensional fracture spacing in the fractured rock case). Each dual media gridblock is connected to other gridblocks in the normal way, but with connections for both media [Pruess and Narasimhan, 1985]. The method can be applied to complex heterogeneous 3-D grids if desired.

In the present application, we consider two types of porous media: a high permeability, low capillary pressure media, and a lower permeability, higher capillary pressure media. Compared to fractured rock applications, we assume a much smaller spacing between the two media, with a correspondingly larger interfacial area. For the case shown in Figure 2, the high permeability zones are separated by only 5 mm, so the average distance from the high permeability to the low permeability zones is only a millimeter or so, depending on the geometric model. The average interfacial area is very high in this case, approximately 768 m² of interface per m³ of porous media. Other conceptual models of the two phase distributions (eg. the gas flowing through parallel cylindrical channels) are easily implemented by adjusting the interfacial area and distance terms in the dual media grid generation step (subroutine MINC in the MESHMAKER module). The properties of the two media, and their distributions are chosen so that the sparging gas will form the characteristic local channels through the high permeability media. Currently, we do not have a technique for determining these parameters based on traditional porous media measurements, and rely instead on fitting. This is a significant limitation to the method, and it is an area where further research could provide important practical developments.

During an air sparging simulation, almost all of the gas flows through the high permeability/low capillary pressure zone. If the gas composition is not in equilibrium with the pore water, this gives rise to a concentration gradient between the nearly water filled low permeability/high capillary pressure zone and the gas filled high permeability zone. Because each media is modeled with a single node separated by some average distance, this diffusive mass transfer between the media is mathematically analogous to the first order interphase mass transfer formulation described earlier, (except that local equilibrium occurs between the gas and water in the low capillary pressure media). For the dual media approach, the mass transfer-interfacial area product, $k_{int}a$ can be calculated from

$$k_{int}a = \frac{(\phi S_w \tau_w D_w / H)A}{d}$$

where $\phi S_w \tau_w D_w$ is the effective porous media diffusion coefficient in the water-filled matrix, A is the average interfacial area between the two media per unit volume of porous media, and d is the average distance from the liquid filled matrix to the gas interface.

A series of numerical simulations were performed to illustrate the method. These were conducted using T2VOC [Falta et al., 1995], modified to account for aqueous phase diffusion. The dual permeability mesh generator (subroutine MINC in the MESHMAKER module) was modified slightly to allow for direct input of interfacial area and distance.

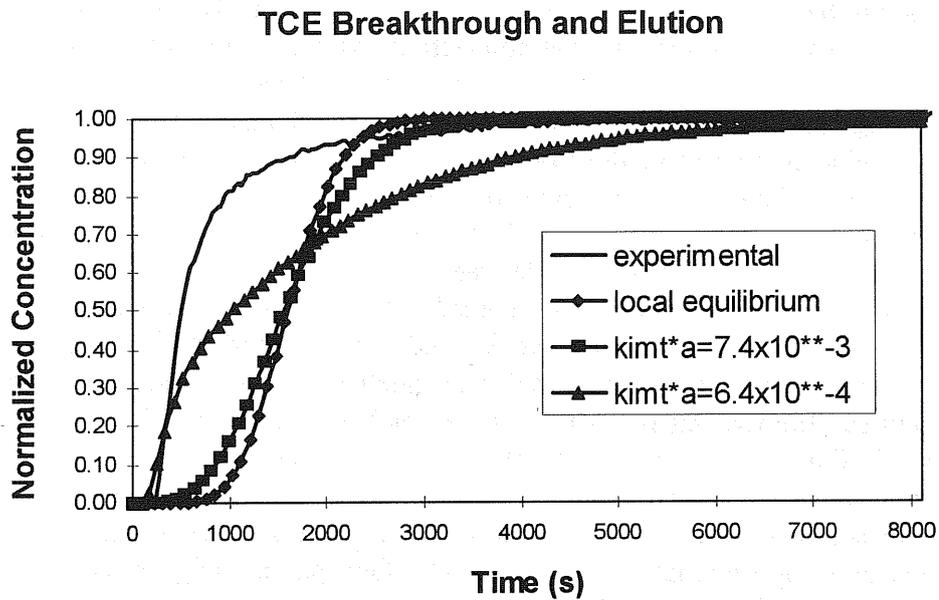


Figure 3. Numerical simulations of air sparging with local kinetic interphase mass transfer at high rates.

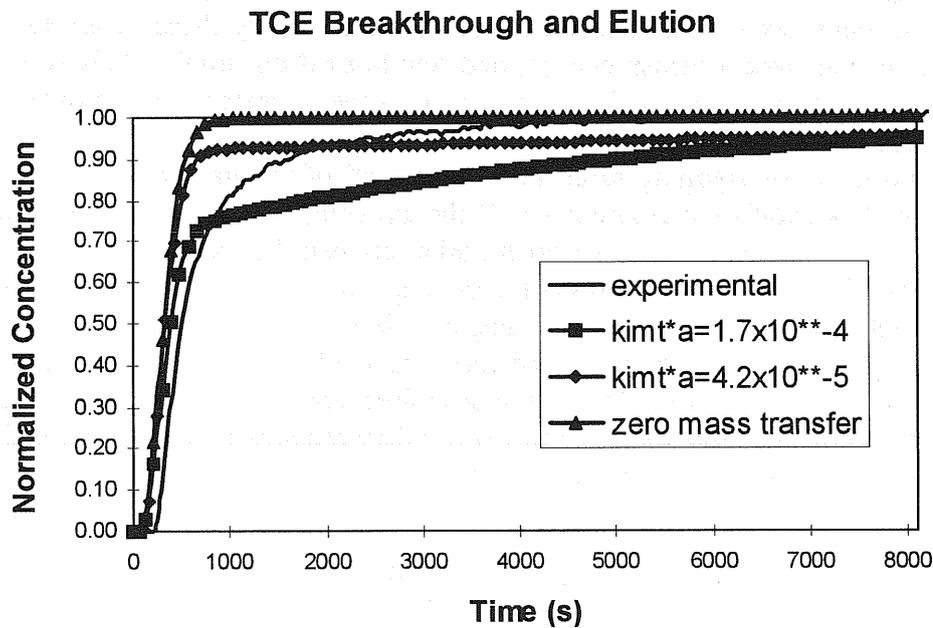


Figure 4. Numerical simulations of air sparging with local kinetic interphase mass transfer at low rates.

Figures 3 and 4 show the results of simulations assuming that all of the gas flows through 30% of the total media, with various rates of interphase mass transfer. At very high rates of interphase mass transfer (Figure 3), the dual media model essentially

duplicates the single media local equilibrium curve, as expected. As the interphase mass transfer rate constant is decreased, the curve shifts dramatically, showing an earlier initial breakthrough, followed by a long period of tailing. The case with a mass transfer coefficient of $6.4 \times 10^{-4} \text{ s}^{-1}$ corresponds to a conceptual model consisting of the gas flowing through parallel cylindrical tubes with diameters of about 1mm. This diameter is similar to the average grain size diameter of the sand in the experiment (about 0.6 to 0.8 mm). In the low mass transfer cases (Figure 4), the simulated breakthrough occurs quickly, followed by extensive tailing. The zero mass transfer case results in simple advection and diffusion through the gas filled 30% of the media, with no interphase mass transfer to the water filled media. The curve in this case is still affected by retardation in the pore water located in the gas zone ($S_w=.25$).

Unfortunately, none of the simulations shown here were able to provide a close match with the experimental data over the entire range. It is possible that the match can be improved by adjusting the relative volumes of the two-phase and liquid zones. However, it is also possible that a higher order mass transfer model is required to match this experiment. Such a higher order model could be implemented using the idea of multiple interacting continua (MINC) as described by Pruess and Narasimhan [1985]. With this approach (which already is included in the MESHMAKER module), the local liquid diffusion would be modeled using several nested blocks, improving the resolution of the local concentration gradients in the stagnant water phase. This and similar approaches will be a focus of our future research in this area.

ACKNOWLEDGEMENTS

This work is supported by the U.S. Department of Energy's Morgantown Energy Technology Center, under Contract Number DE-RO21-95MC33082 with Michigan Technological University, with a subcontract to Clemson University.

REFERENCES

- Falta, R.W., K. Pruess, S. Finsterle, and A. Battistelli, T2VOC User's Guide, *Lawrence Berkeley Laboratory Report LBL-36400*, March, 1995
- Hein, G.L., N.J. Hutzler, J.S. Gierke, and R.W. Falta, Three-Dimensional Experimental Testing of a Two-Phase Flow-Modeling Approach to Air Sparging, *Ground Water Monitoring and Remediation*, Vol. 17, No. 3, 1997.
- McCray, J.E. and R.W. Falta, Numerical Simulations of Air Sparging for Subsurface NAPL Remediation, *Ground Water Vol. 35, No. 1*, 1997.
- Pruess, K. and T. N. Narasimhan, A practical method for modeling fluid flow and heat flow in fractured porous media. *Society of Petroleum Engineers Journal*, 25(1), 14-26, February, 1985.
- Sleep, B.E., and J.F. Sykes, Modeling the transport of volatile organics in variably saturated media, *Water Resources Research*, Vol. 25, No. 1, 81-92 1989.