Comparison of two-domain models for simulating bromide transport in three different column setups

B. Arora[1], B. P. Mohanty[*2], J. T. McGuire[3], J.M. Köhne[4], and P. Castiglione[5]

1. Department of Water Management and Hydrological Science, Texas A&M University, College Station.
2. Department of Biological and Agricultural Engineering, Texas A&M University, College Station.
3. Department of Geology and Geophysics, Texas A&M University , College Station.
4. The Helmholtz Centre for Environmental Research, Halle, Germany.
5. Department of Land Resources and Environmental Sciences, Montana State University, Bozeman.

* Corresponding Author's contact: bmohanty@tamu.edu

36639

INTRODUCTION

Macropores and fractures in soils present critical pathways for vertical and lateral movement of contaminants through the subsurface zone to surface and ground water. This study is intended to improve our understanding of solute transport in macroporous soils and to quantify interdomain (macropore-matrix) solute transfer. In this study, three experimental designs with soil-macropore systems are considered in increasing order of complexity: 1) a homogeneous soil column, 2) a central macropore column with 0.1 cm macropore diameter, and 3) a soil column with multiple macropores in one-half of the column cross-section and plain matrix in the other half. The multiple macropore design is intended for a more realistic representation of the soil structure. The objectives of this study are: 1) to study the effect of geometry (number of macropores, density/area fraction of macropores, etc.) on flow and conservative transport in macroporous soils through controlled lab experiments, and 2) to compare single-porosity model (SPM), mobile-immobile model (MIM), and dual-permeability model (DPM) with first and second order water transfer functions (WTFs) in simulating experimental data.

THEORY

Model	Water flow	Water transfer term	Solute transport	1st order Solute transfer term
SPM	Richards' eq.	-	CDE	-
MIM	Richards' eq. (mobile region)	$\Gamma_w = \omega (S_e^f - S_e^m)$	CDE (mobile region)	$\Gamma_s = \alpha_s (c_f - c_m) + \begin{cases} \Gamma_w c_f, \Gamma_w > 0 \\ \Gamma_w c_m, \Gamma_w < 0 \end{cases}$
DPM - 1st order	2 Richards' eqs. (2 mobile regions)	$\Gamma_w = \alpha_w (h_f - h_m)$, $\alpha_w = \frac{\beta}{a^2} \gamma_w K_a(h)$	2 CDE (2 mobile regions)	$\Gamma_s = \alpha_s (1 - w_f) \theta_m (c_f - c_m) + \begin{cases} \Gamma_w c_f, \Gamma_w > 0 \\ \Gamma_w c_m, \Gamma_w < 0 \end{cases}$, $\alpha_s = \frac{\beta}{a^2} D_a(\theta)$
DPM - 2nd order	2 Richards' eqs. (2 mobile regions)	$\Gamma_w = \alpha_w \frac{(\bar{h}_m - h_i)^2 - (h_f - h_i)^2}{(\bar{h}_m - h_i)}$, $\alpha_w = \frac{\beta K_m}{2a^2}$	2 CDE (2 mobile regions)	$\Gamma_s = \alpha_s (1 - w_f) \theta_m (c_f - c_m) + \begin{cases} \Gamma_w c_f, \Gamma_w > 0 \\ \Gamma_w c_m, \Gamma_w < 0 \end{cases}$, $\alpha_s = \frac{\beta}{a^2} D_a(\theta)$

Symbols: *h*-pressure head, c-concentration, θ-water content, m-matrix domain (immobile), f-fracture domain (mobile), i-initial, Γ_w (Γ_s)-water (solute) transfer rate, ω–first-order water transfer rate coefficient, *Se*–effective water saturation, K_a (D_a)-hydraulic conductivity (diffusion coefficient) in interface region, *a*–aggregate half-width, β–geometry factor, γ_w–scaling factor, w_f –volumetric fraction of fracture system

METHODOLOGY

a. Experimental Approach

- Column setup:

Domain	Measurements
Soil matrix	TDR probes –water content, solute concentration Mini tensiometers –matric potential Bromide specific probes –bromide concentration
Soil macropore and interface region	TDR coil probes –water content Mini tensiometers –matric potential Bromide specific probes –bromide concentration

- Experimental designs:

	Homogeneous	Central Macropore	Multiple Macropore
Size of column	75 cm x 24 cm	75 cm x 24 cm	75 cm x 24 cm
Size of macropore		1 macropore (0.1 cm dia)	19 macropores (0.1 cm dia each)
w_f (Volume fraction)		1.7e-05 (cm^3/cm^3)	3.3e-04 (cm^3/cm^3)

b. Numerical Modeling

Simulations are performed with all four models using modified Hydrus-1D (Simunek et al., 2002). Initial and boundary conditions are selected based on experiments.

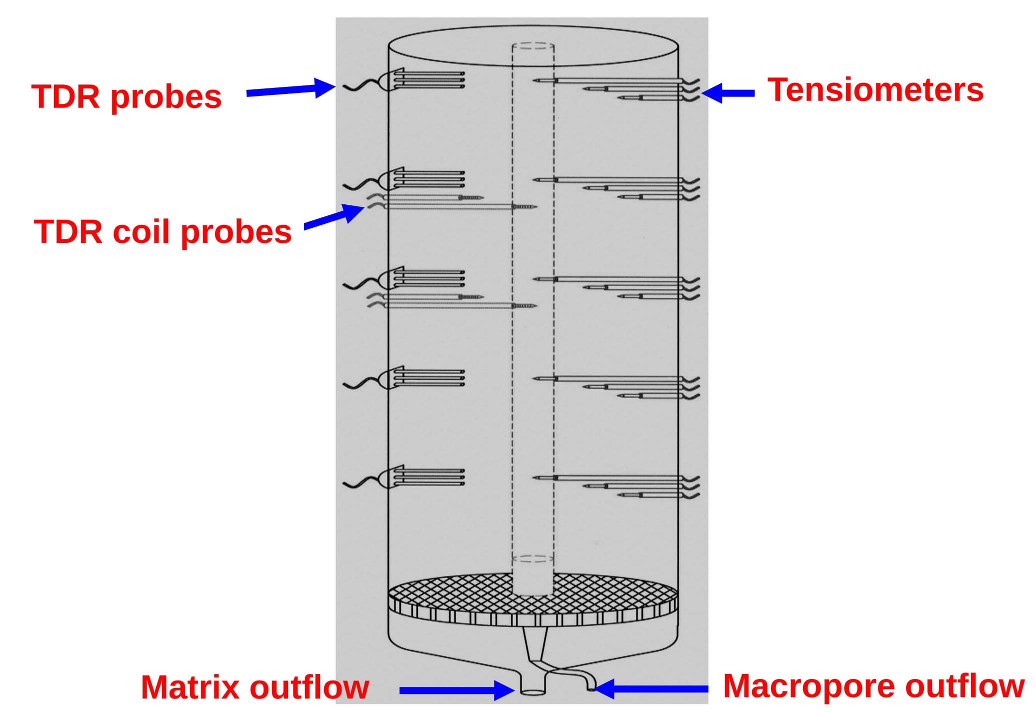


Fig 1. Central macropore column

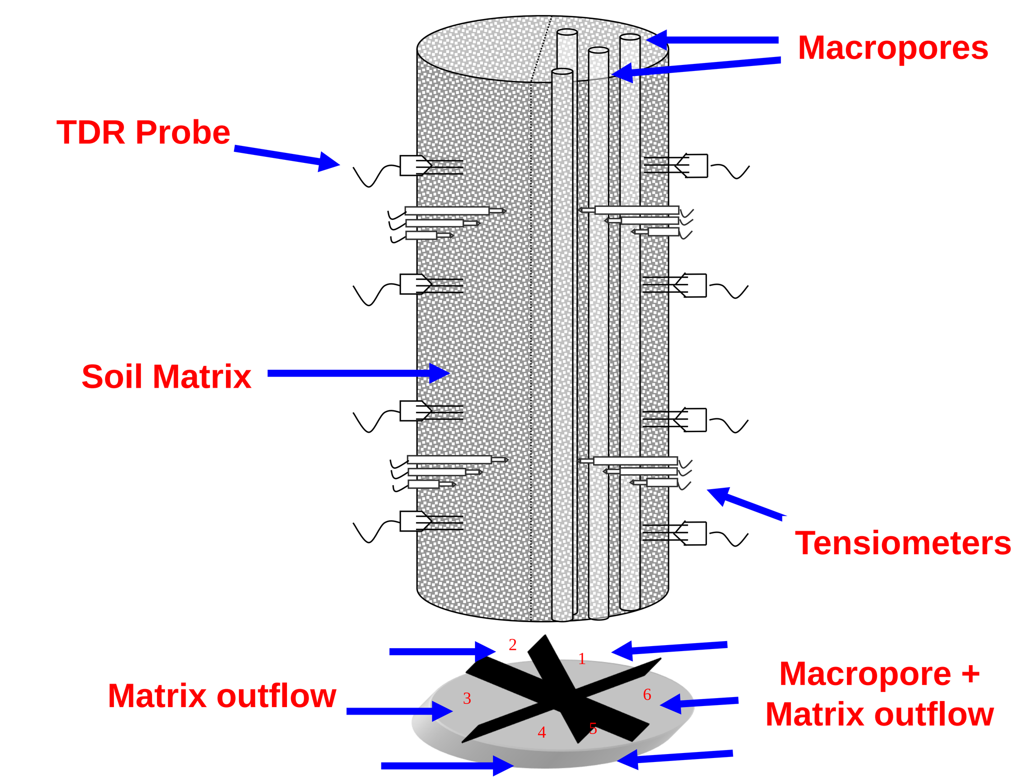
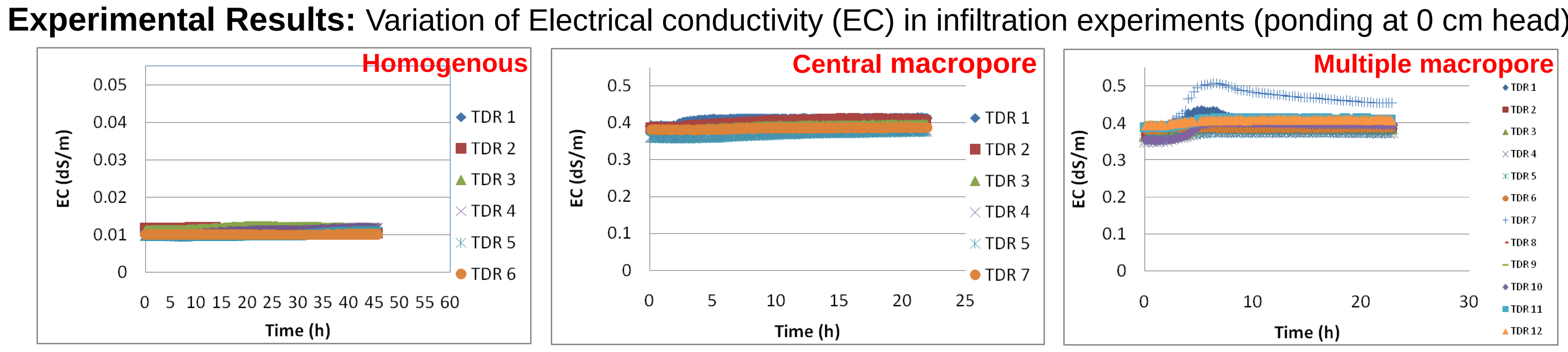


Fig 2. Multiple macropore column

RESULTS

a. Experimental Results: Variation of Electrical conductivity (EC) in infiltration experiments (ponding at 0 cm head)

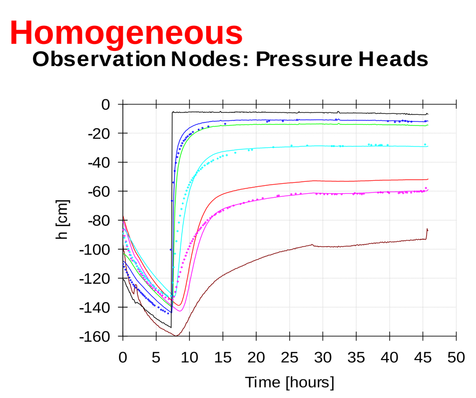


EC variation with depth is observed as the number and volume fraction of macropores increases.

b. Numerical Results

Infiltration experiment with 0 cm ponding is simulated by DPM 1st order WTF. Pressure head variations are shown here.

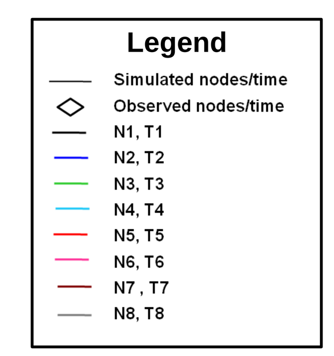
Homogeneous



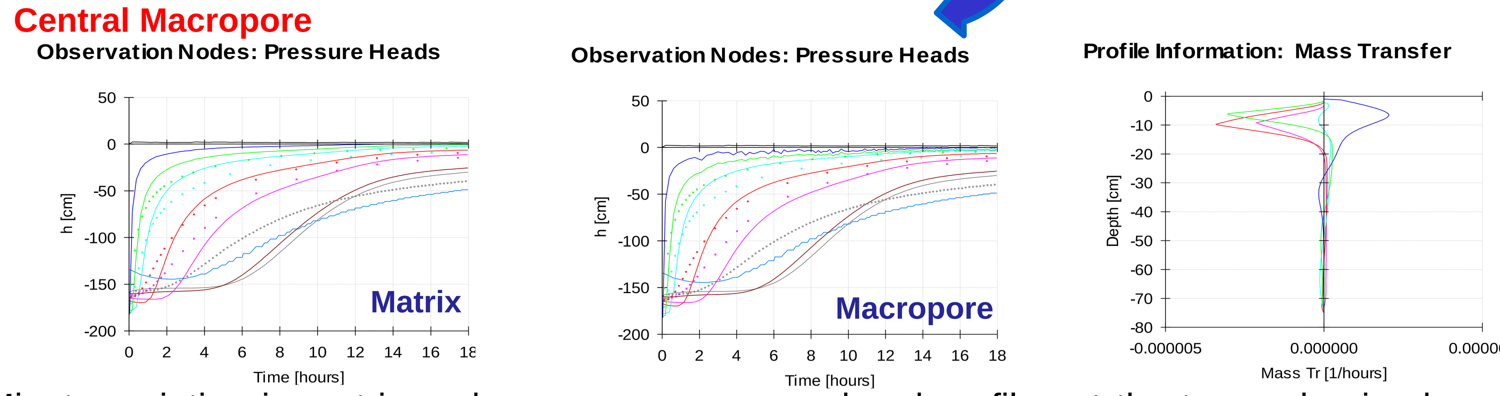
R^2	0.9915
MBE	0.0023
SSQ	0.0413

Matrix parameters

θr	0.2
θs	0.37
α	0.0045
n	1.843
Ks	0.1348



Central Macropore



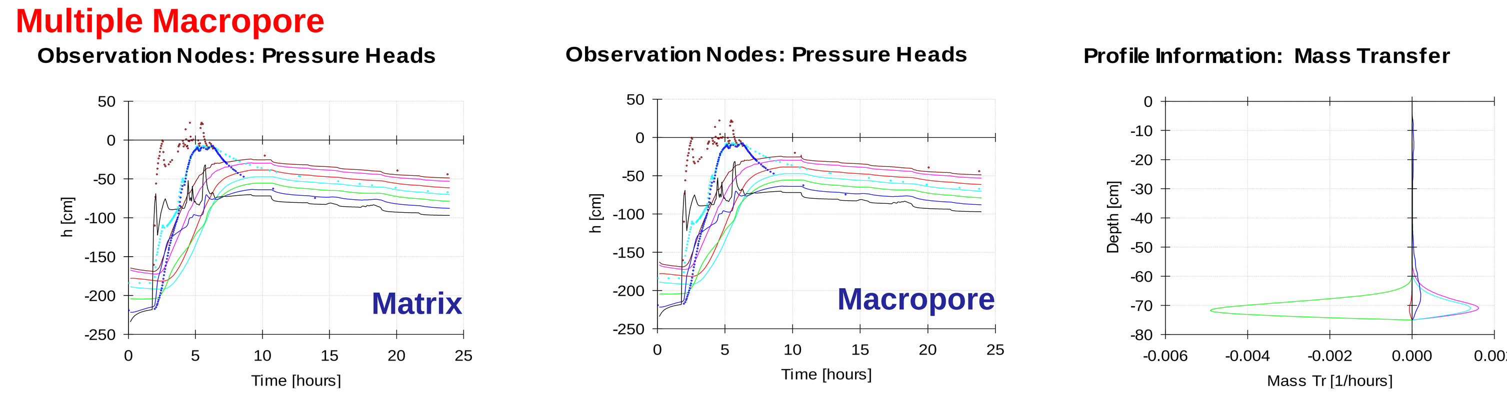
R^2	0.9753
MBE	0.0034
SSQ	0.5930

Macropore parameters

θr	0.078
θs	0.39
α	0.01
n	2
Ks	8.265

Minute variation in matrix and macropore pressure head profiles at the top nodes is observed. Variation at top nodes only could be attributed to the small size of the macropore (0.1 cm diameter) reflecting early attainment of equilibrium between the two domains. Mass transfer graph corroborates observation of inequilibrium at top nodes only.

Multiple Macropore

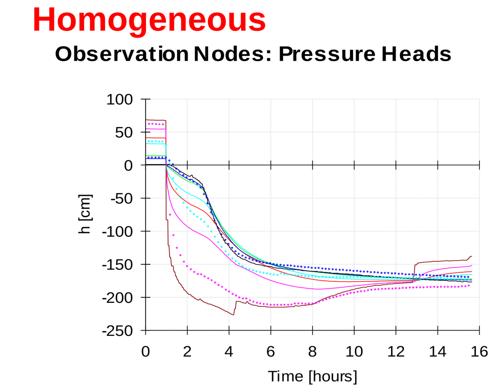


R^2	0.7055
MBE	0.03
SSQ	16.44

DPM 1st order WTF is not able to capture all the pressure head fluctuations observed in the experiment.

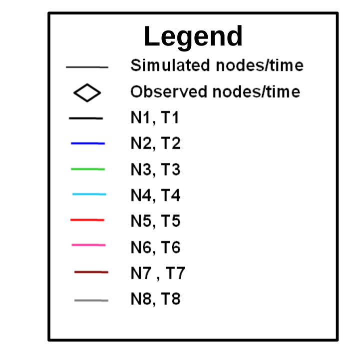
Drainage experiment is simulated by DPM 1st order WTF. Pressure head variations are shown here.

Homogeneous

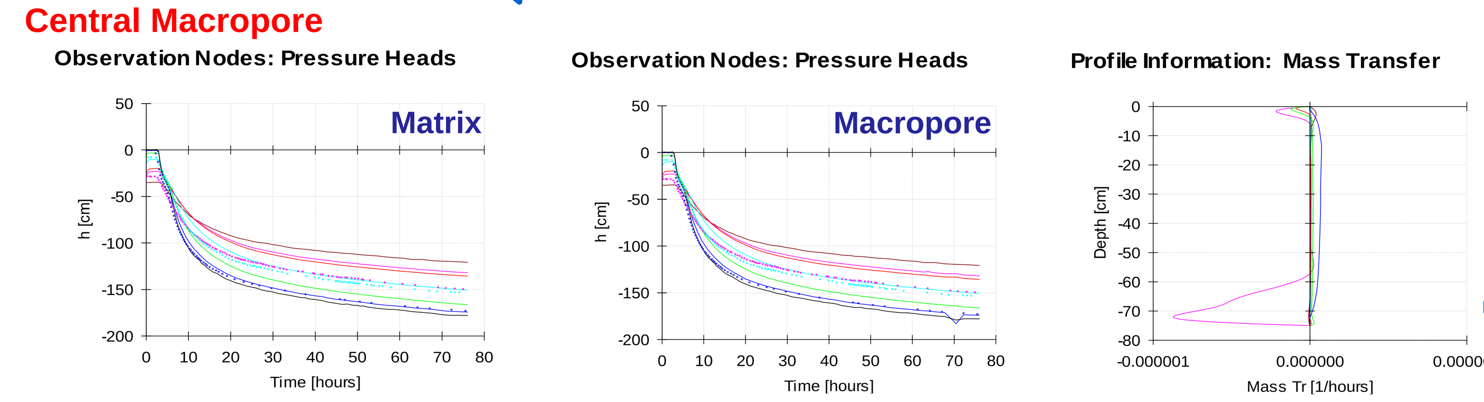


R^2	0.9863
MBE	0.0012
SSQ	0.1803

Matrix parameters



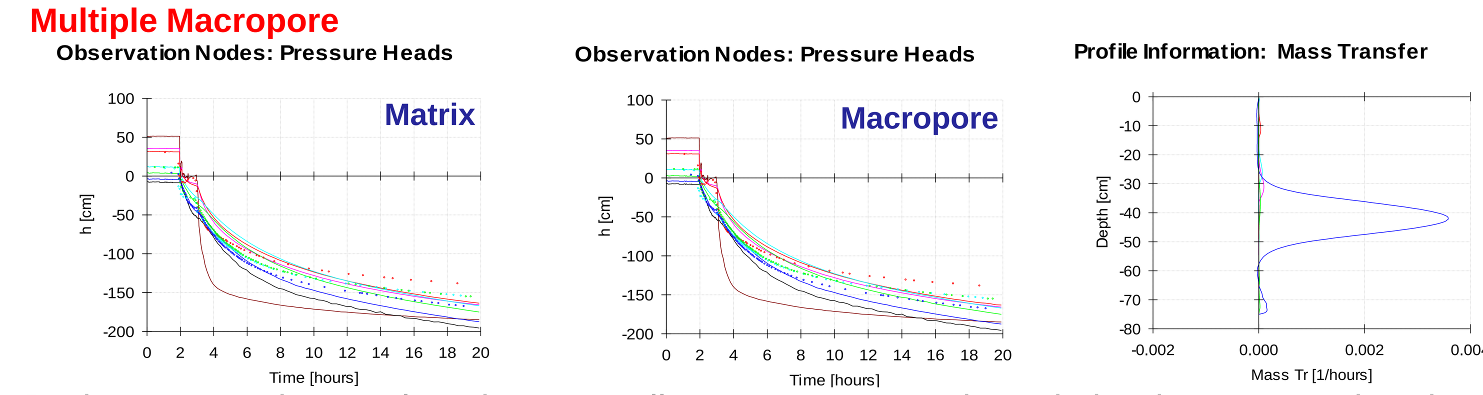
Central Macropore



R^2	0.9962
MBE	0.0014
SSQ	12.44

Macropore parameters

Multiple Macropore



R^2	0.9834
MBE	0.2147
SSQ	2.766

Drainage experiment also shows small macropore –matrix variation in pressure head profiles of the central macropore system. Drainage in multiple macropore system is simulated better than infiltration.

IMPLICATIONS AND FUTURE WORK

- Experimental analysis of variation in EC suggests that matrix parameters change with the size and volume fraction of macropores though not to the same degree.
- Numerical analysis suggests that DPM with 1st order water transfer function can simulate physical non-equilibrium correctly but correct soil matrix and macropore parameters need to be established from homogenous and central macropore experiments. (Same matrix and macropore parameters were used in both infiltration and drainage experiments.)
- The importance of this study is the realization of a distributed macropore system in laboratory soil columns and parameter estimation in numerical models through the use of two-domain models.
- Some questions remain:
  - Does solute behave differently than flow in a distributed macropore system?
  - What degree of model complexity (SPM, MIM, DPM) is adequate to describe preferential flow in macroporous soils?
- Future work: We are conducting several controlled soil column experiments with different physical, chemical and biological controls to understand the effect of coupled processes on flow and contaminant transport in soils. The focus is on flow-induced redox geochemistry within fractured/macroporous and layered vadose zone.

Fig 3. Soil columns for future studies.

SELECTED REFERENCES

Simunek, J., N. J. Jarvis, M. T. van Genuchten, and A. Gärdenäs. 2002. Review and Comparison of Models for Describing Non-equilibrium and Preferential Flow and Transport in the Vadose Zone. Journal of Hydrology, 272, 14-35.

Castiglione, P., B. P. Mohanty, P. J. Shouse, J. Simunek, M. T. van Genuchten, and A. Santini. 2003. Lateral Water Diffusion in an Artificial Macroporous System: Modeling and Experimental Evidence. Vadose Zone Journal, 2(2), 212-221.

Köhne, J. M., and B. P. Mohanty. 2005. Water Flow Processes in a Soil Column with a Cylindrical Macropore: Experiment and Hierarchical Modeling. Water Resources Research, 41(3), W03010, doi:10.1029/2004WR003303.

ACKNOWLEDGEMENT

Funding support from NSF - Hydrological Sciences grant is acknowledged.