Modeling Pulsed Air Sparging Mass Removal of DNAPL on a Lab Scale using a Dual-Media Approach

Darby J. VanAntwerp

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Overview

- Objectives
- Previous Modeling Attempts
- Lab Experiment
- Single Domain Results
- Dual Domain Approach and Results
- Summary

Objectives

- Obtain a better understanding of contaminant mass removal in air sparging
  - Rate-limited mass transfer effects
  - Pulsed Air-Sparging
- Validate multiphase fluid flow model T2VOC for predicting contaminant mass removal

T2VOC Code

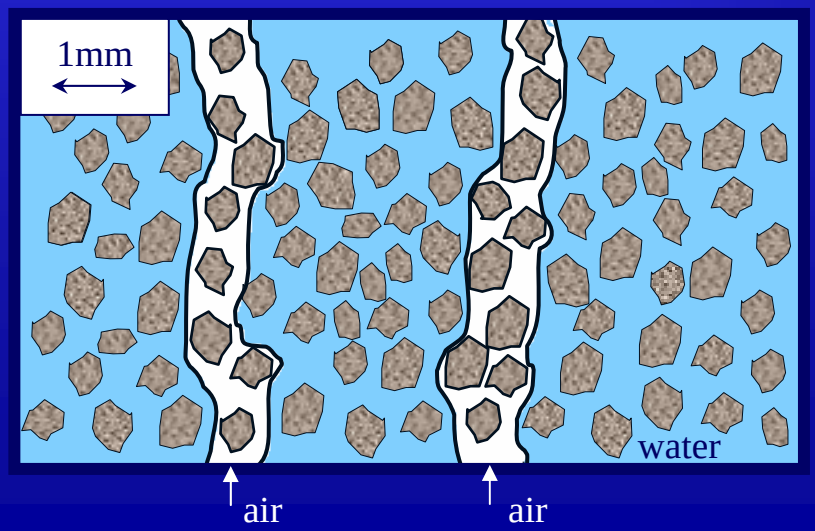
- Developed from TOUGH Codes at U.C. Berkeley
  (**t**ransport **o**f **u**nsaturated **g**roundwater and **h**eat)

- 3-d numerical simulator for multiphase flow and transport of organic chemicals in variably saturated media

(Falta, et al. 1995)

Previous Modeling Attempts

- Conventional multiphase flow approaches have accurately modeled the sparge gas plume*
  - Large scale heterogeneities can be accounted for: i.e. capillary and permeability barriers
  - Local effects not resolved: important controls on mass transfer and removal
  - Local chemical equilibrium assumption: can overestimate interphase mass transfer



*(Hein et al., 1997; McCray and Falta, 1997)

Previous Modeling Attempts

- Interphase mass transfer has been accounted for in some codes*
  - These models do not account for transient 2D or 3D multiphase flow that occurs during air sparging
  - Use conventional first order mass transfer:

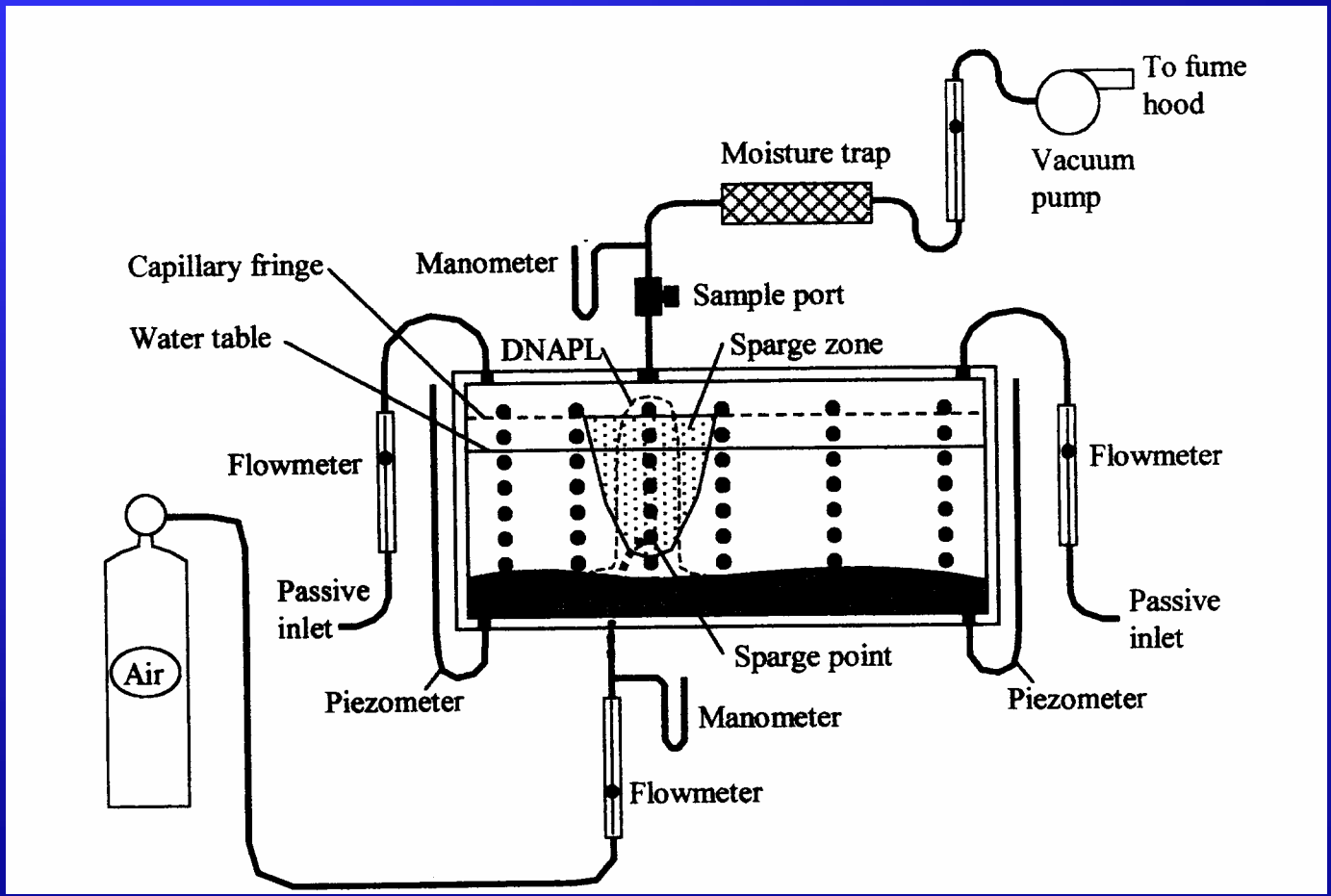
$$Q_{imt} = \underbrace{k_{imt}a}(C_w H - C_g)$$

Mass transfer coefficient x interfacial area

  - Difficult to implement in multiphase flow models due to separate mass balances on each phase of contaminant

*(Braida and Ong, 1998; Elder et al., 1999)

Experiment Set-Up



(Heron et al., 2002)

Initial Contaminant Distribution

- 100 ml PCE injected
- Water table lowered and raised to vertically smear NAPL

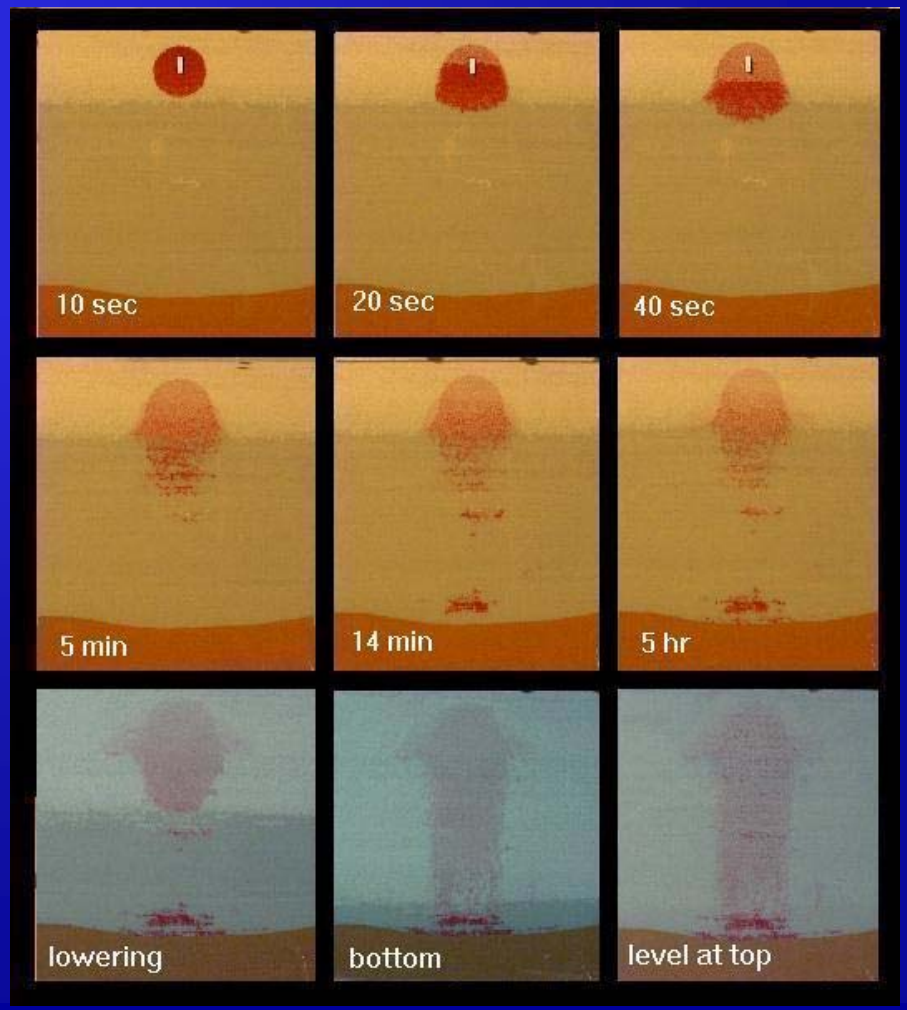
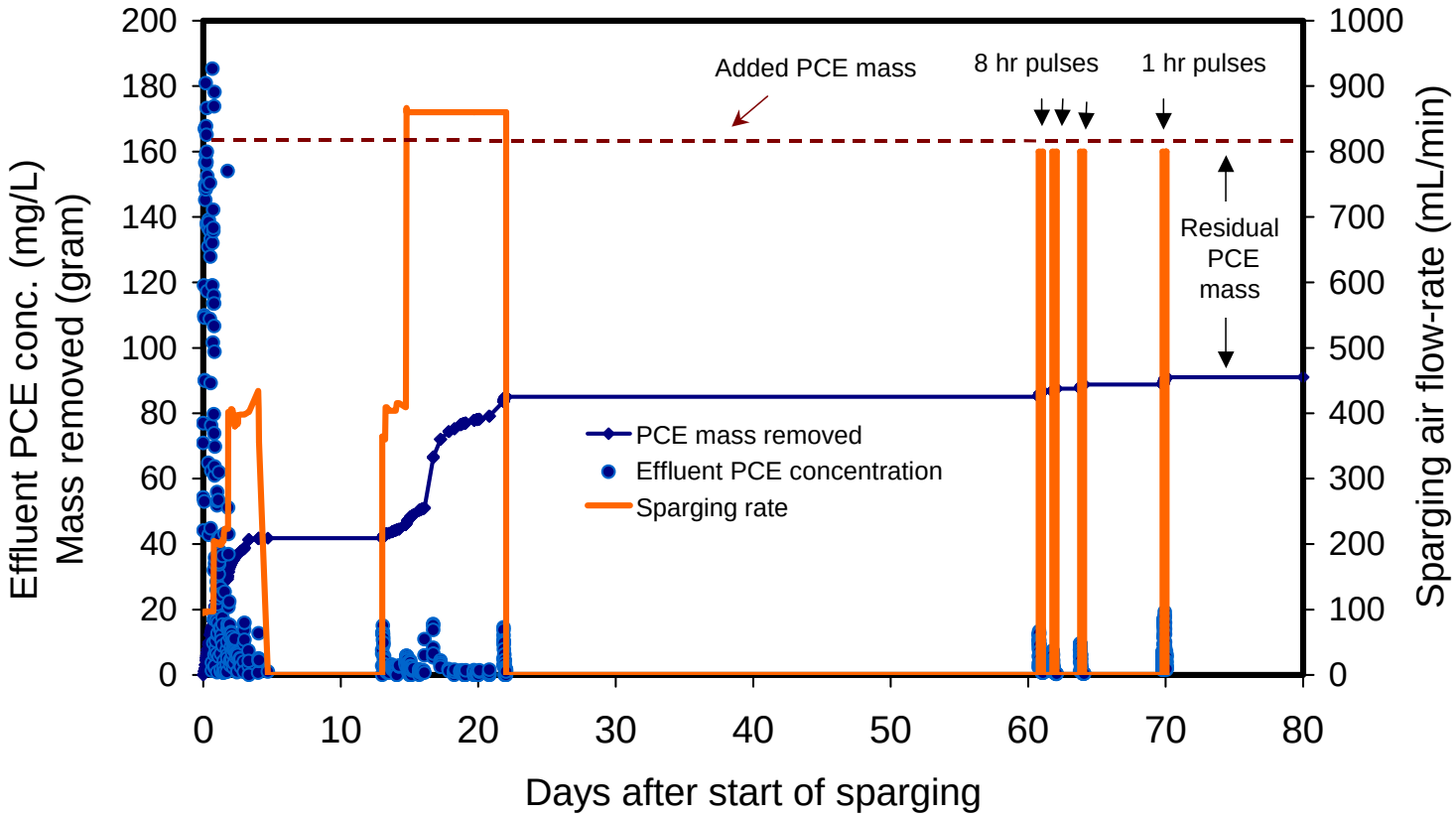


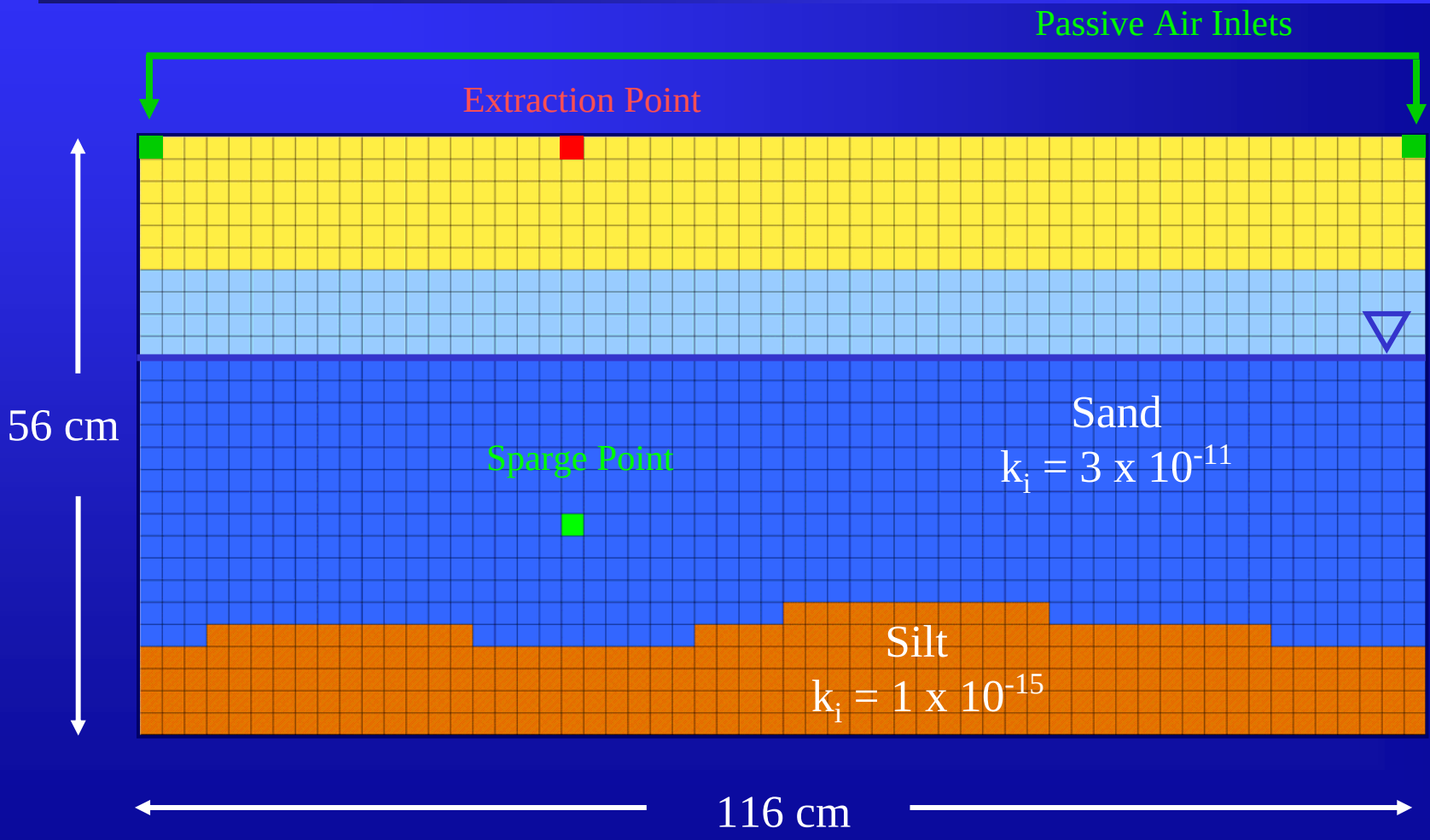
Photo courtesy of J. S. Gierke

Experiment Data

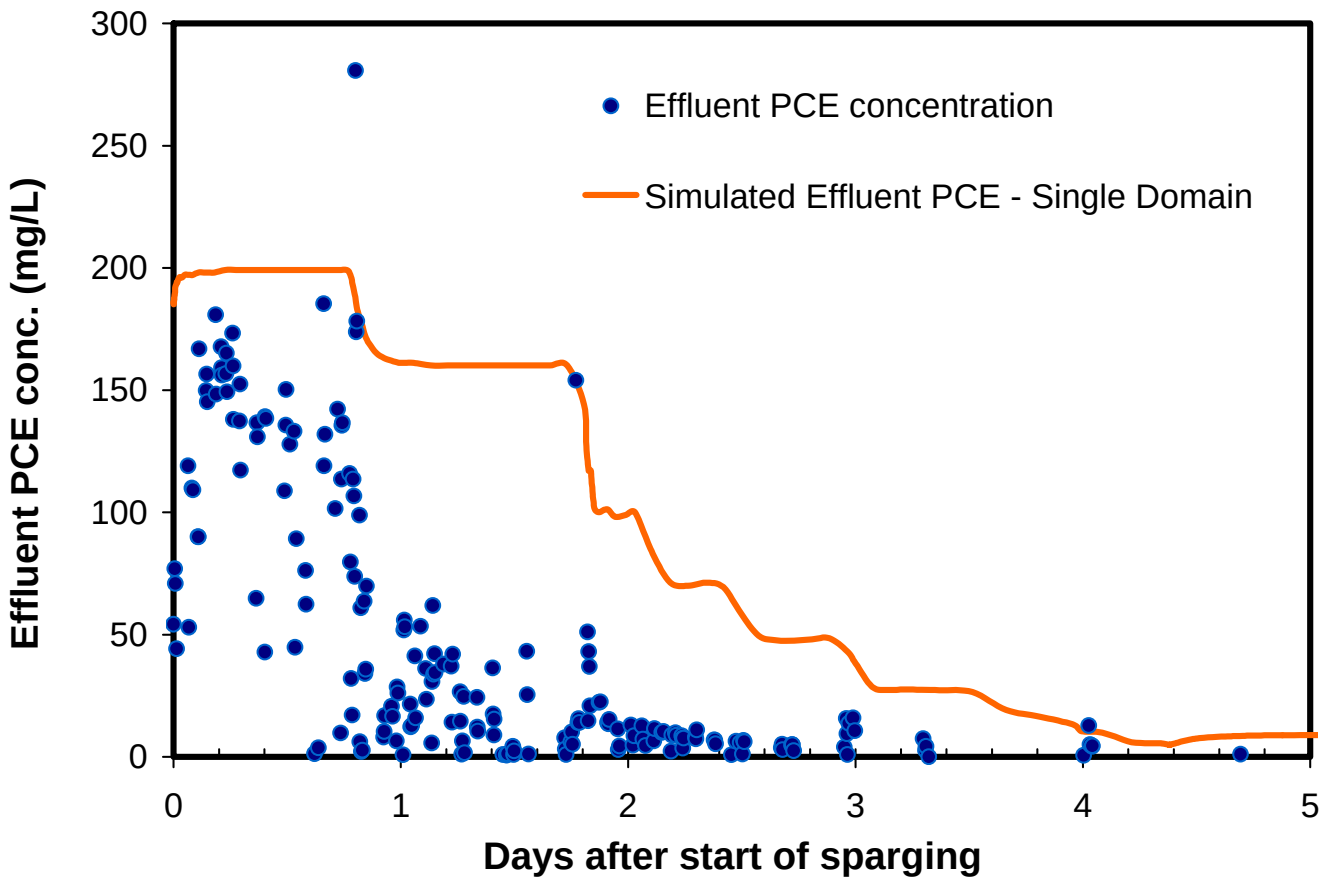


(Heron et al., 2002)

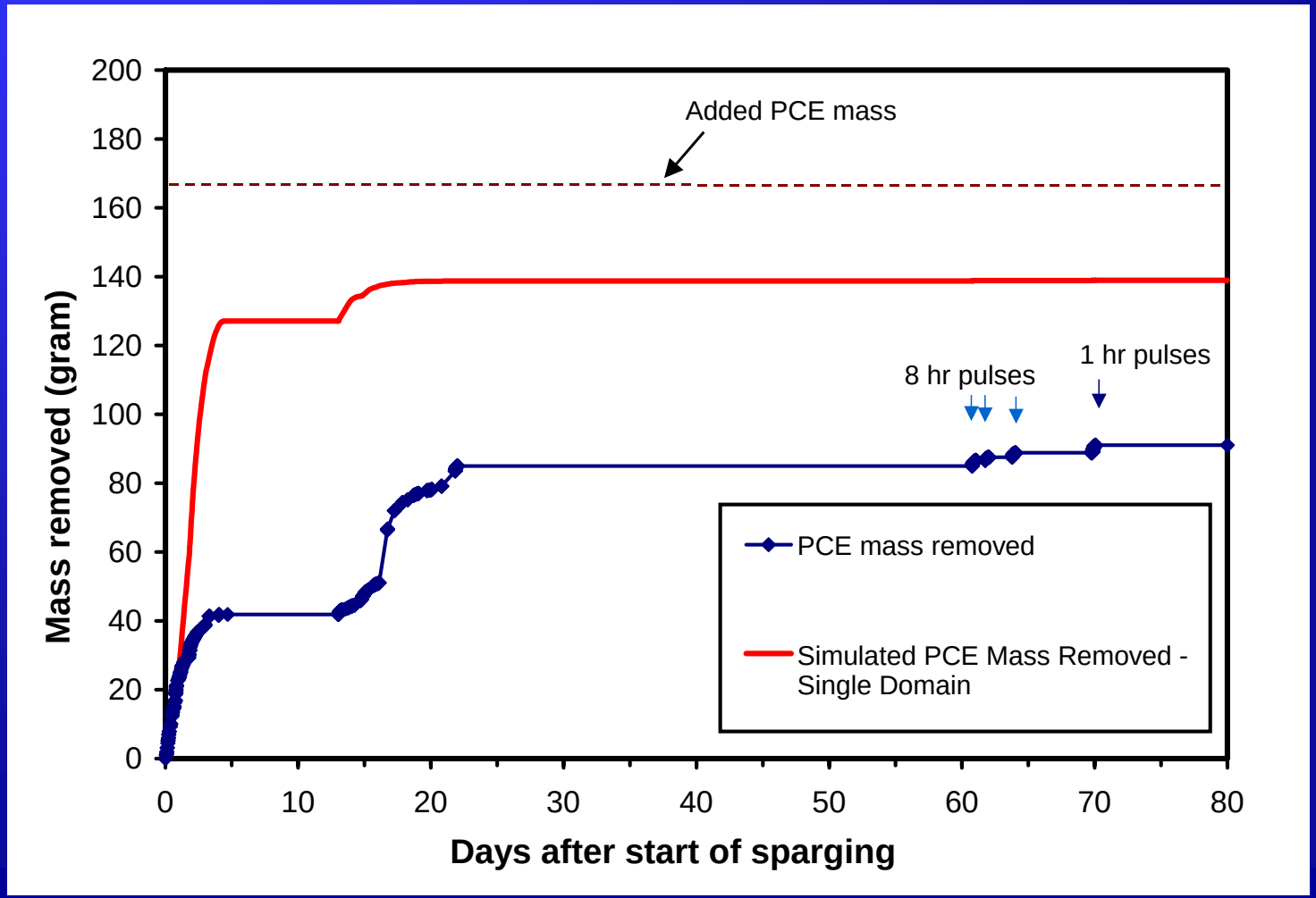
Conceptual Model



Single Domain Simulation Results:
Effluent Concentrations



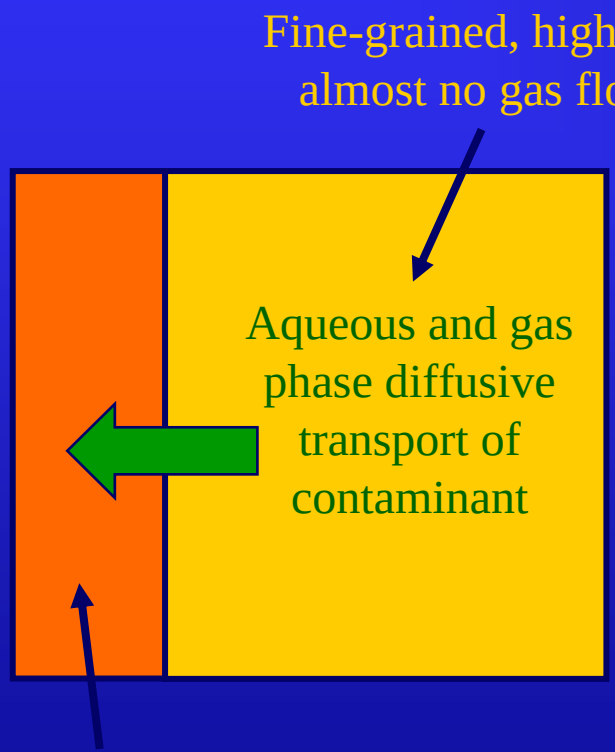
Single Domain Simulation Results:
Total Mass Removed

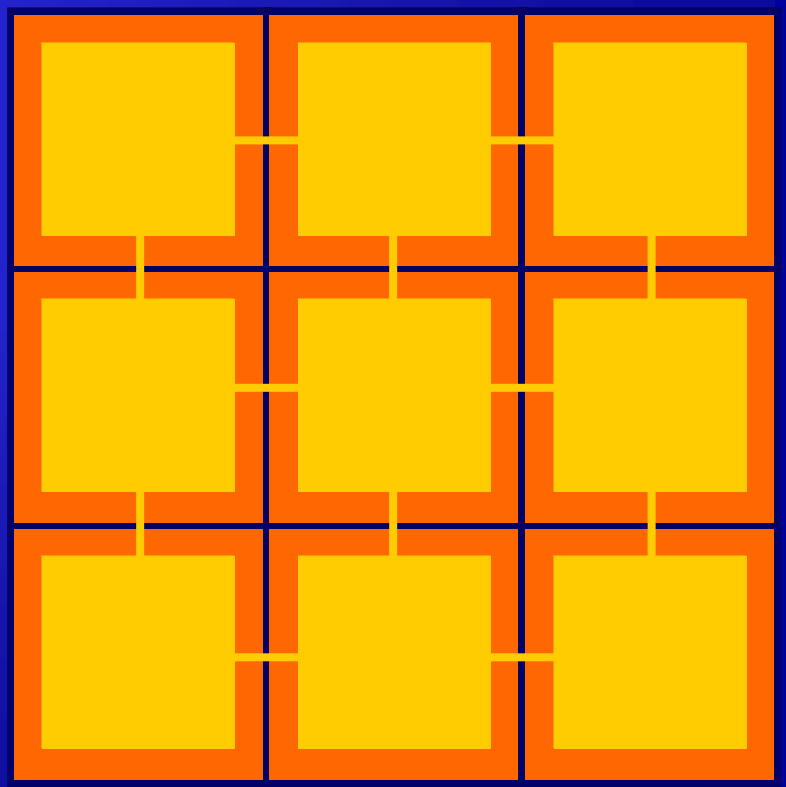


Dual-Domain Approach for Air Sparging*

Conceptual Model

Model Grid



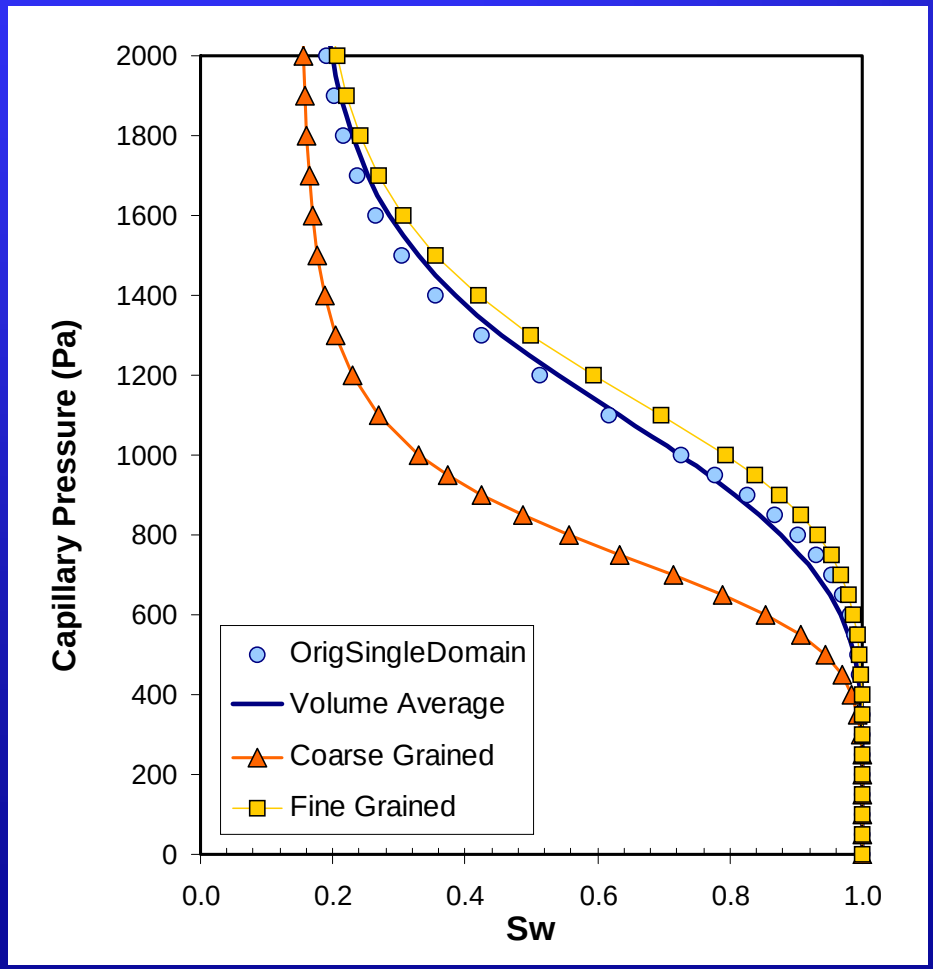


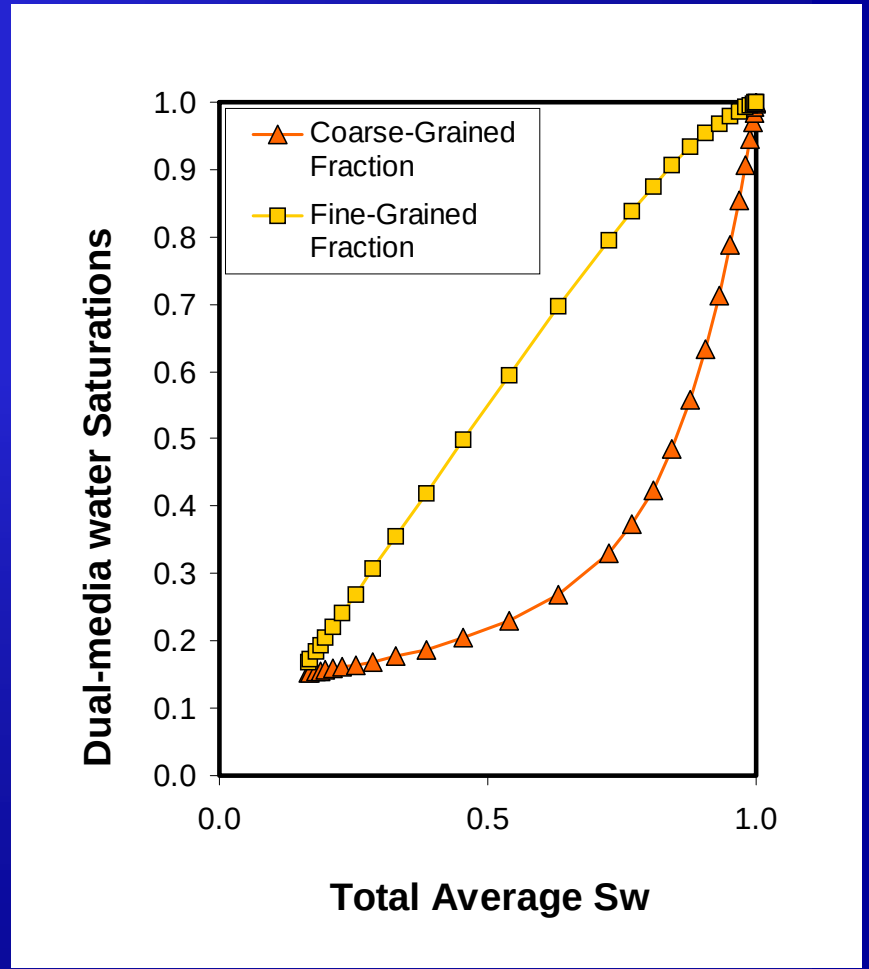
*(Falta, R. W., 2000)

Mass Rate Limitations

- Accounts for rate-limited mass transfer by:
  - Local equilibruim between flowing gas and porewater within coarse grained fraction
  - 1st order kinetic interphase mass transfer in adjacent fine-grained fraction
- Relative contributions of each region are determined by media volume fractions and water saturation in adjacent media

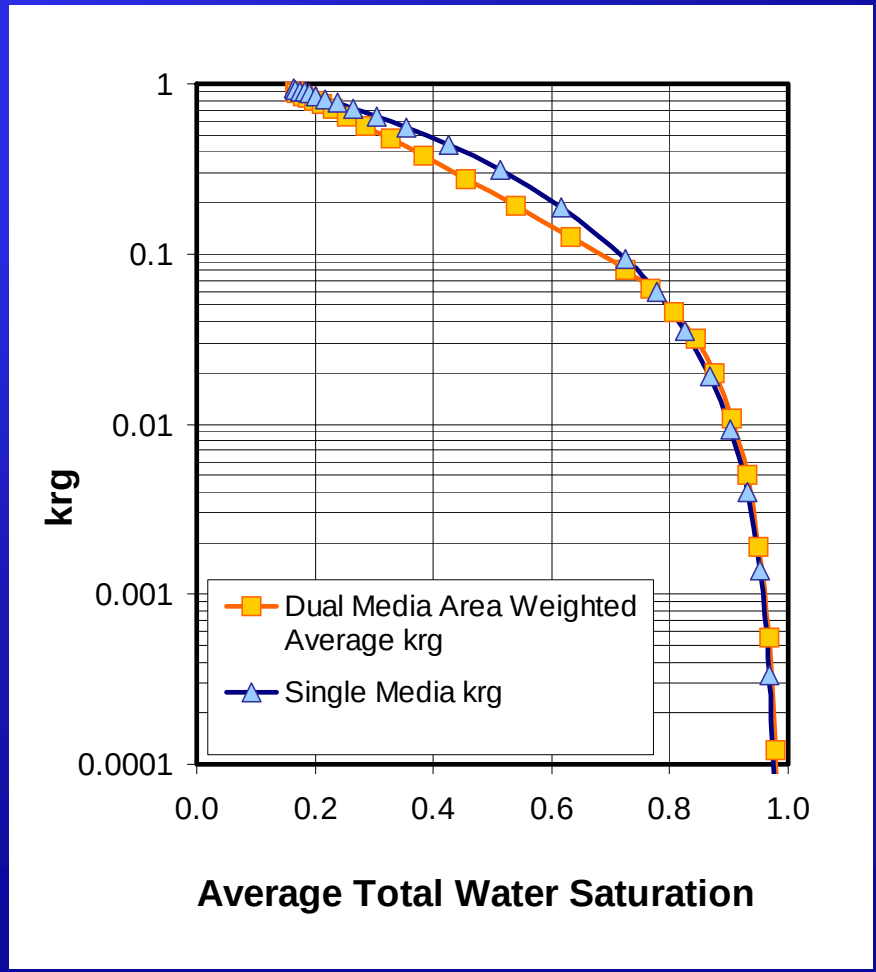
Dual-Domain Capillary Parameters





Dual-Domain Relative Permeabilities

$$k_{rg} = \left(\frac{S_g - S_{gr}}{1 - S_{wr}} \right)^n$$



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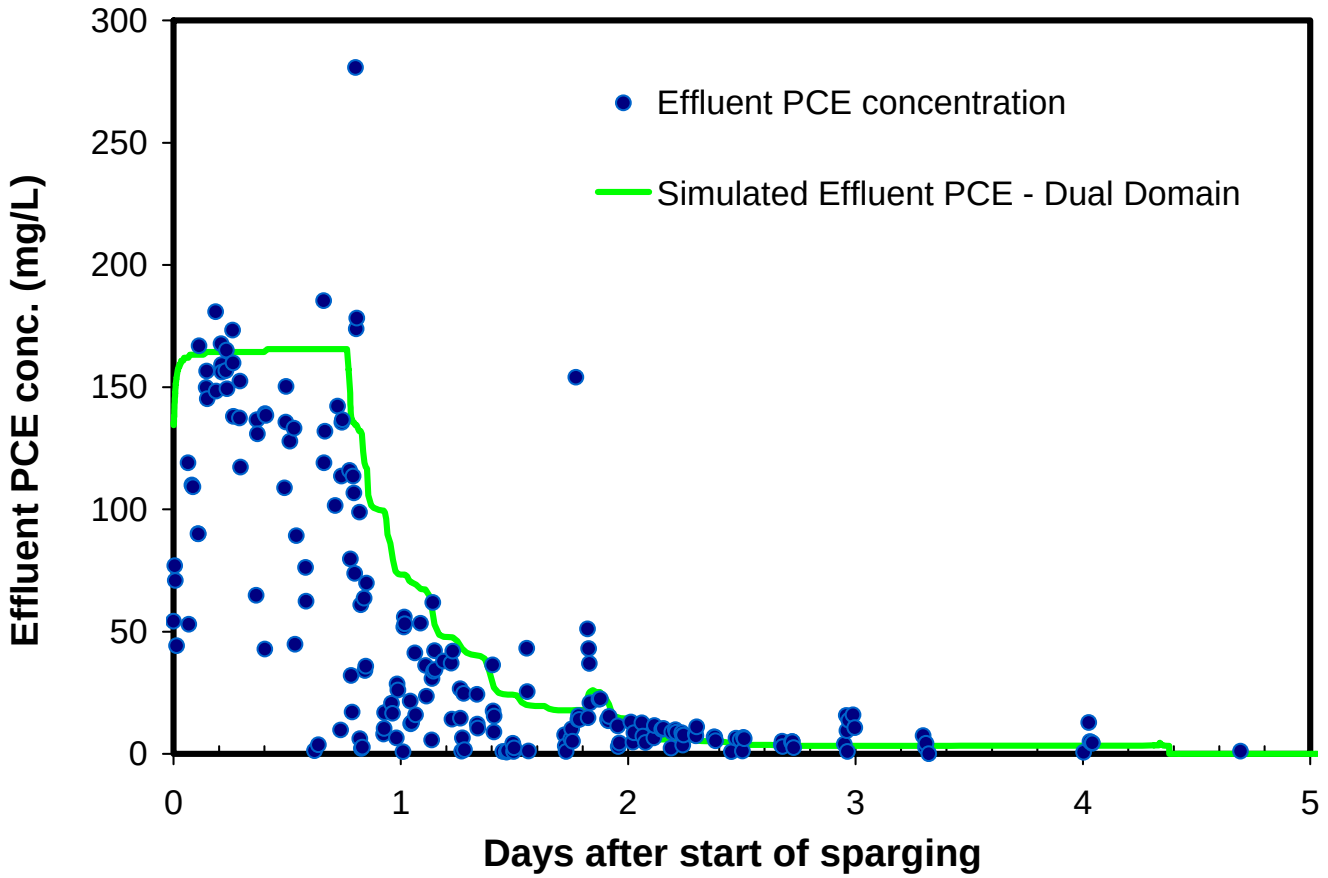

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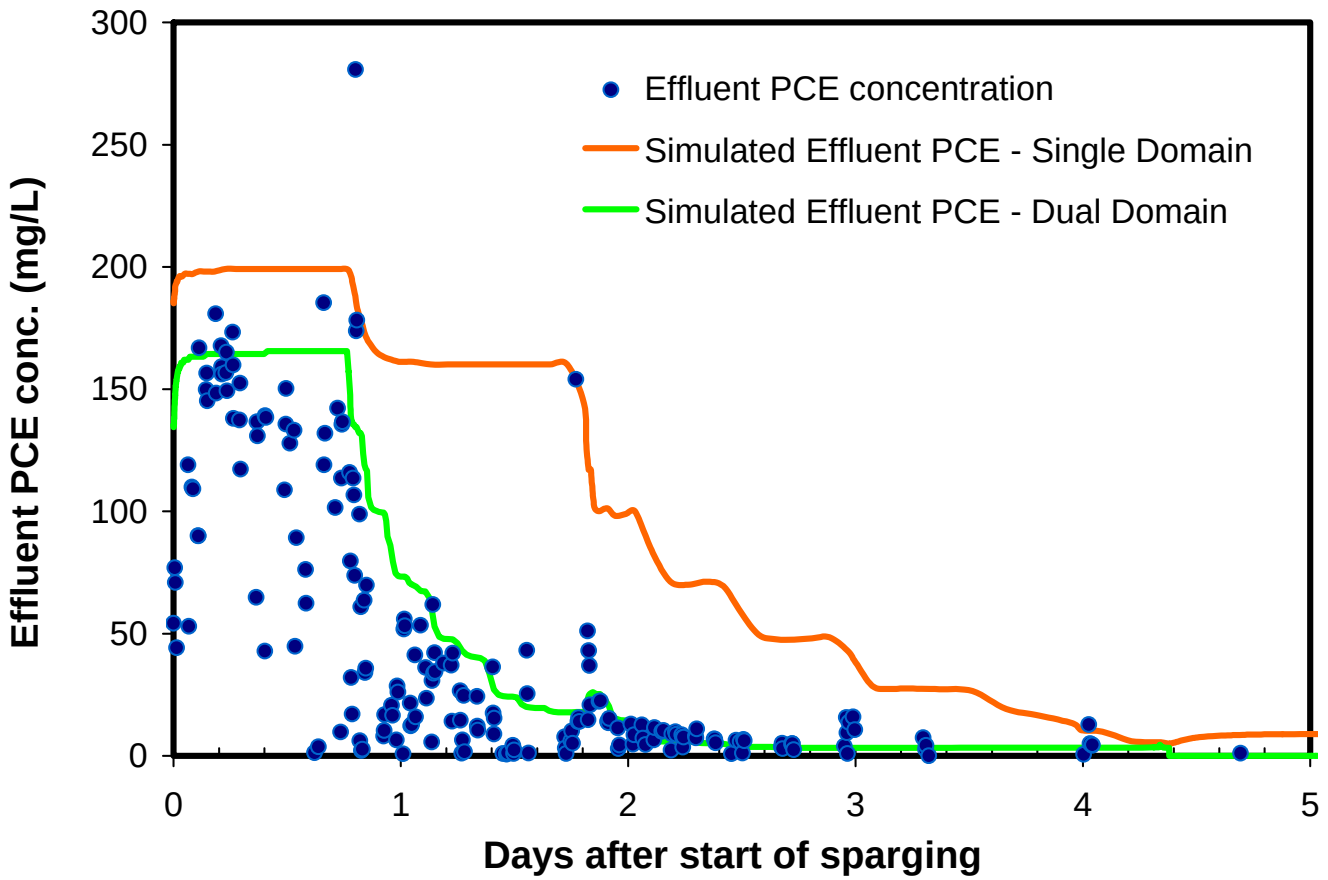
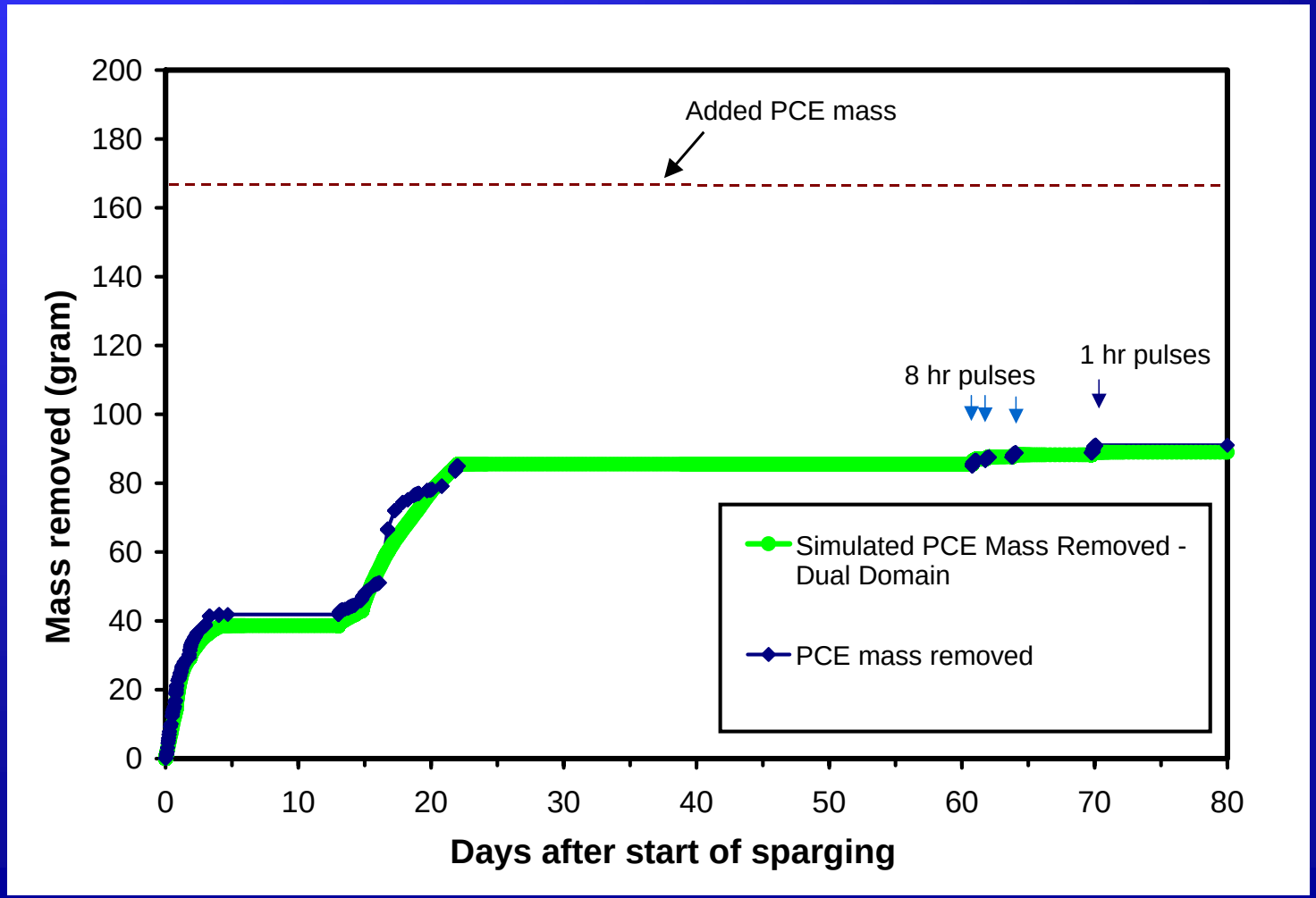


Dual Domain Simulation Results:
Total Mass Removed



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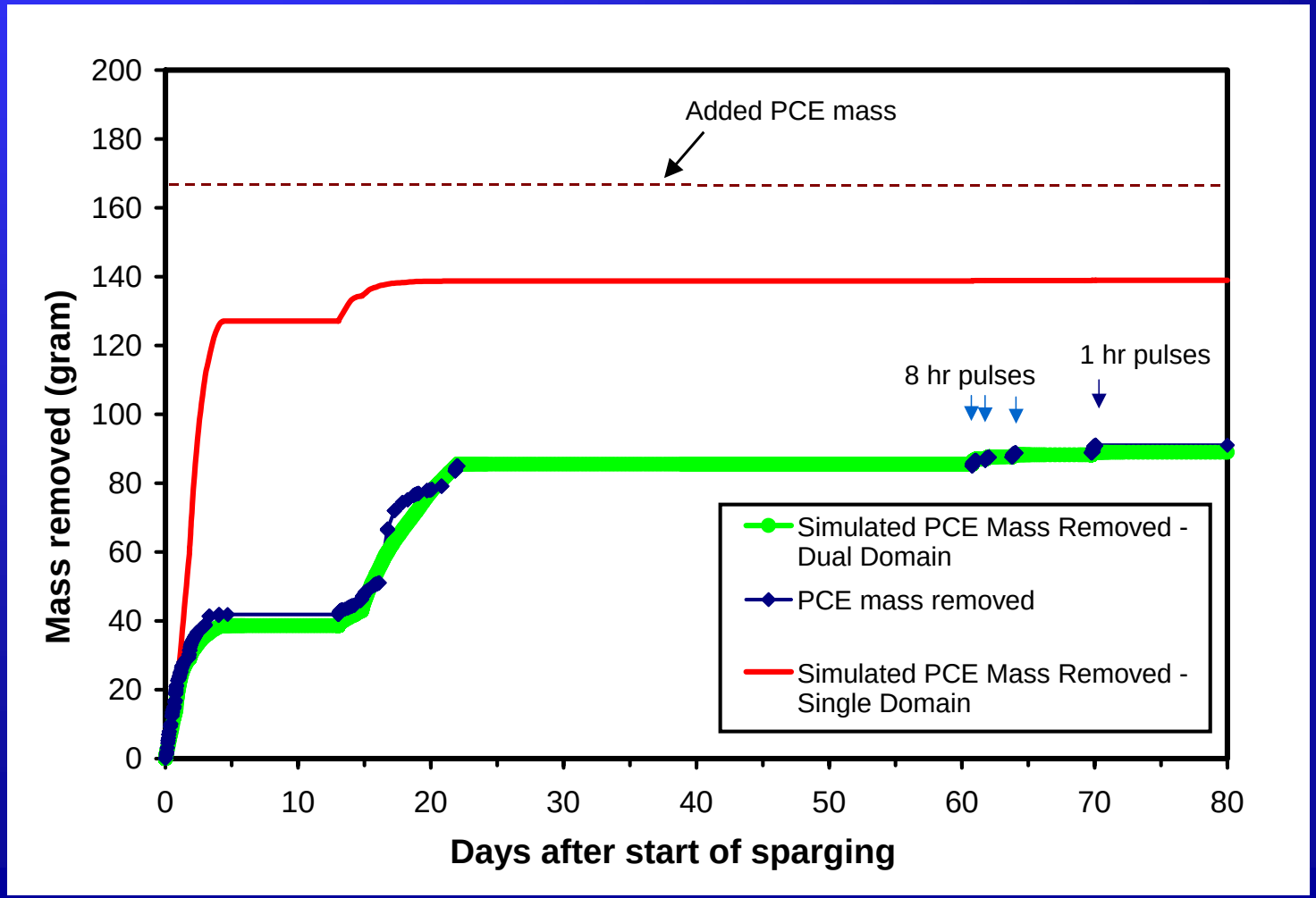

Summary

- Kinetic interphase mass transfer is an important factor in air sparging mass removal
- T2VOC can be adapted through the dual-domain approach to accurately model rate-limited mass transfer
- Two-dimensional NAPL distribution and aqueous dissolution between pulses being examined
- Field-scale modeling studies need to be performed to assess scale dependency and applicability of method

Acknowledgements

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DoD EPA DOE SERDP
Strategic Environmental Research and Development Program

References:

Elder, C. R., C. H. Benson, and G. Eykholt, Factors affecting mass removal during in situ air sparging, *J. Geothech. Geoenviron. Eng.,* 125(11), 1999.

Braida, W.J., and S. K. Ong, Air Sparging: Air-water mass transfer coefficients, Water Resour. Res., 34(12), 3245-3253, 1998.

Falta, R. W., K. Pruess, S. Finsterle, and A. Battistelli, T2VOC user's guide, Rep. LBL-36400, Lawrence Berkely Lab., Berkeley, Calif., March 1995.

Falta, R. W., 2000. Numerical modeling of kinetic interphase mass transfer during air sparging using a dual-media approach, Water Resources Research. pp. 3391-3400.

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. Groundwater Monit. Rem., 17(3), 1997.

Heron, G., Gierke, J. S., Faulkner, B., Mravik, S., Wood, L., and Enfield, C. G., 2002. Pulsed air sparging in aquifers contaminated with dense nonaqueous phase liquids. Ground Water Monit. & Rem., 22(4): 73.

Questions??