History of Solute Transport Modeling Codes

Vivek Bedekar

Σ²Π S.S. Papadopulos & Associates, Inc.
Environmental and Water-Resource Consultants

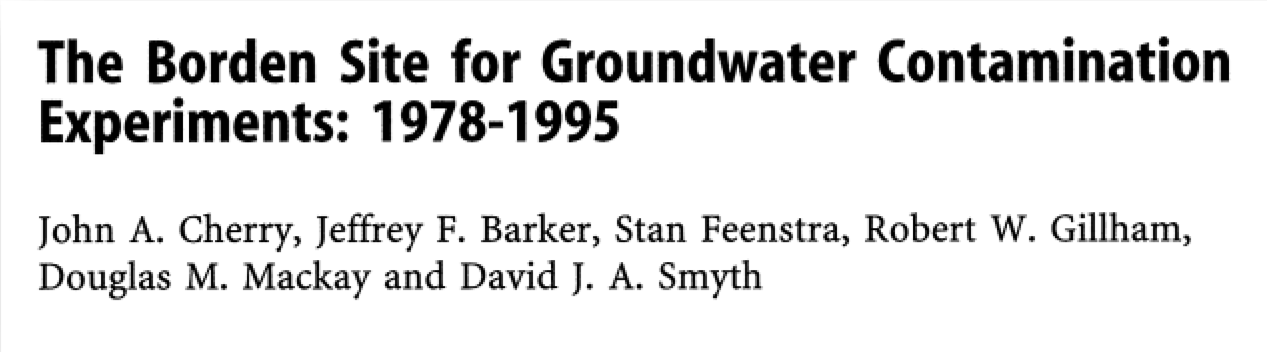
CWEMF 2024

Folsom, CA

September 24, 2024

History of Solute Transport

- Experiments



The Borden Site for Groundwater Contamination Experiments: 1978-1995

John A. Cherry, Jeffrey F. Barker, Stan Feenstra, Robert W. Gillham,
Douglas M. Mackay and David J. A. Smyth

Toxic Substances Hydrology Program

Cape Cod Toxic Substances Hydrology Research Site

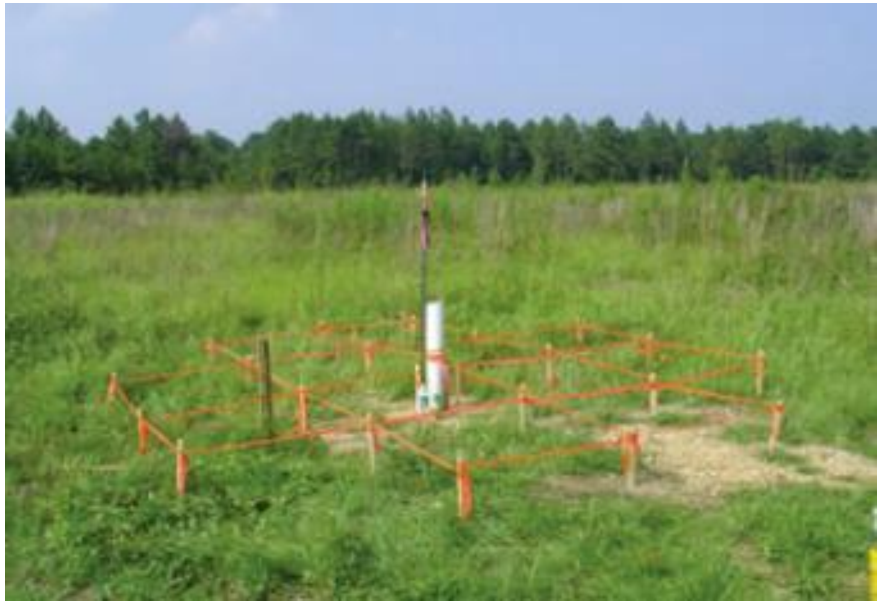
Physical, Chemical, and Biological Processes that Control the Fate of Contaminants in Ground Water

Array with more than 12,000 sampling points used for ground-water tracer experiments

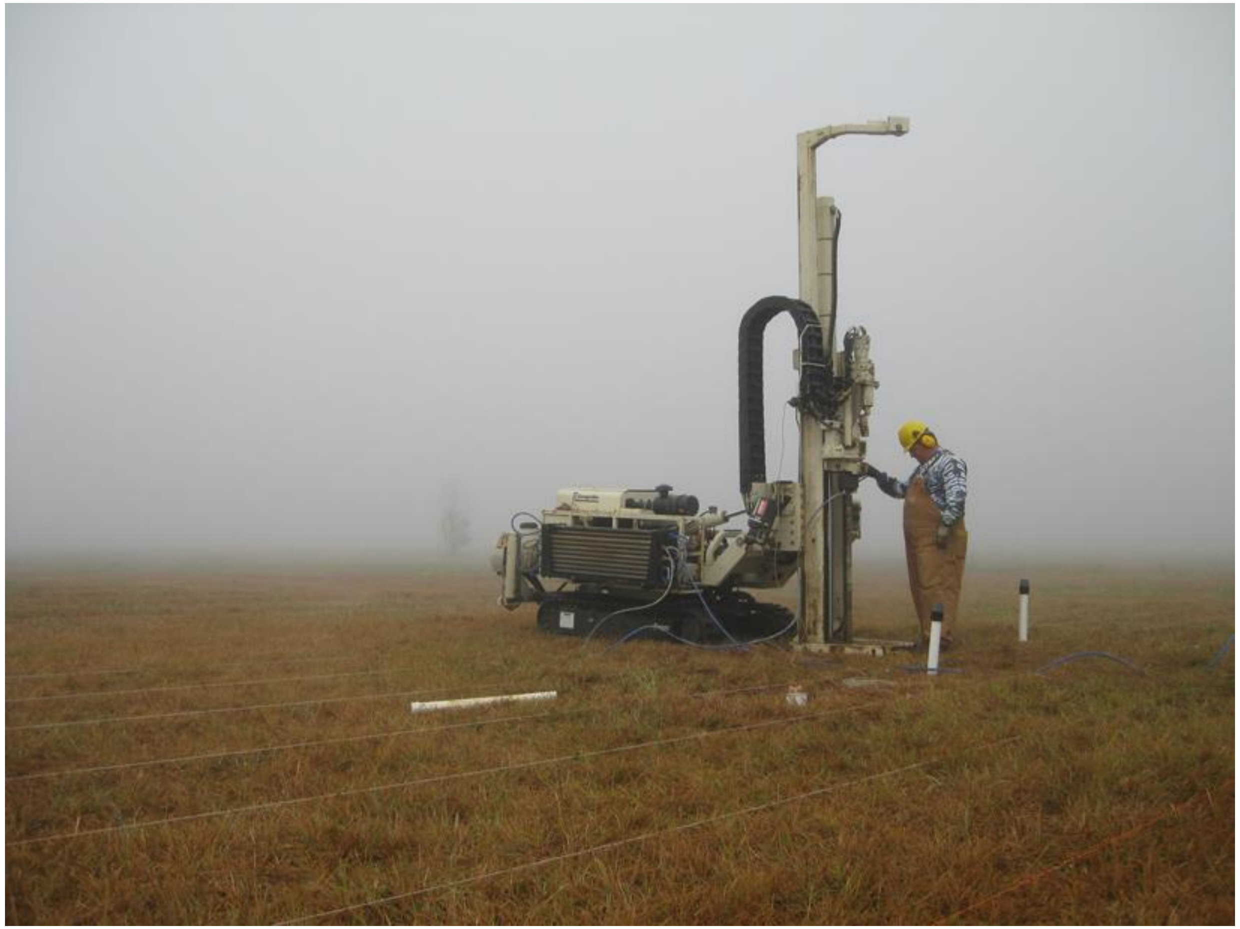
Studied since 1983

https://pubs.usgs.gov/fs/2006/3096/pdf/fs2006_3096.pdf

Macro-dispersion Experiment (MADE) Site



Zheng, C., Bianchi, M. and Gorelick, S.M. (2011), Lessons Learned from 25 Years of Research at the MADE Site. Groundwater, 49: 649-662. https://doi.org/10.1111/j.1745-6584.2010.00753.x



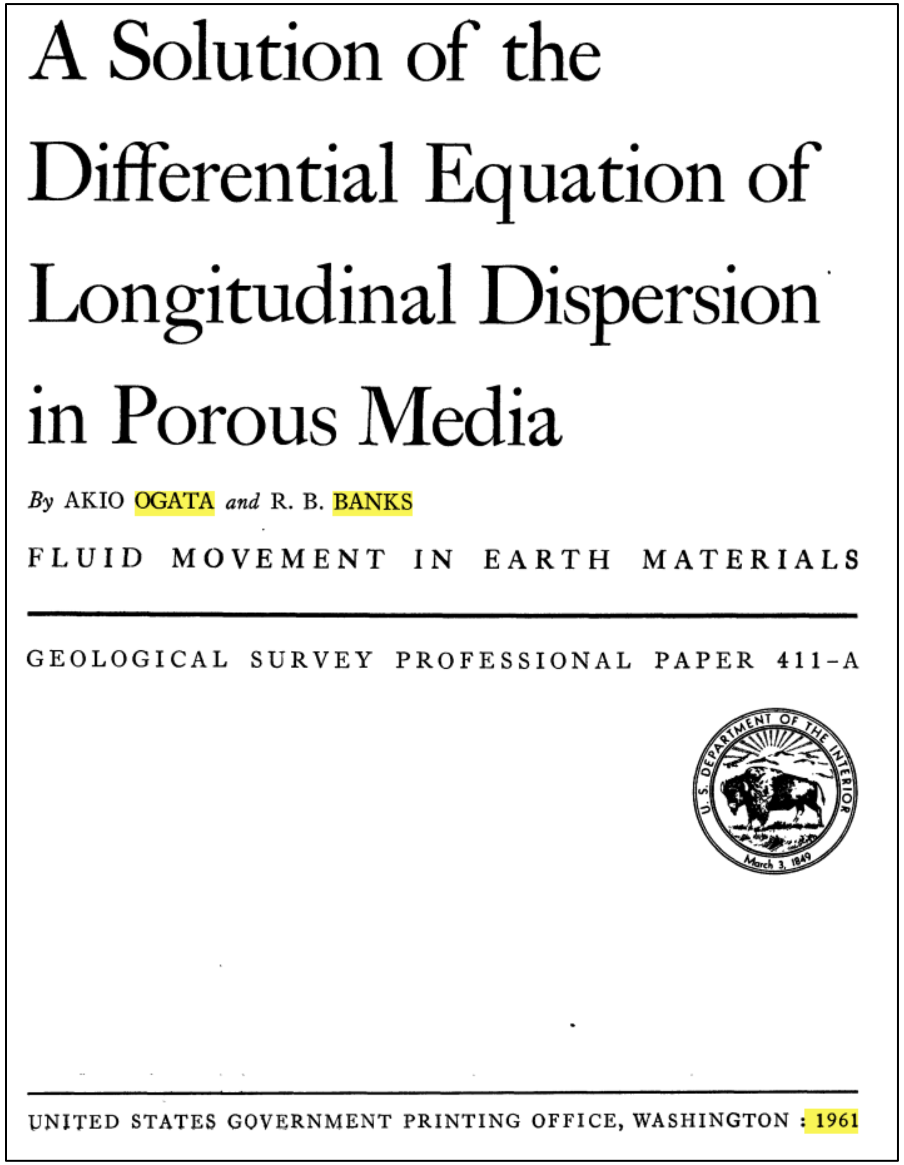
Gómez-Hernández, J. J., J. J. Butler Jr., and A. Fiori (2016), Groundwater transport in highly heterogeneous aquifers, Eos, 97, doi:10.1029/2016EO047263. Published on 3 March 2016.

History of Solute Transport

- Experiments
- Theory, Analytical Solutions

History of Solute Transport

- Experiments
- Theory, Analytical Solutions



A Solution of the Differential Equation of Longitudinal Dispersion in Porous Media

By AKIO OGATA and R. B. BANKS

FLUID MOVEMENT IN EARTH MATERIALS

GEOLOGICAL SURVEY PROFESSIONAL PAPER 411-A

U.S. DEPARTMENT OF THE INTERIOR
March 3, 1849

UNITED STATES GOVERNMENT PRINTING OFFICE, WASHINGTON : 1961

History of Solute Transport

- Experiments
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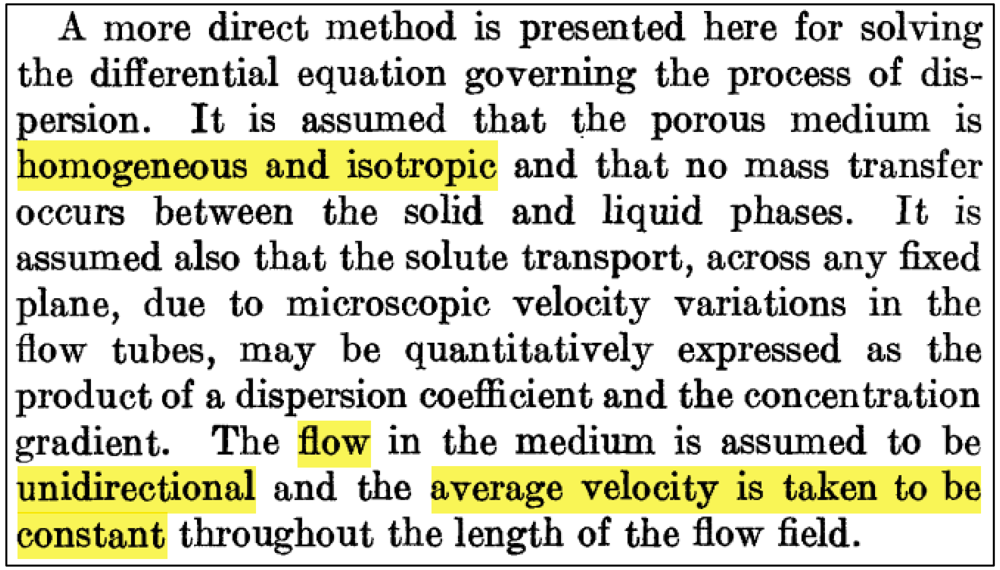
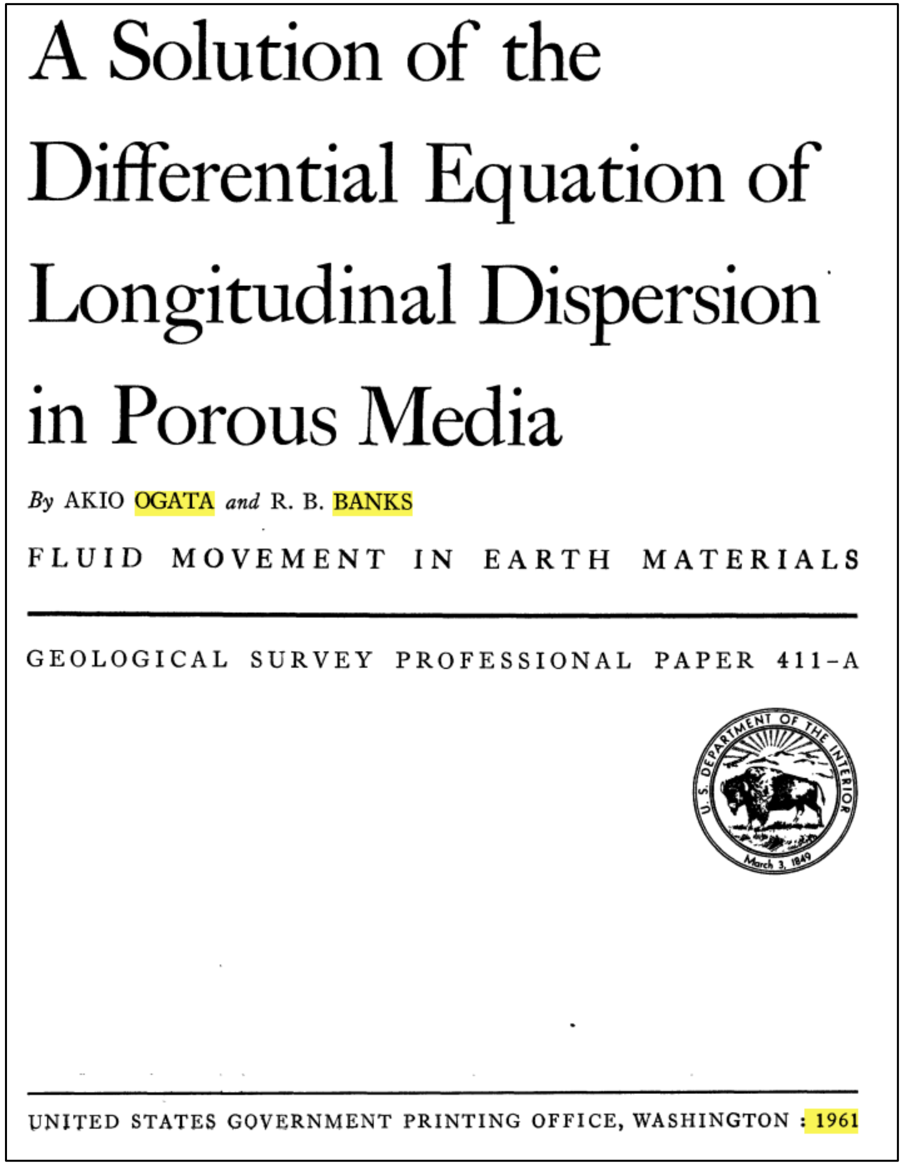


A more direct method is presented here for solving the differential equation governing the process of dispersion. It is assumed that the porous medium is homogeneous and isotropic and that no mass transfer occurs between the solid and liquid phases. It is assumed also that the solute transport, across any fixed plane, due to microscopic velocity variations in the flow tubes, may be quantitatively expressed as the product of a dispersion coefficient and the concentration gradient. The flow in the medium is assumed to be unidirectional and the average velocity is taken to be constant throughout the length of the flow field.



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History of Solute Transport

- Experiments
- Theory, Analytical Solutions
- Numerical Models

History of Solute Transport

- Experiments
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  - 1970s (Mainframe)
  - 1980s
  - 1990s (PCs)

History of Solute Transport

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- Theory, Analytical Solutions
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  - Initial developments from reservoir engineering

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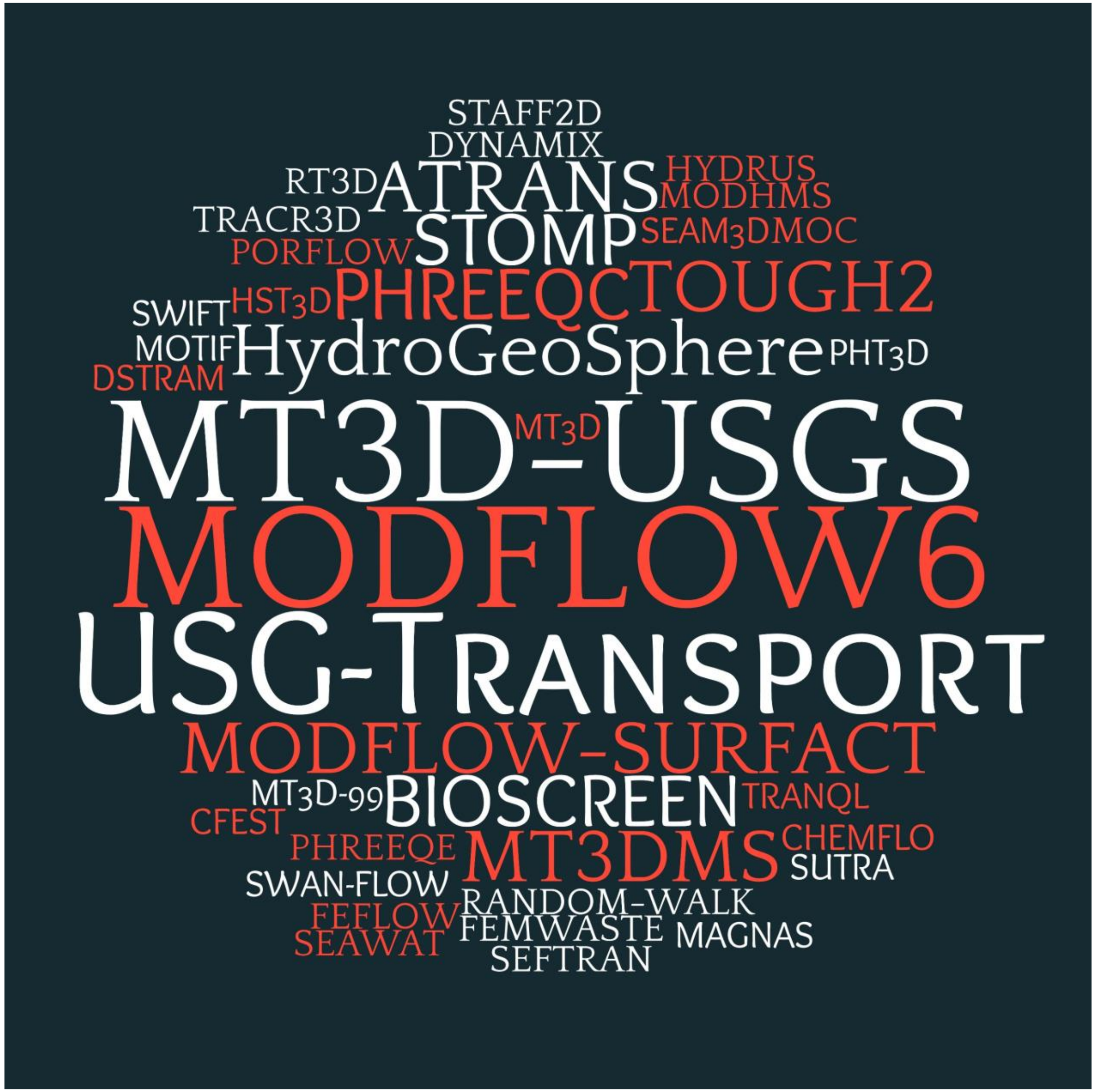


Advection-Dispersion Equation

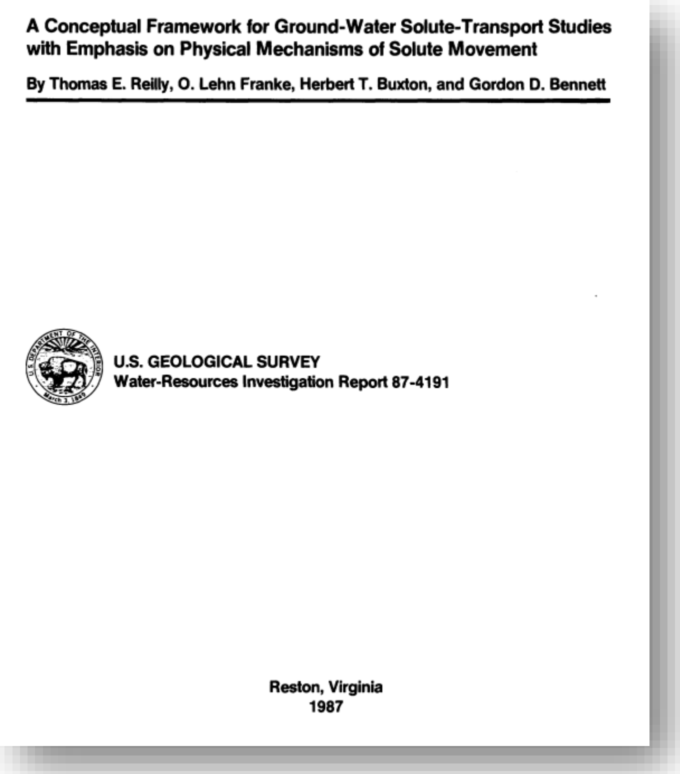
$$\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(q_i C)$$

$$-\frac{\partial}{\partial x_i}(q_i C)$$

Advection

$$\frac{\partial}{\partial x_i}\left(\theta D_{ij}\frac{\partial C}{\partial x_j}\right)$$

Dispersion



A Conceptual Framework for Ground-Water Solute-Transport Studies with Emphasis on Physical Mechanisms of Solute Movement

By Thomas E. Reilly, O. Lehn Franke, Herbert T. Buxton, and Gordon D. Bennett

U.S. GEOLOGICAL SURVEY
Water-Resources Investigation Report 87-4191

Reston, Virginia
1987

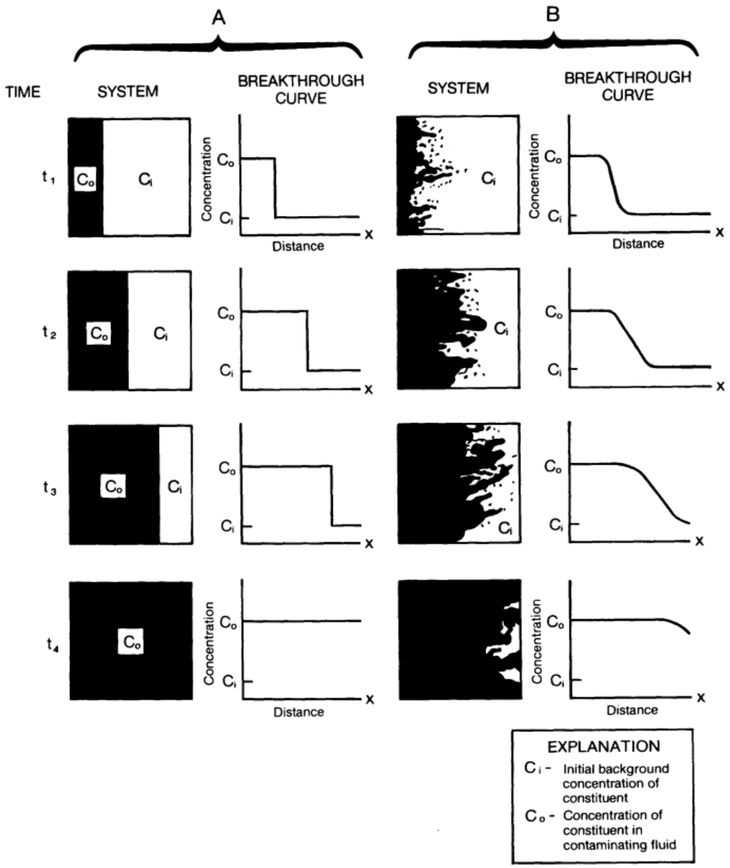


Figure 9. Advance of a tracer for: (A) a sharp front and (B) an irregular advance.

Figure 7. (A) Approximate fluid velocity distribution in a single pore; and
(B) Tortuous paths of fluid movement in an unconsolidated porous medium.

Numerical Models

- Advection-dispersion-reaction model
  - Heterogeneity (physical, geochemical)

Numerical Models

- Advection-dispersion-reaction model
    - Heterogeneity (physical, geochemical); Scale

Numerical Models

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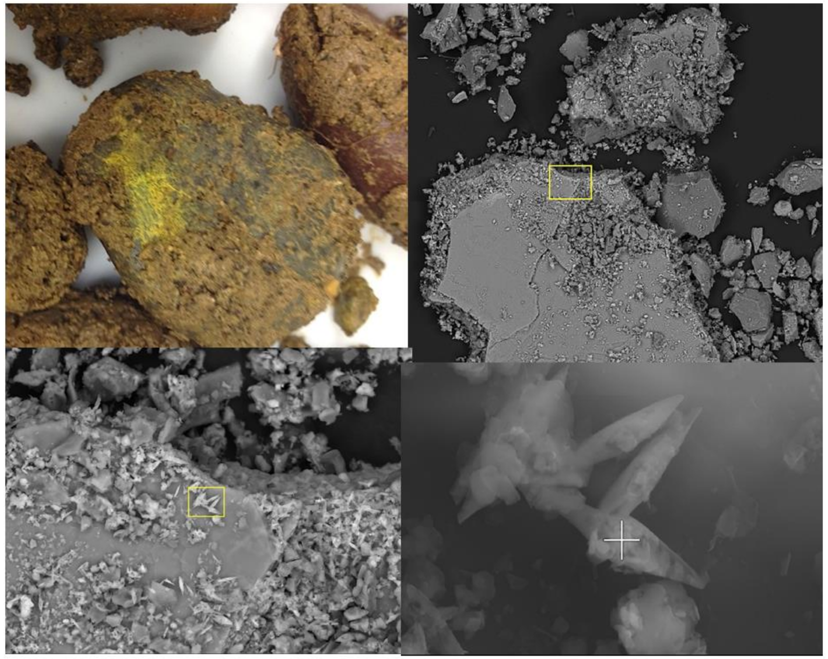


Photo of gravel with fine yellow precipitate

EMPA* image (160x) of clay particle with fine surface precipitate

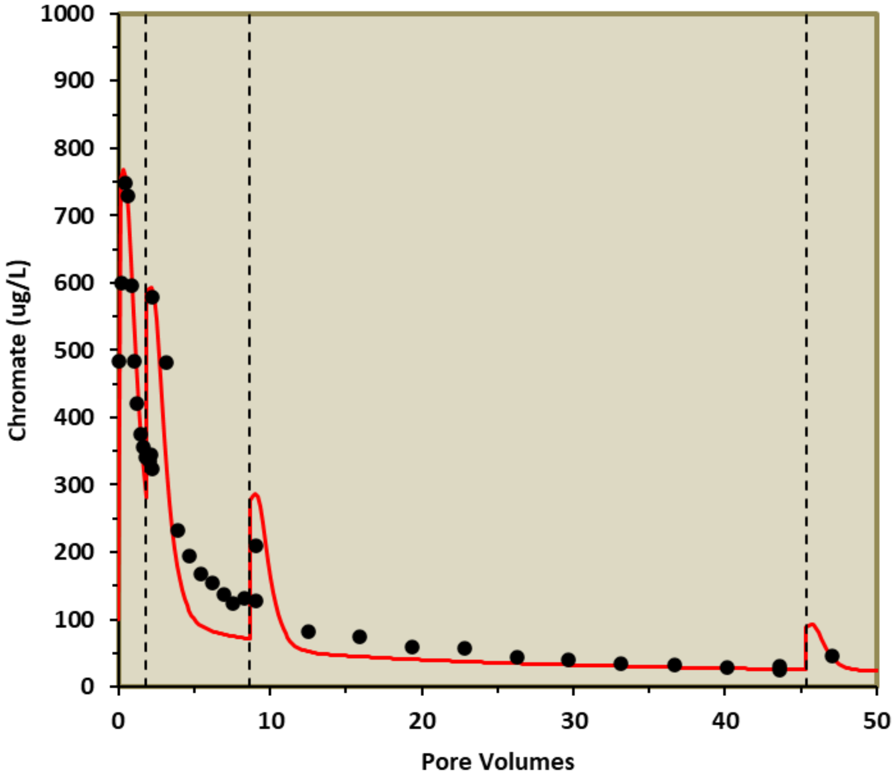
**Electron micro-probe*

EMPA image (950x) of fine bladed precipitates

EMPA image (6000x) of bladed precipitates - cross shows location of elemental analysis

Numerical Models

- Advection-dispersion-reaction model
    - Heterogeneity (physical, geochemical); Scale



Numerical Models

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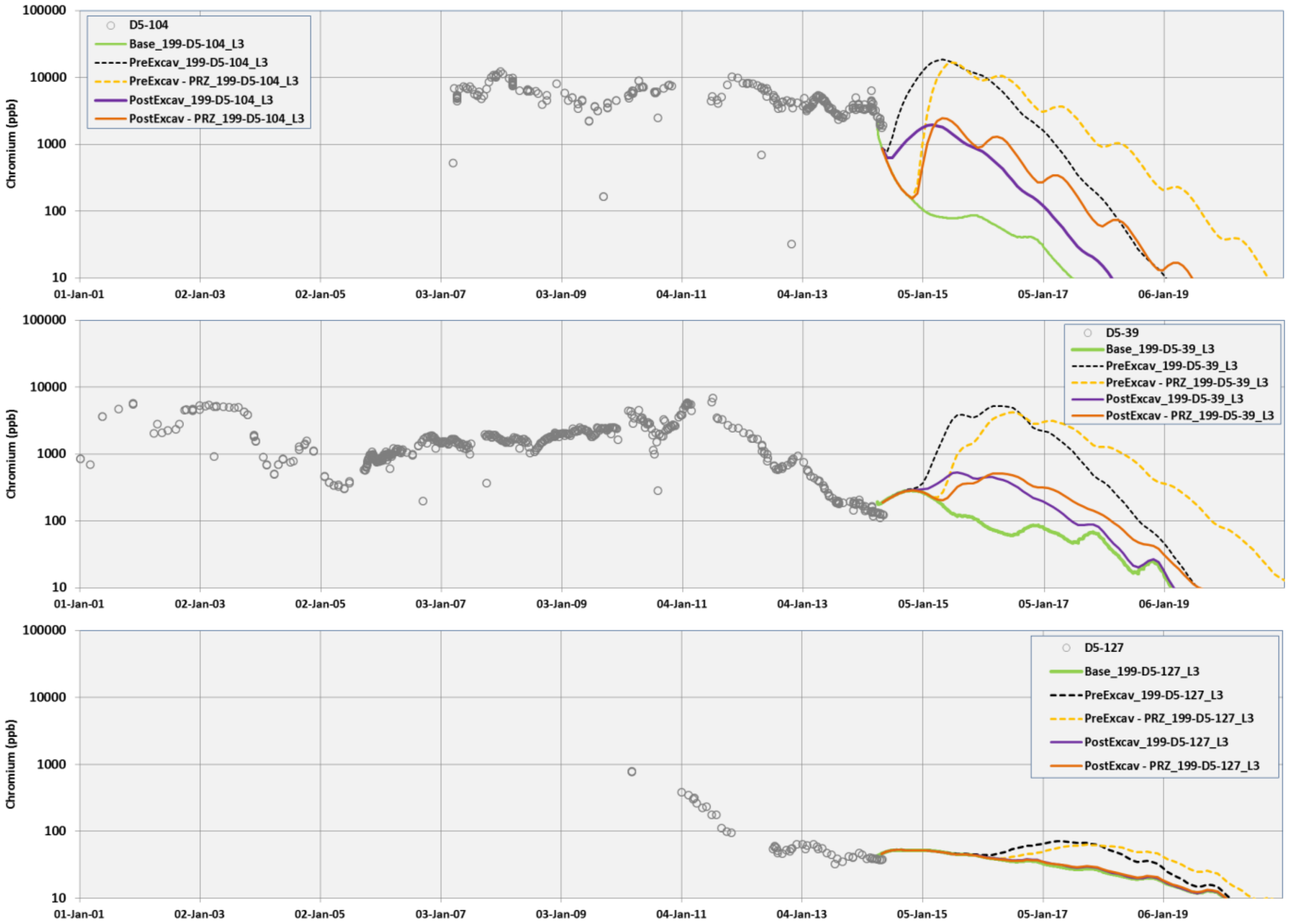

Numerical Models

- Advection-dispersion-reaction model
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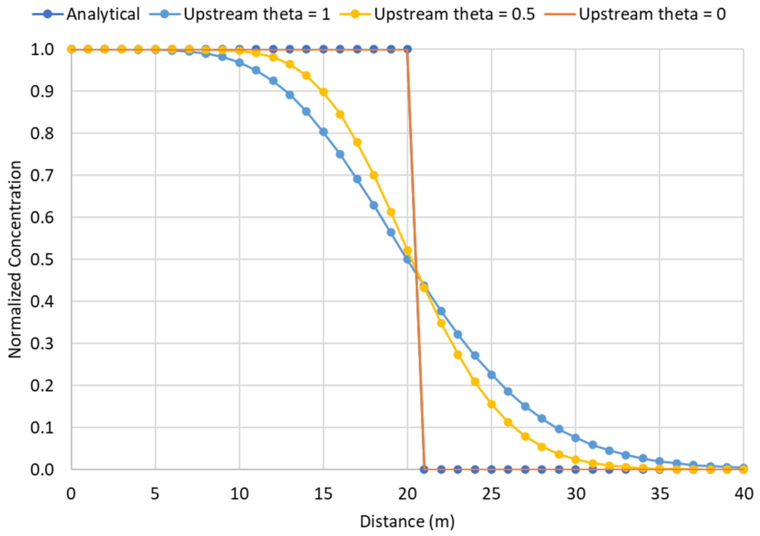
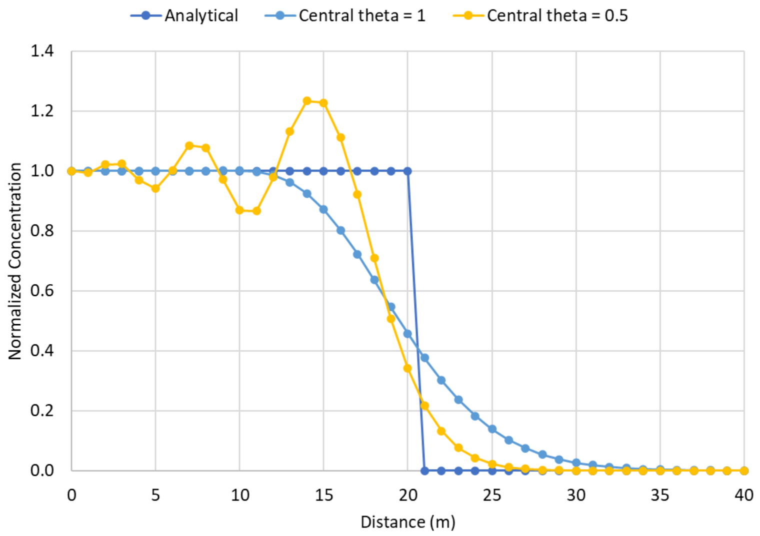
- Numerical methods
  - Particle based methods, finite-elements, finite-differences, finite-volumes

Numerical Models

- Advection-dispersion-reaction model
  - Heterogeneity (physical, geochemical); Scale
- Numerical methods
  - Particle based methods, finite-elements, finite-differences, finite-volumes
- Challenges and techniques
  - Oscillations and numerical dispersion
  - Space-weighting schemes
  - Time-weighting schemes
  - Total Variation Diminishing (TVD) schemes





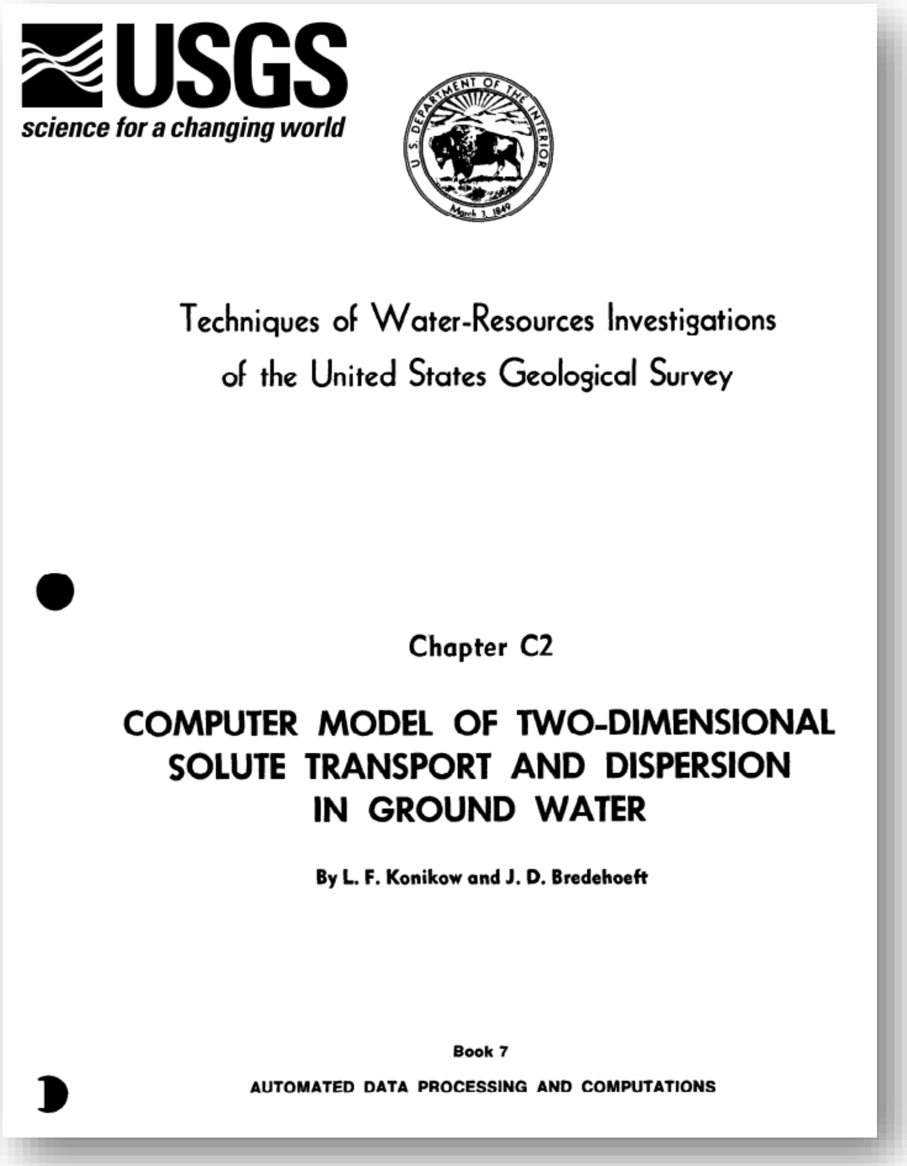
MODFLOW-family of Codes

- MODFLOW laid the foundation in early 1980s

Precursor to MOC3D

- Particle-based methods

Konikow, L.F., and Bredehoeft, J.D., 1978, Computer model of two-dimensional solute transport and dispersion in ground water: U.S. Geological Survey Techniques of Water-Resources Investigations, book 7, chap. C2, 90 p.



USGS
science for a changing world

Techniques of Water-Resources Investigations
of the United States Geological Survey

Chapter C2

COMPUTER MODEL OF TWO-DIMENSIONAL
SOLUTE TRANSPORT AND DISPERSION
IN GROUND WATER

By L. F. Konikow and J. D. Bredehoeft

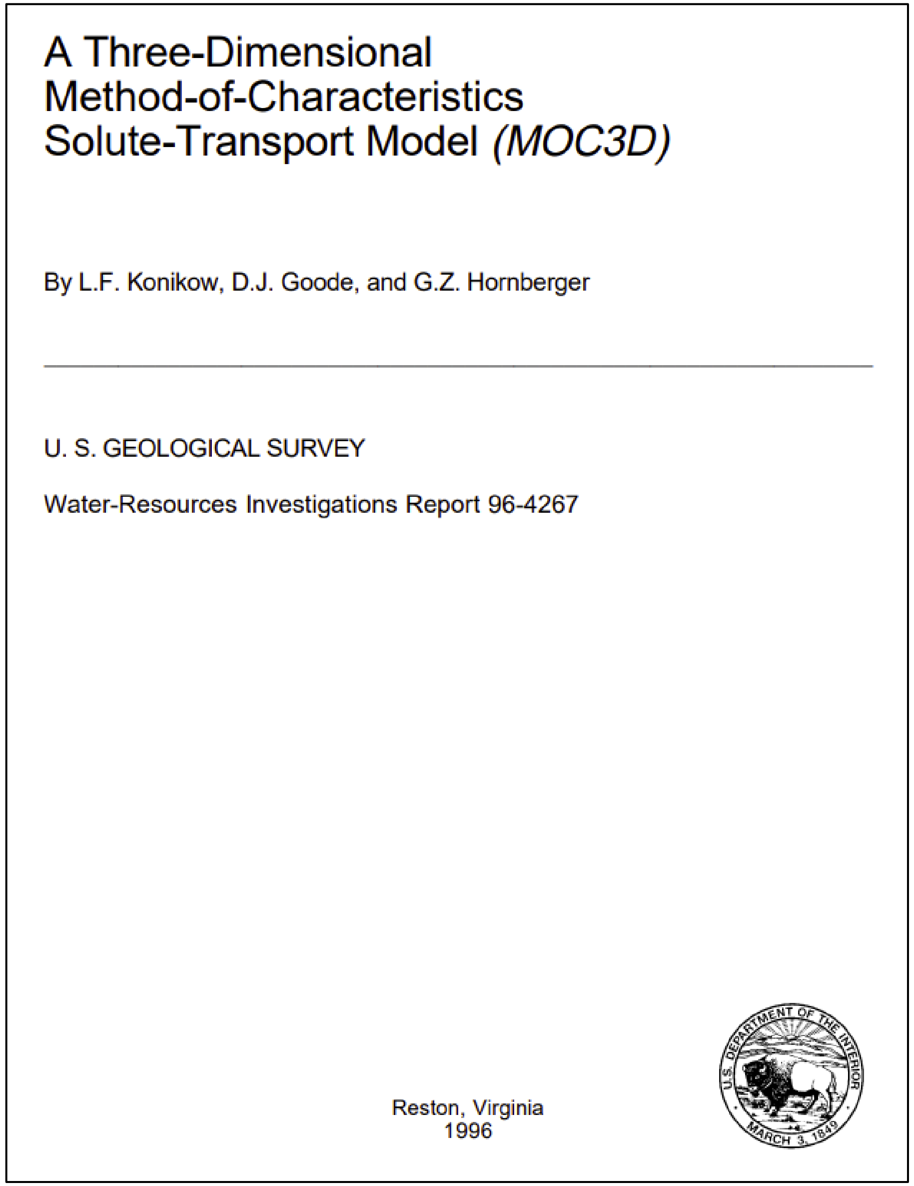
Book 7

AUTOMATED DATA PROCESSING AND COMPUTATIONS

MOC3D

- Particle-based methods

Konikow, L.F., Goode, D.J., and Hornberger, G.Z., 1996, A Three- Dimensional Method-of-Characteristics Solute-Transport Model (MOC3D): U.S. Geological Survey Water-Resources Investigations Report 96-4267, 87 p.



A Three-Dimensional
Method-of-Characteristics
Solute-Transport Model *(MOC3D)*

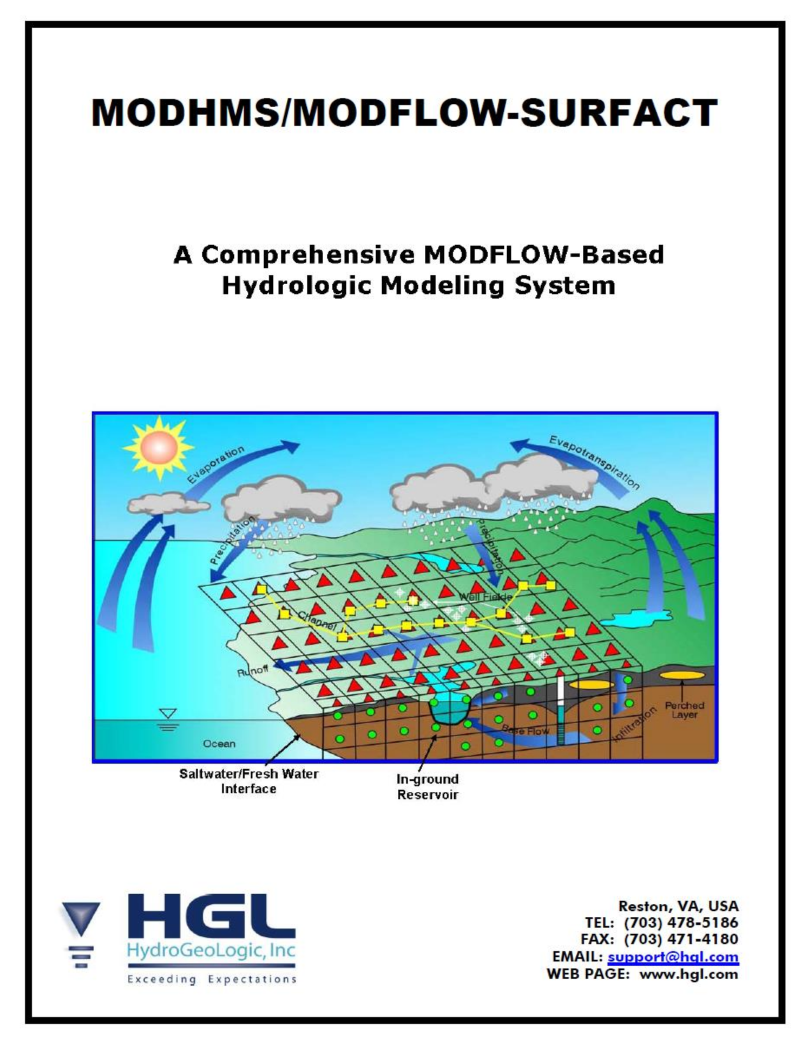
By L.F. Konikow, D.J. Goode, and G.Z. Hornberger

U. S. GEOLOGICAL SURVEY

Water-Resources Investigations Report 96-4267

Reston, Virginia
1996

MODFLOW-SURFACT

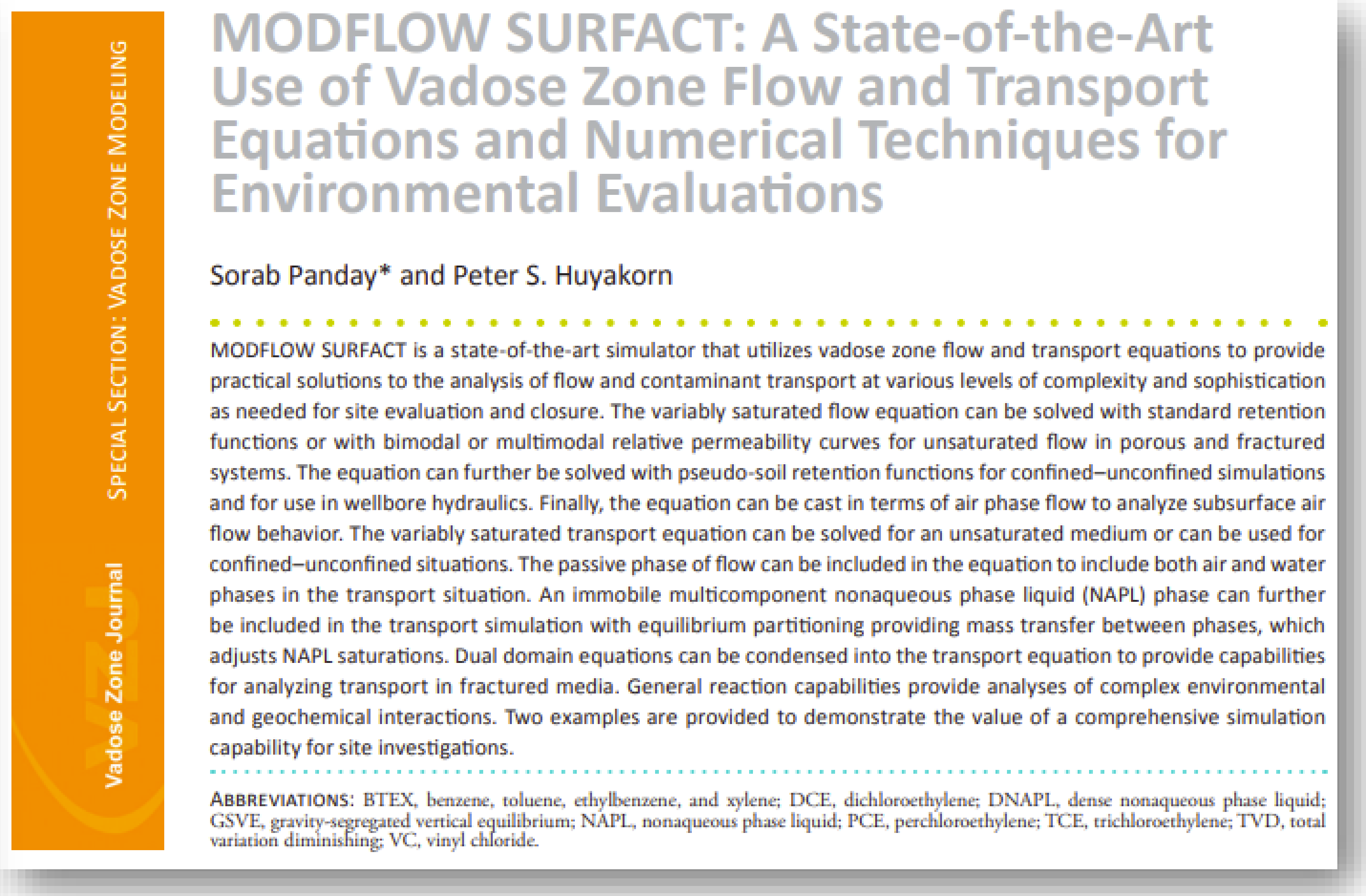


MODHMS/MODFLOW-SURFACT

A Comprehensive MODFLOW-Based
Hydrologic Modeling System

HGL
HydroGeoLogic, Inc
Exceeding Expectations

Reston, VA, USA
TEL: (703) 478-5186
FAX: (703) 471-4180
EMAIL: support@hgl.com
WEB PAGE: www.hgl.com



SPECIAL SECTION: VADOSE ZONE MODELING

Vadose Zone Journal

MODFLOW SURFACT: A State-of-the-Art Use of Vadose Zone Flow and Transport Equations and Numerical Techniques for Environmental Evaluations

Sorab Panday* and Peter S. Huyakorn

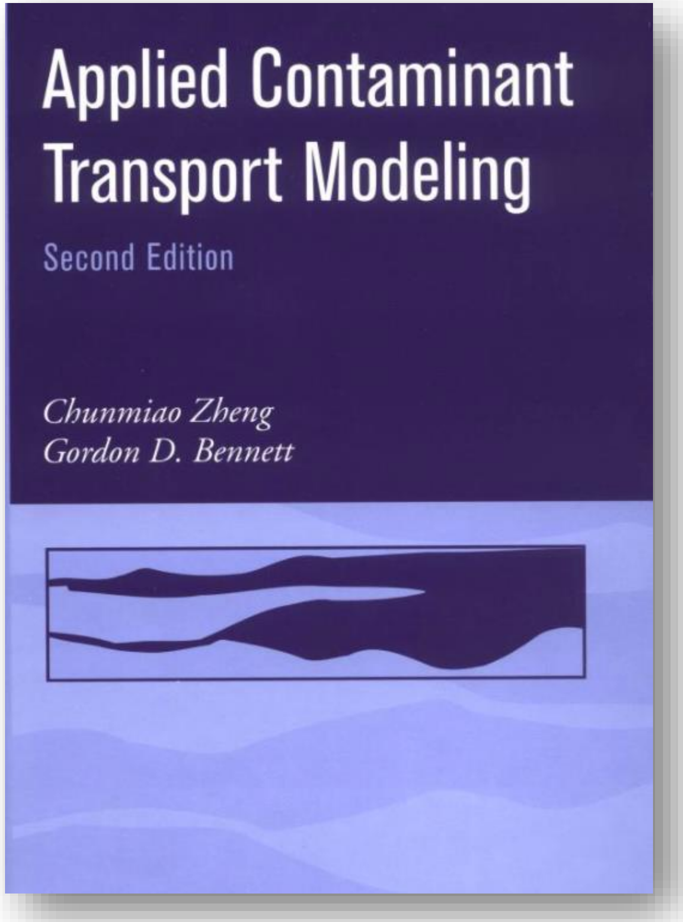
MODFLOW SURFACT is a state-of-the-art simulator that utilizes vadose zone flow and transport equations to provide practical solutions to the analysis of flow and contaminant transport at various levels of complexity and sophistication as needed for site evaluation and closure. The variably saturated flow equation can be solved with standard retention functions or with bimodal or multimodal relative permeability curves for unsaturated flow in porous and fractured systems. The equation can further be solved with pseudo-soil retention functions for confined–unconfined simulations and for use in wellbore hydraulics. Finally, the equation can be cast in terms of air phase flow to analyze subsurface air flow behavior. The variably saturated transport equation can be solved for an unsaturated medium or can be used for confined–unconfined situations. The passive phase of flow can be included in the equation to include both air and water phases in the transport situation. An immobile multicomponent nonaqueous phase liquid (NAPL) phase can further be included in the transport simulation with equilibrium partitioning providing mass transfer between phases, which adjusts NAPL saturations. Dual domain equations can be condensed into the transport equation to provide capabilities for analyzing transport in fractured media. General reaction capabilities provide analyses of complex environmental and geochemical interactions. Two examples are provided to demonstrate the value of a comprehensive simulation capability for site investigations.

ABBREVIATIONS: BTEX, benzene, toluene, ethylbenzene, and xylene; DCE, dichloroethylene; DNAPL, dense nonaqueous phase liquid; GSVE, gravity-segregated vertical equilibrium; NAPL, nonaqueous phase liquid; PCE, perchloroethylene; TCE, trichloroethylene; TVD, total variation diminishing; VC, vinyl chloride.

S. Panday, N. Brown, T. Foreman, V. Bedekar, J. Kaur, and P.S. Huyakorn, 2009. Simulating Dynamic Water Supply Systems in a Fully Integrated Surface-Subsurface Flow and Transport Model. Vadose Zone Journal, v. 8, no. 4, pp. 858-872.

MT3D

- MT3D (1990), MT3DMS (1999)



Applied Contaminant Transport Modeling

Second Edition

Chunmiao Zheng
Gordon D. Bennett

Contract Report SERDP-99-1
December 1999

US Army Corps of Engineers
Engineer Research and Development Center

Strategic Environmental Research and Development Program

MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems; Documentation and User's Guide

by Chunmiao Zheng, P. Patrick Wang
University of Alabama

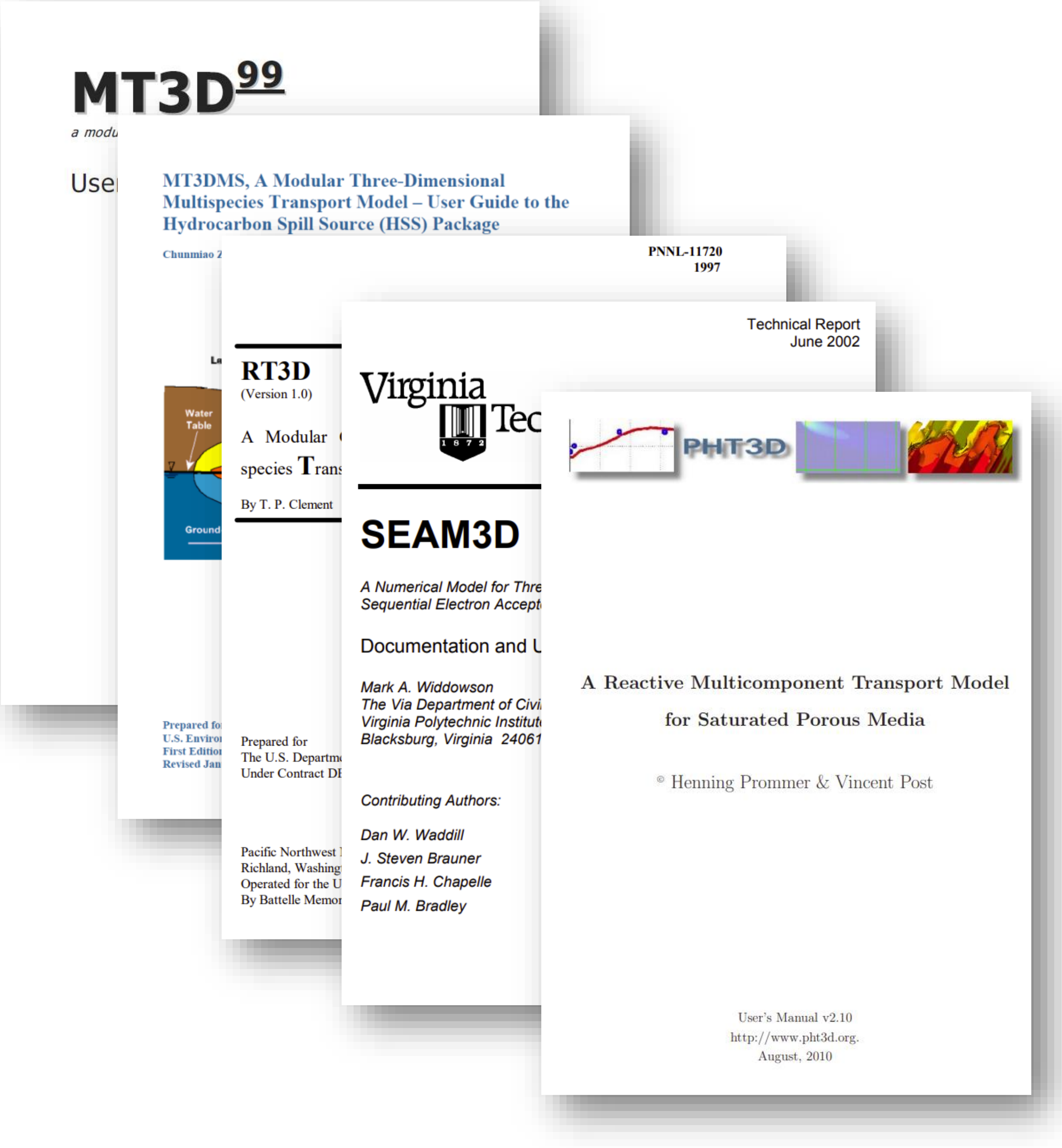
Approved For Public Release; Distribution Is Unlimited

SERDP
Strategic Environmental Research and Development Program
Improving Mission Readiness through Environmental Research

Prepared for Headquarters, U.S. Army Corps of Engineers

MT3D

- MT3D (1990), MT3DMS (1999)
- Reactive transport capabilities
  - MT3D-99, MT3D-HSS, RT3D, SEAM3D, PHT3D (MT3D-PHREEQC)



MT3D^{99}

a modu

Use

MT3DMS, A Modular Three-Dimensional Multispecies Transport Model – User Guide to the Hydrocarbon Spill Source (HSS) Package

Chunmiao Z

Prepared fo
U.S. Enviro
First Editio
Revised Jan

PNNL-11720
1997

RT3D
(Version 1.0)

A Modular
species Trans

By T. P. Clement

Prepared for
The U.S. Departm
Under Contract DE

Pacific Northwest
Richland, Washing
Operated for the U
By Battelle Memor

Technical Report
June 2002

Virginia Tec

SEAM3D

A Numerical Model for Thre
Sequential Electron Accept

Documentation and U

Mark A. Widdowson
The Via Department of Civi
Virginia Polytechnic Institut
Blacksburg, Virginia 24061

Contributing Authors:

Dan W. Waddill
J. Steven Brauner
Francis H. Chapelle
Paul M. Bradley

PHT3D

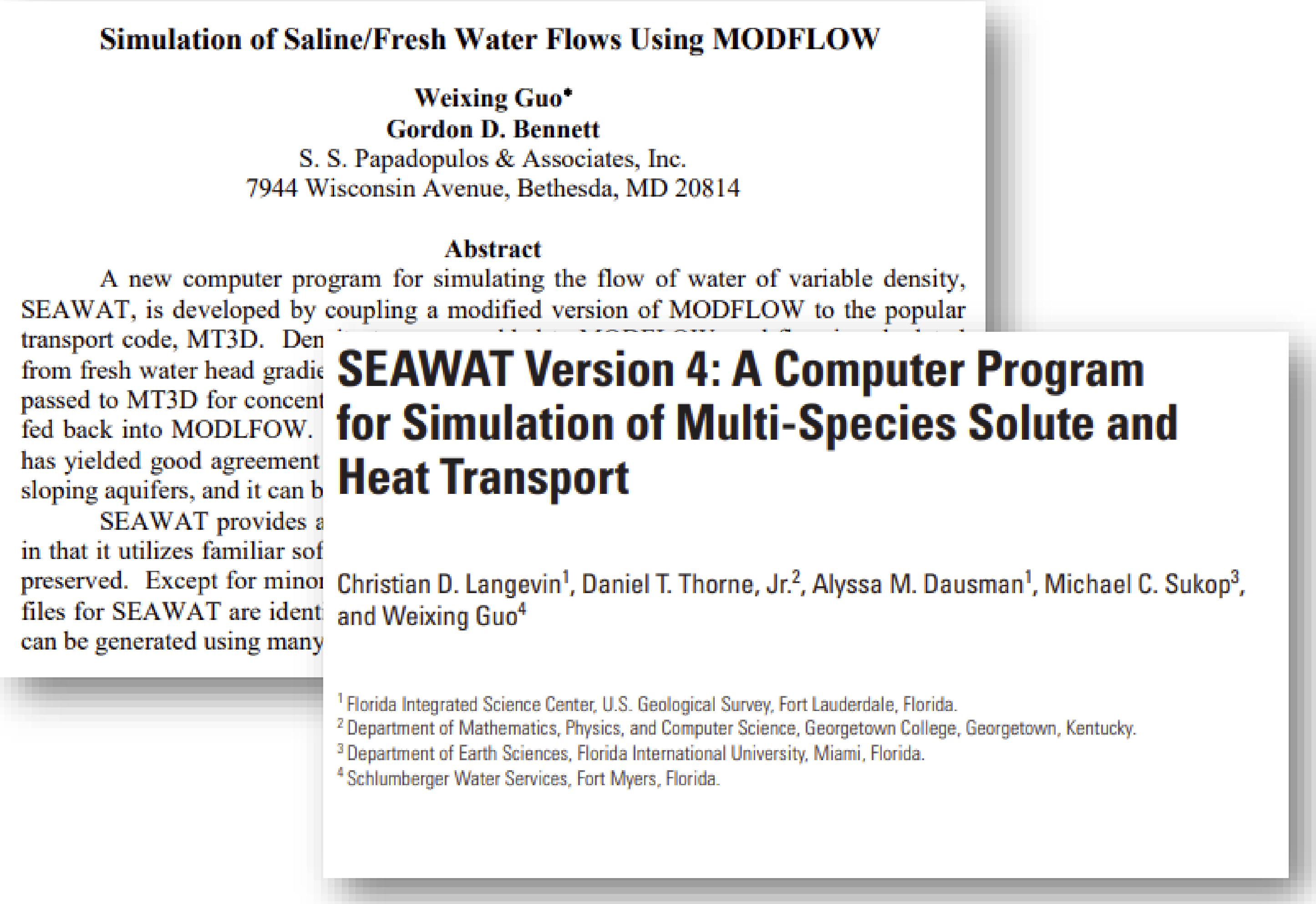
A Reactive Multicomponent Transport Model
for Saturated Porous Media

© Henning Prommer & Vincent Post

User's Manual v2.10
http://www.pht3d.org.
August, 2010

MT3D

- MT3D (1990), MT3DMS (1999)
- Reactive transport capabilities
  - MT3D-99, MT3D-HSS, RT3D, SEAM3D, PHT3D (MT3D-PHREEQC)
- Variable density - SEAWAT



Simulation of Saline/Fresh Water Flows Using MODFLOW

Weixing Guo*
Gordon D. Bennett
S. S. Papadopulos & Associates, Inc.
7944 Wisconsin Avenue, Bethesda, MD 20814

Abstract

A new computer program for simulating the flow of water of variable density, SEAWAT, is developed by coupling a modified version of MODFLOW to the popular transport code, MT3D. Den
from fresh water head gradie
passed to MT3D for concent
fed back into MODLFOW.
has yielded good agreement
sloping aquifers, and it can b
SEAWAT provides a
in that it utilizes familiar sof
preserved. Except for minor
files for SEAWAT are ident
can be generated using many

SEAWAT Version 4: A Computer Program for Simulation of Multi-Species Solute and Heat Transport

Christian D. Langevin[1], Daniel T. Thorne, Jr.[2], Alyssa M. Dausman[1], Michael C. Sukop[3], and Weixing Guo[4]

[1] Florida Integrated Science Center, U.S. Geological Survey, Fort Lauderdale, Florida.
[2] Department of Mathematics, Physics, and Computer Science, Georgetown College, Georgetown, Kentucky.
[3] Department of Earth Sciences, Florida International University, Miami, Florida.
[4] Schlumberger Water Services, Fort Myers, Florida.

MT3D

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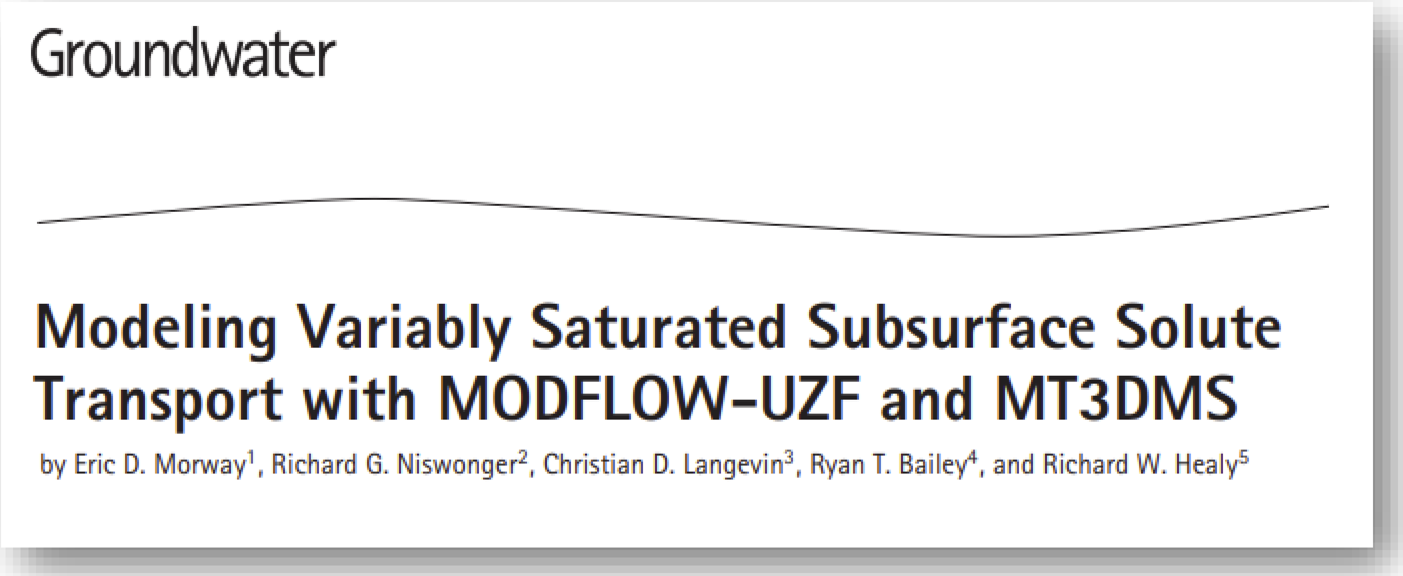
- Unsaturated zone transport



Groundwater

Modeling Variably Saturated Subsurface Solute Transport with MODFLOW-UZF and MT3DMS

by Eric D. Morway[1], Richard G. Niswonger[2], Christian D. Langevin[3], Ryan T. Bailey[4], and Richard W. Healy[5]

MT3D

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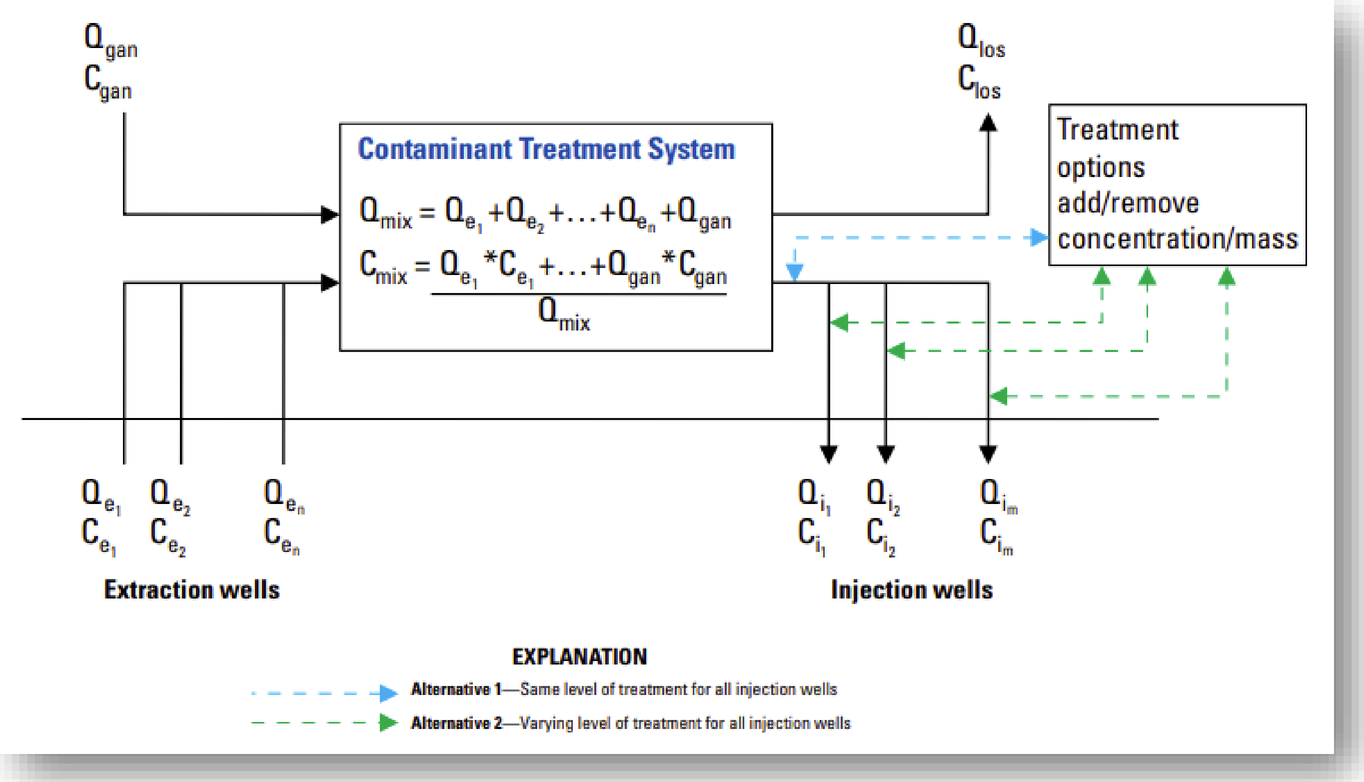
- Pump and treat systems



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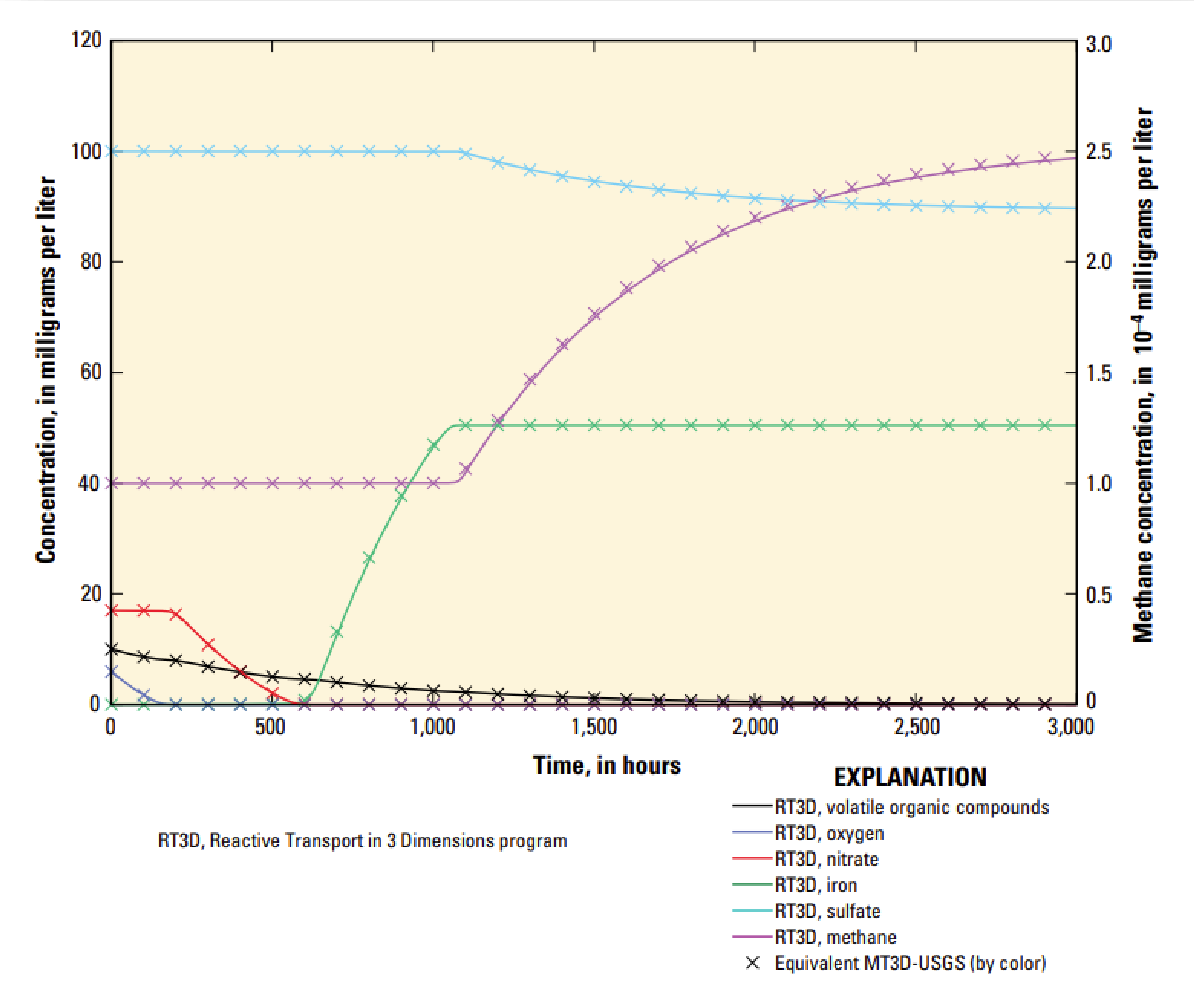

RT3D, Reactive Transport in 3 Dimensions program

MT3D

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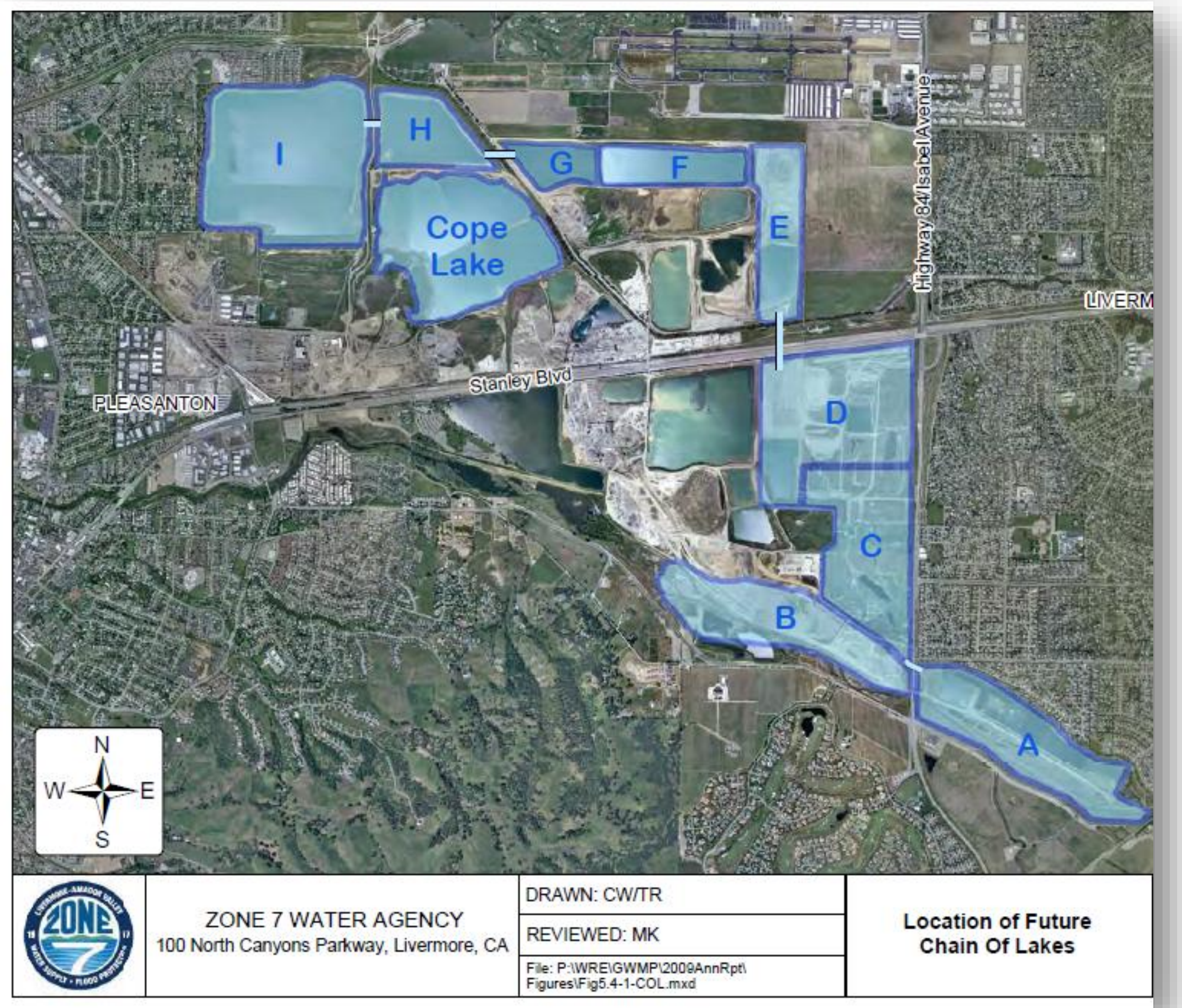

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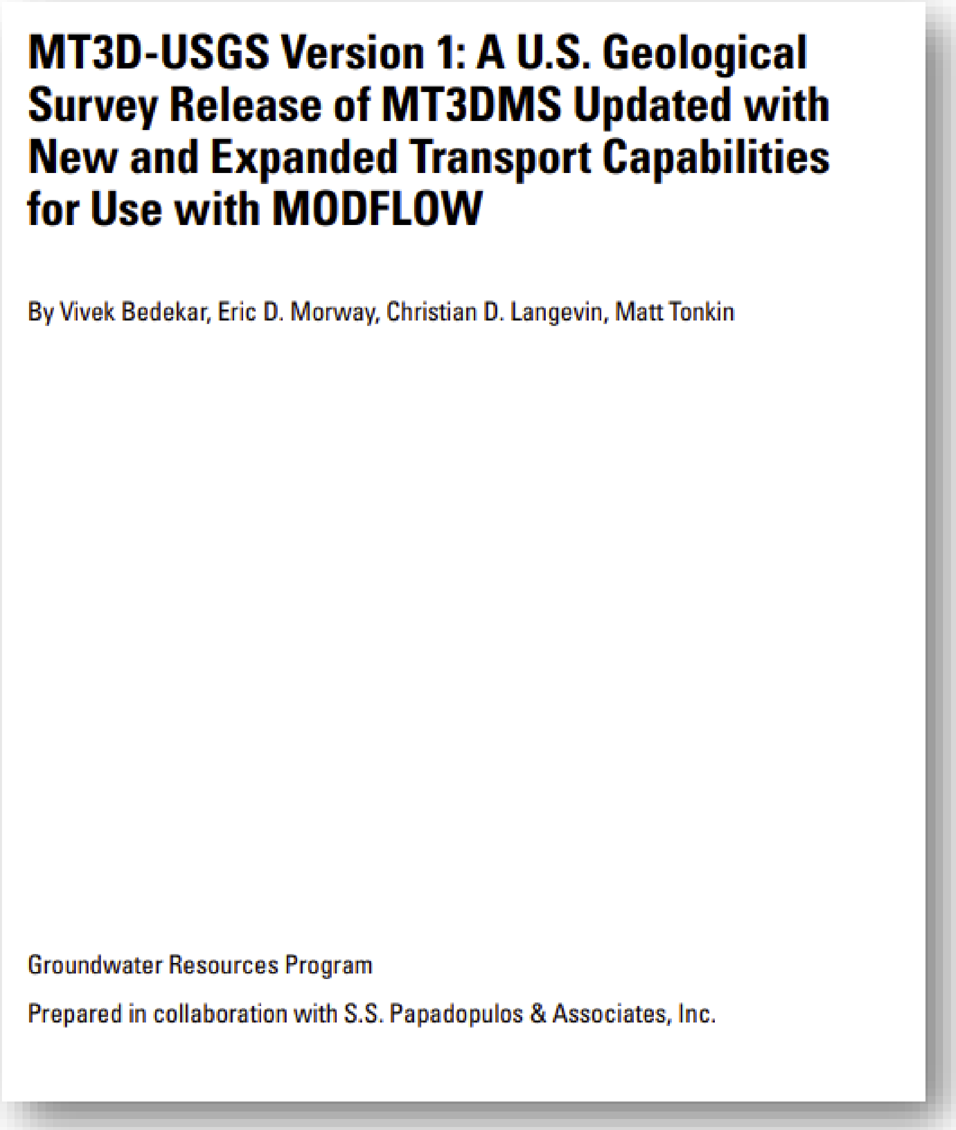
- MT3D-USGS



MT3D-USGS Version 1: A U.S. Geological Survey Release of MT3DMS Updated with New and Expanded Transport Capabilities for Use with MODFLOW

By Vivek Bedekar, Eric D. Morway, Christian D. Langevin, Matt Tonkin

Groundwater Resources Program

Prepared in collaboration with S.S. Papadopulos & Associates, Inc.

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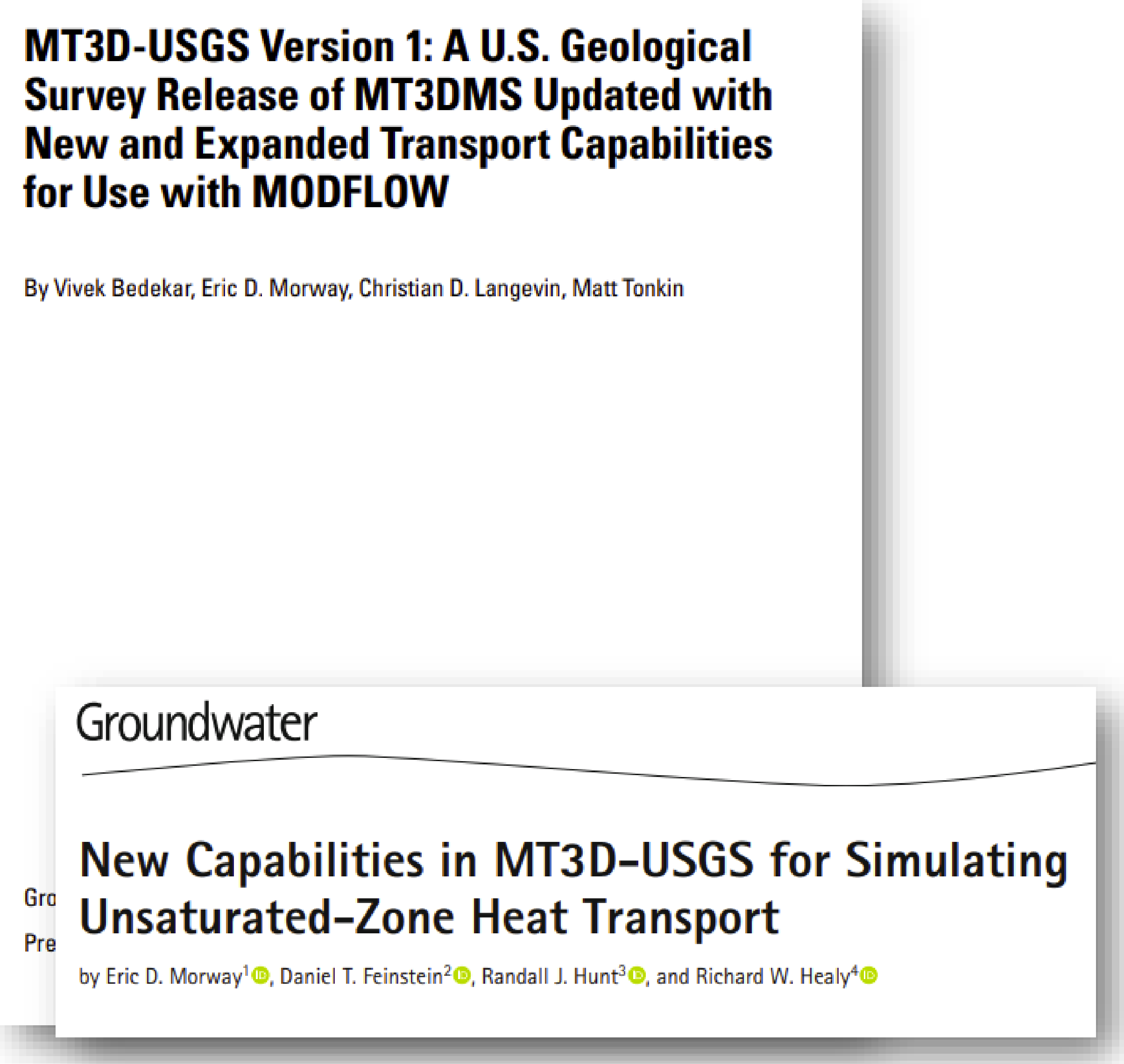
- Heat transport



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By Vivek Bedekar, Eric D. Morway, Christian D. Langevin, Matt Tonkin

Gro

Pre

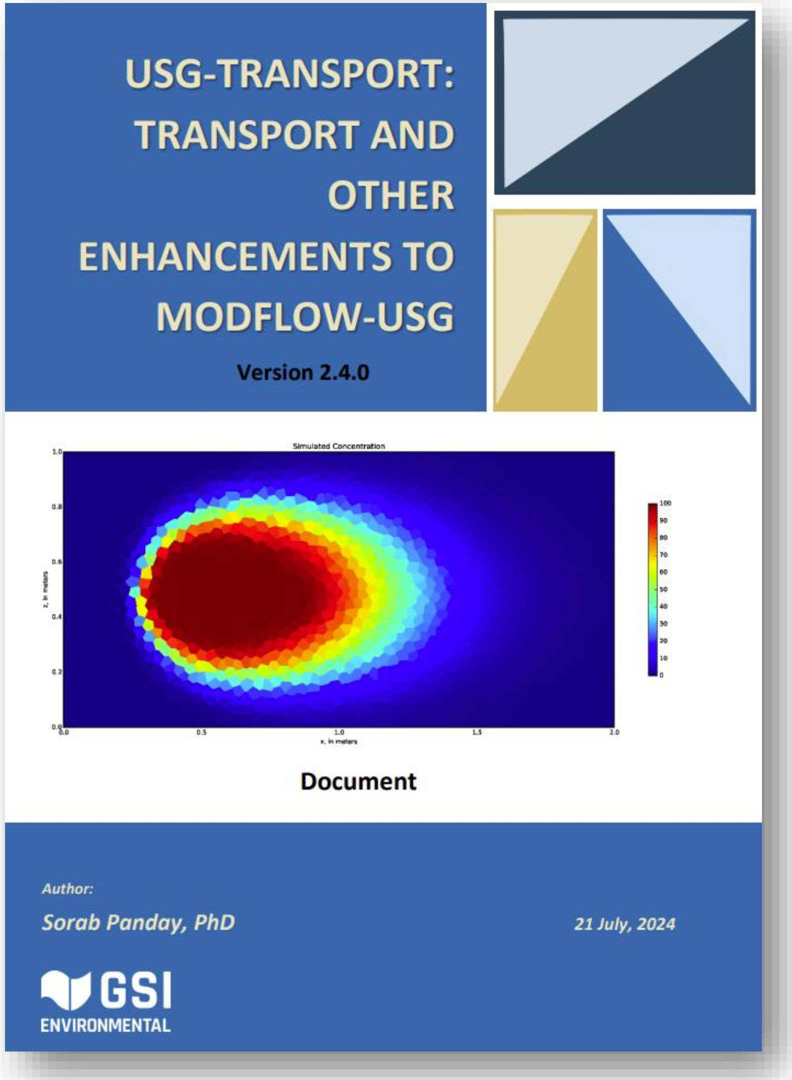
Groundwater

New Capabilities in MT3D-USGS for Simulating Unsaturated-Zone Heat Transport

by Eric D. Morway[1], Daniel T. Feinstein[2], Randall J. Hunt[3], and Richard W. Healy[4]

MODFLOW-USG-Transport

- Grid flexibility like finite-element grids, mass conservative solutions of the finite-volume approach



USG-TRANSPORT: TRANSPORT AND OTHER ENHANCEMENTS TO MODFLOW-USG

Version 2.4.0

Document

Author:

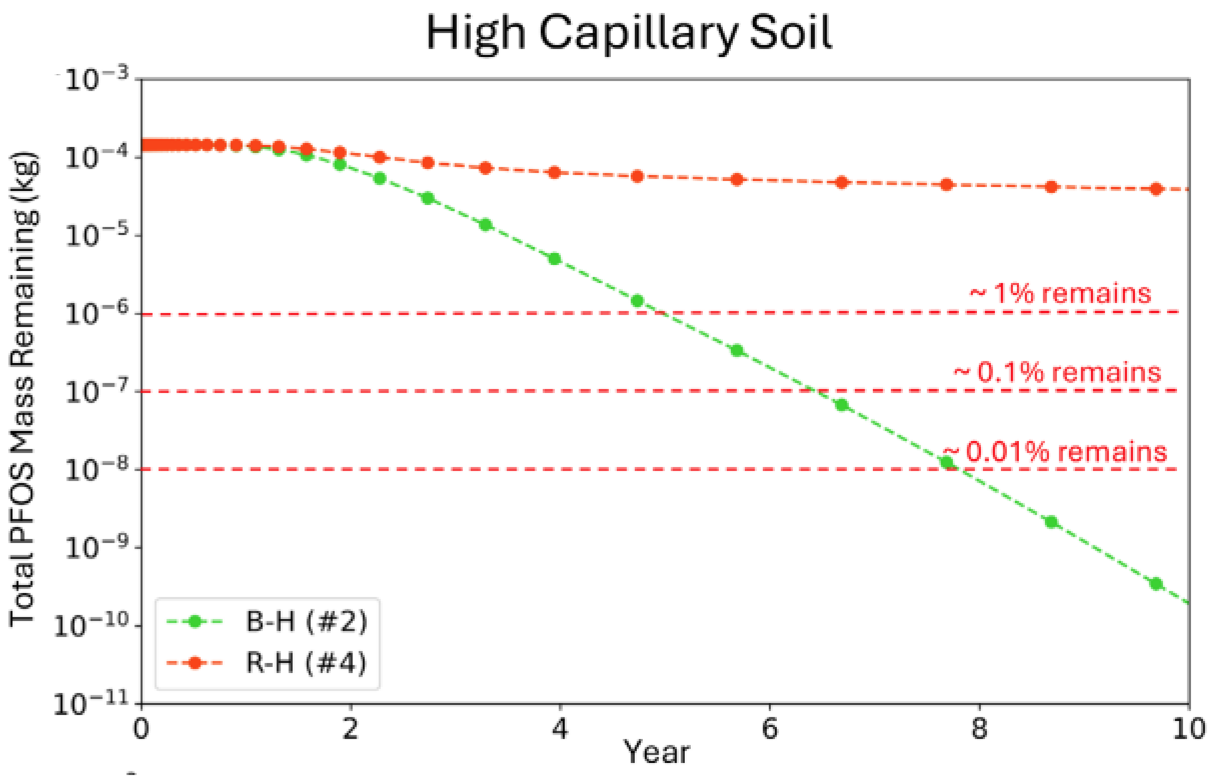
Sorab Panday, PhD

21 July, 2024

GSI ENVIRONMENTAL

MODFLOW-USG-Transport

- Grid flexibility like finite-element grids, mass conservative solutions of the finite-volume approach
- Capabilities
  - **Vadose zone transport**
  - Variable density
  - Dual-porosity
  - Matrix diffusion
  - Time varying materials
  - Heat
  - PFAS
  - PHREEQC support (PHT-USG)



S.S. Papadopulos & Associates, Inc.
Environmental and Water-Resource Consultants

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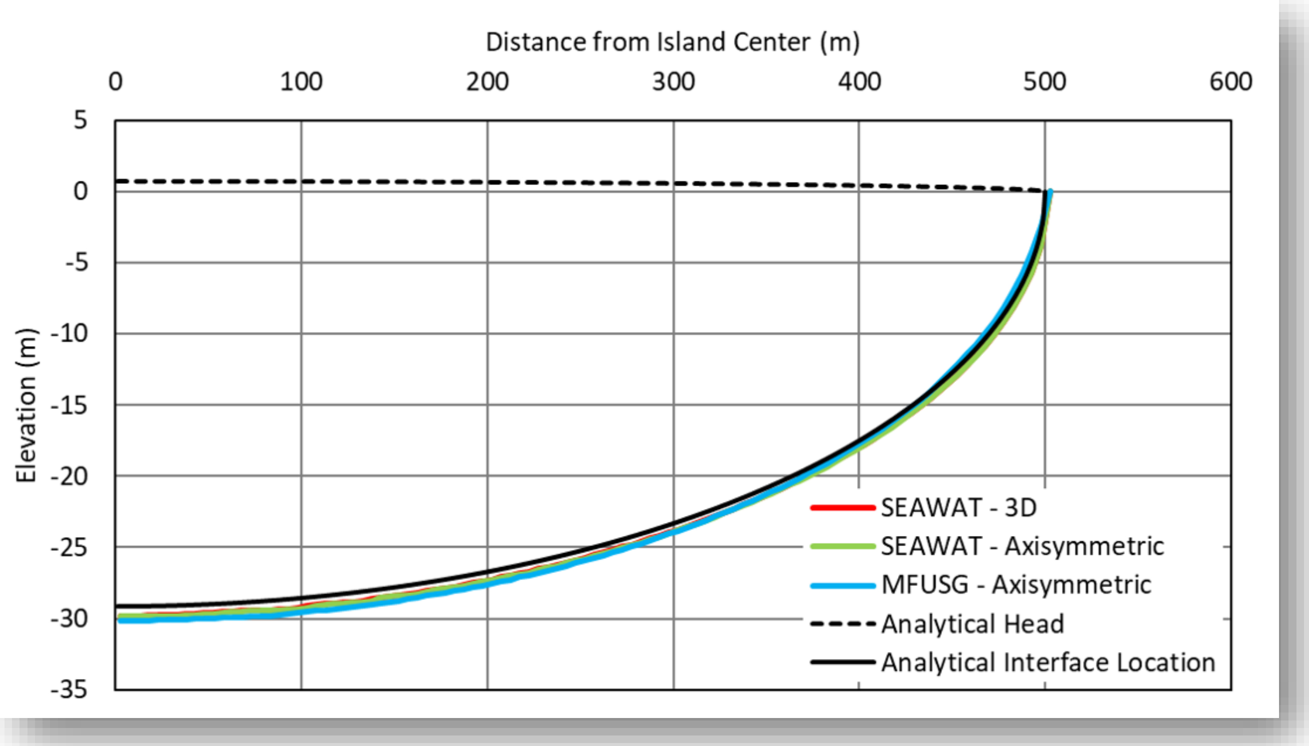
  - PFAS
  - PHREEQC support (PHT-USG)



MODFLOW-USG-Transport

- Grid flexibility like finite-element grids, mass conservative solutions of the finite-volume approach
- Capabilities
  - Vadose zone transport
  - Variable density
  - **Dual-porosity**
  - Matrix diffusion
  - Time varying materials
  - Heat
  - PFAS
  - PHREEQC support (PHT-USG)

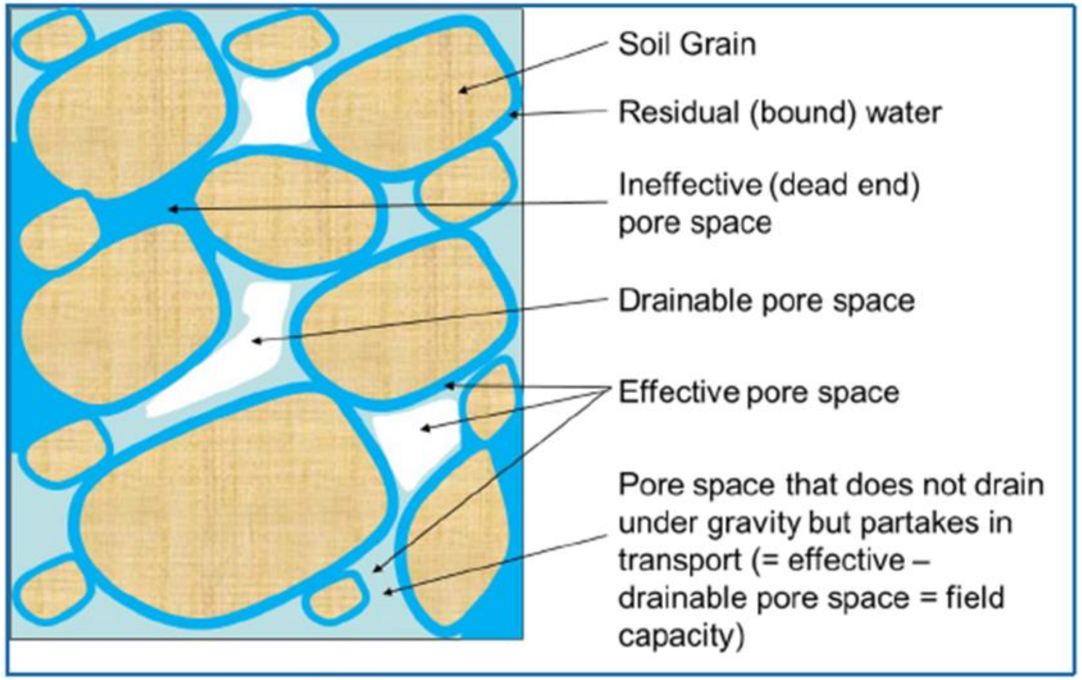


Figure 1. *Porosity Definitions*

MODFLOW-USG-Transport

- Grid flexibility like finite-element grids, mass conservative solutions of the finite-volume approach
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  - **Matrix diffusion**
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  - Heat
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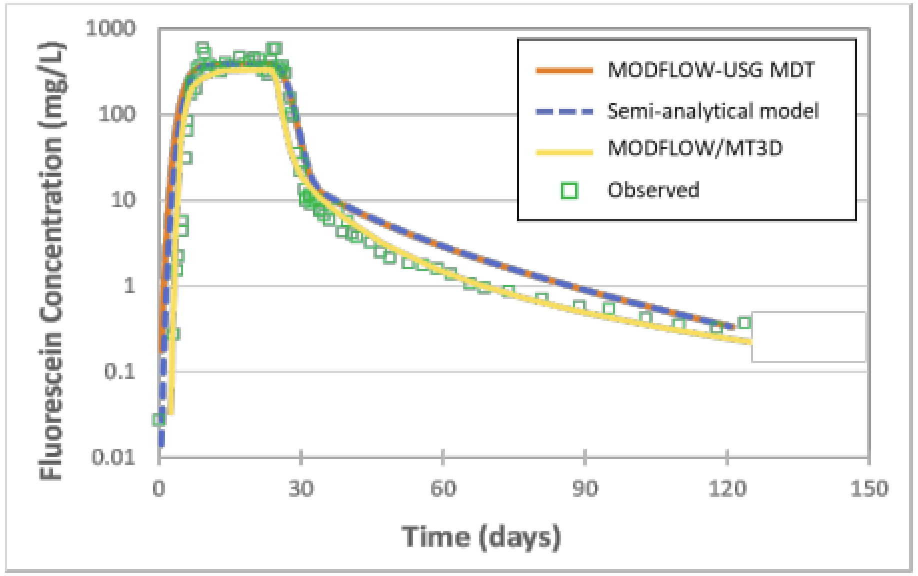

Figure Ex 13. *Comparison of MODFLOW-USG MDT model (50 model cells) output with Chapman et al. (2012) MODFLOW/MT3DMS model (8,988 model cells), semi-analytical model (50 model cells), and observed concentrations.*

MODFLOW-USG-Transport

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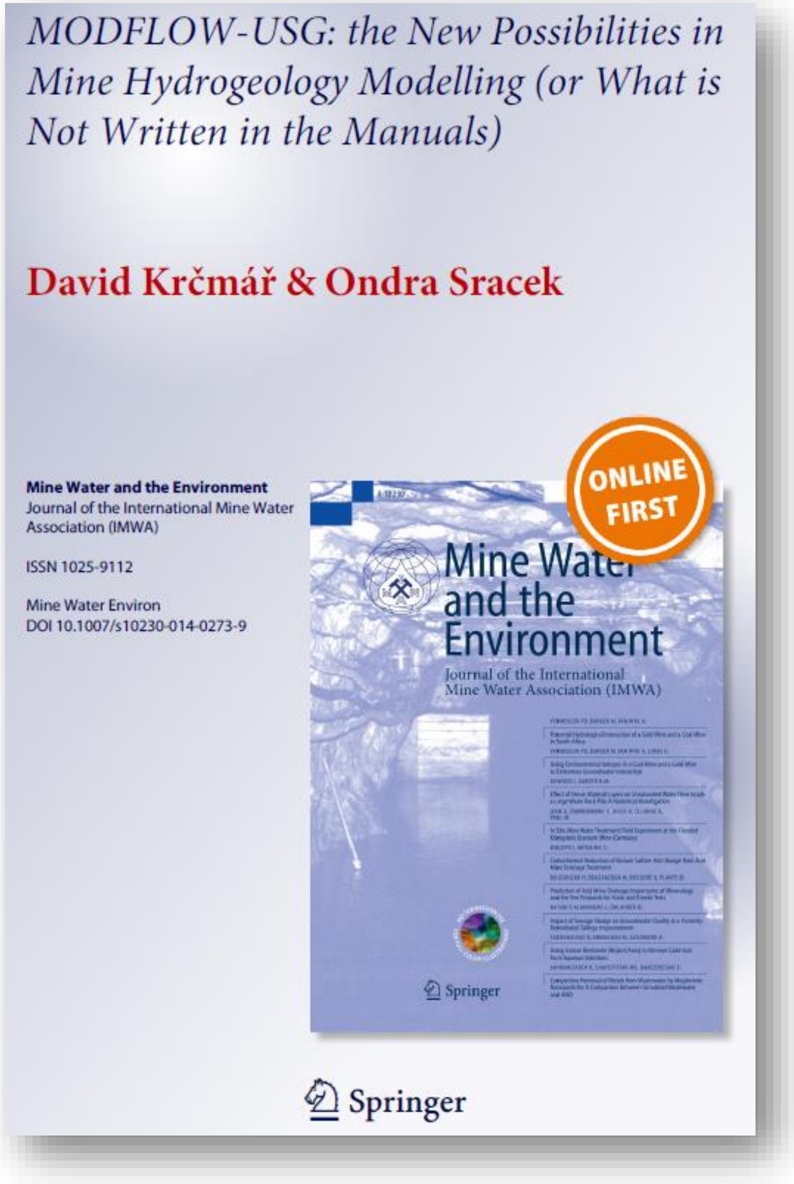

MODFLOW-USG: the New Possibilities in Mine Hydrogeology Modelling (or What is Not Written in the Manuals)

David Krčmář & Ondra Sracek

Mine Water and the Environment
Journal of the International Mine Water Association (IMWA)

ISSN 1025-9112

Mine Water Environ
DOI 10.1007/s10230-014-0273-9

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MODFLOW-USG-Transport

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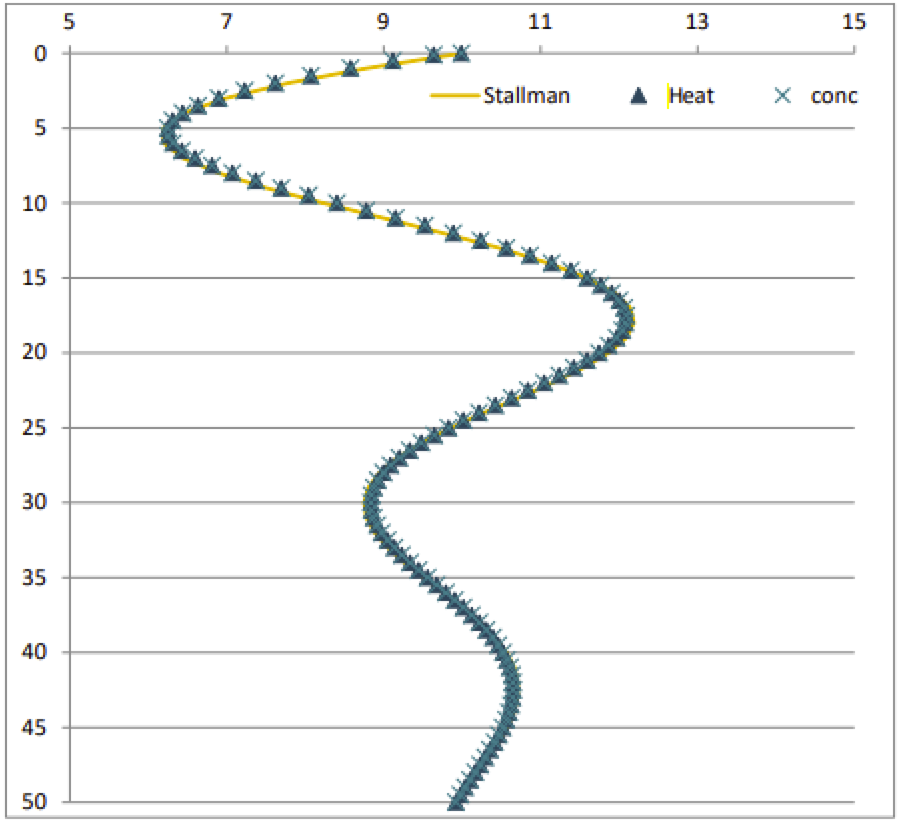

Figure H1: *Comparison of temperature profile simulated with MODFLOW-USG as heat or equivalent solute transport against the Stallman (1965) analytical solution at 10 years.*

MODFLOW-USG-Transport

- Grid flexibility like finite-element grids, mass conservative solutions of the finite-volume approach
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  - Vadose zone transport
  - Variable density
  - Dual-porosity
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  - **PFAS**
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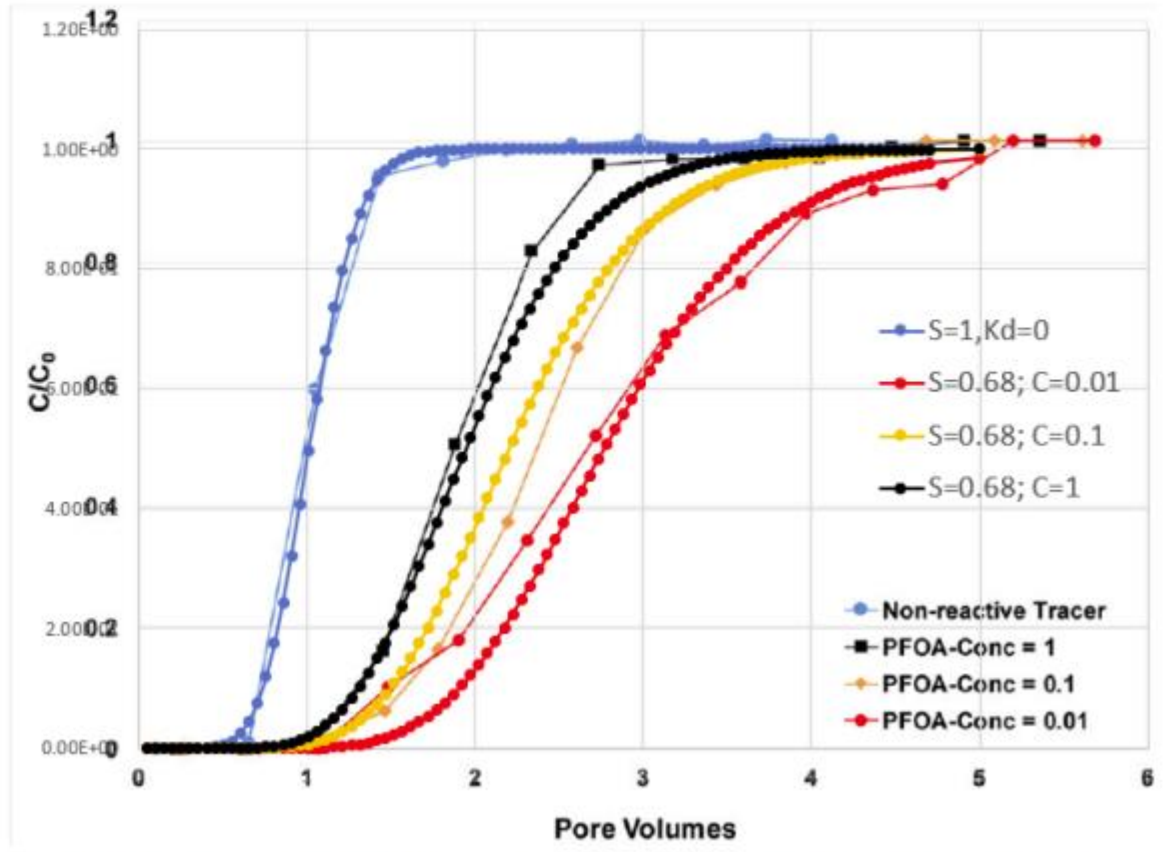
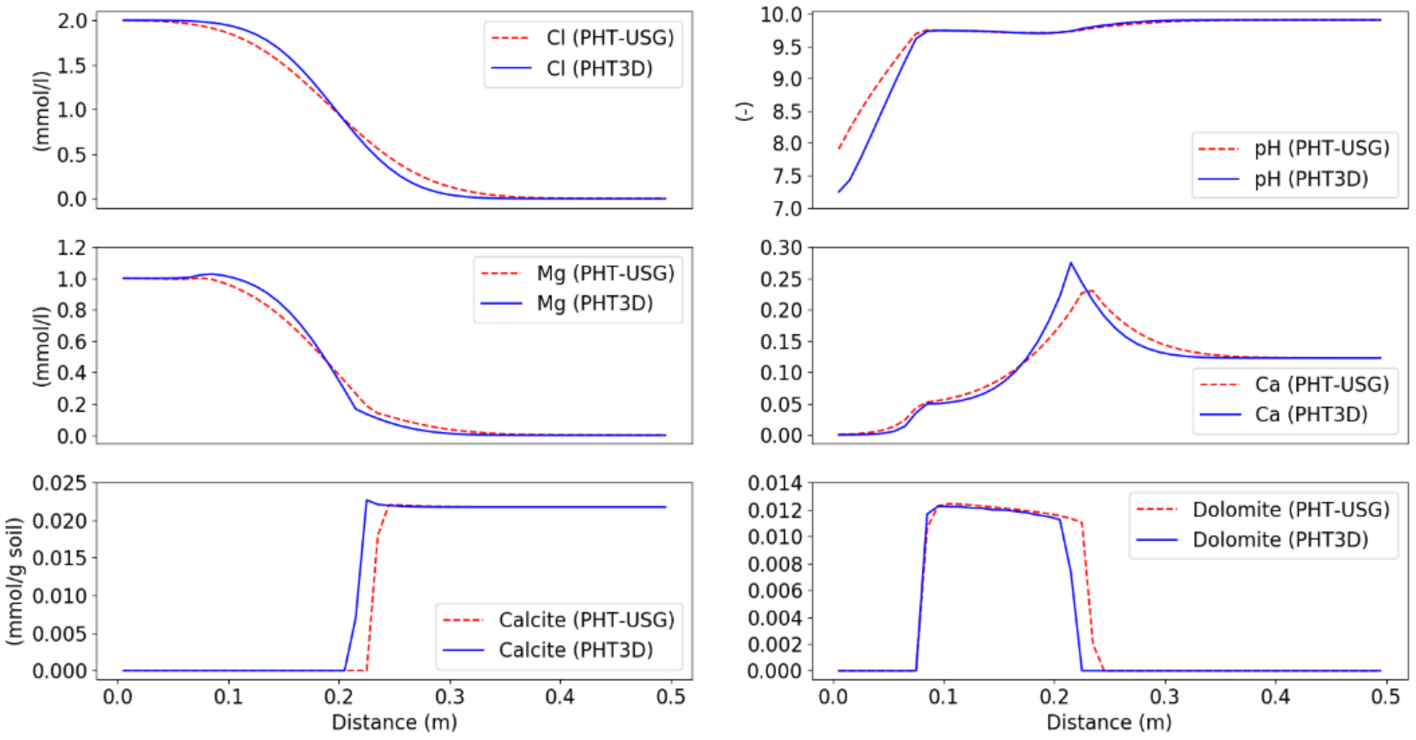


Figure ***Ex 17.*** *Breakthrough of PFOA for different concentration cases compared to Lyu (2018) experimental results.*

MODFLOW-USG-Transport

- Grid flexibility like finite-element grids, mass conservative solutions of the finite-volume approach
- Capabilities
  - Vadose zone transport
  - Variable density
  - Dual-porosity
  - Matrix diffusion
  - Time varying materials
  - Heat
  - PFAS
  - **PHREEQC support (PHT-USG)**



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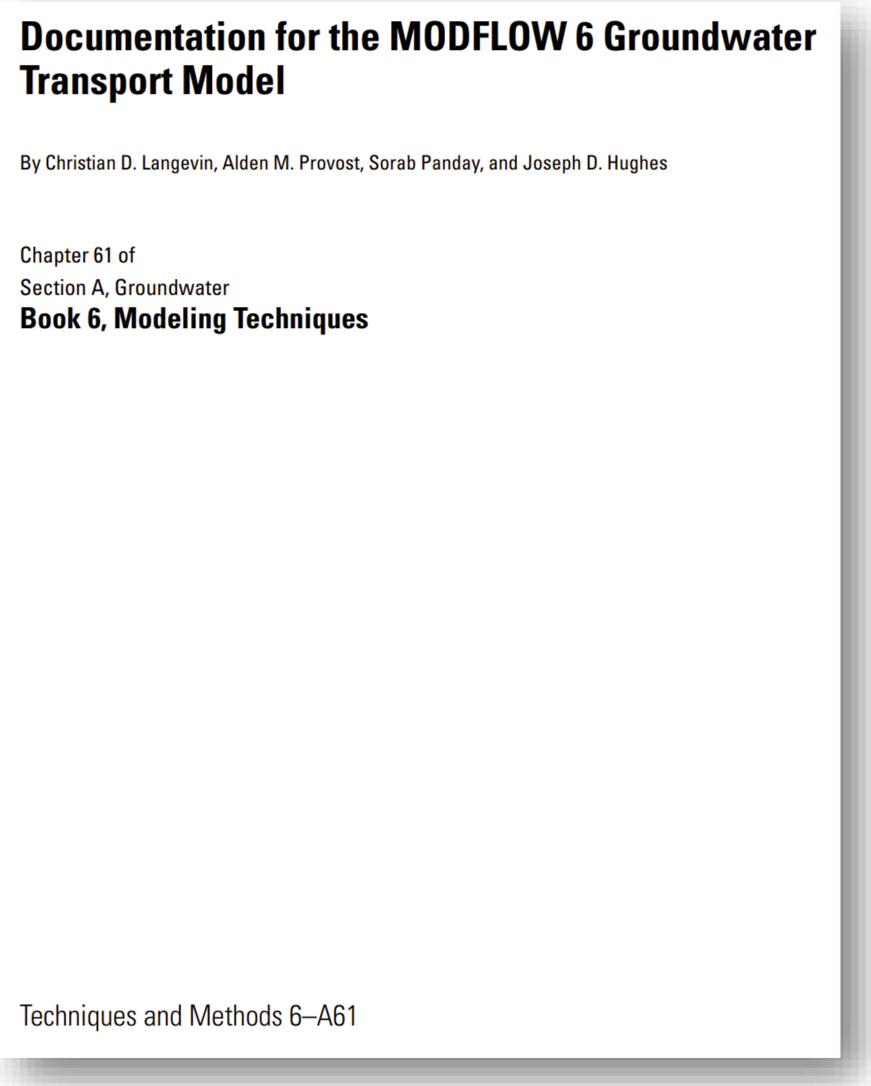
MODFLOW-6

- Capabilities similar to MODFLOW-USG-Transport
- Groundwater Transport Model (GWT)



Documentation for the MODFLOW 6 Groundwater Transport Model

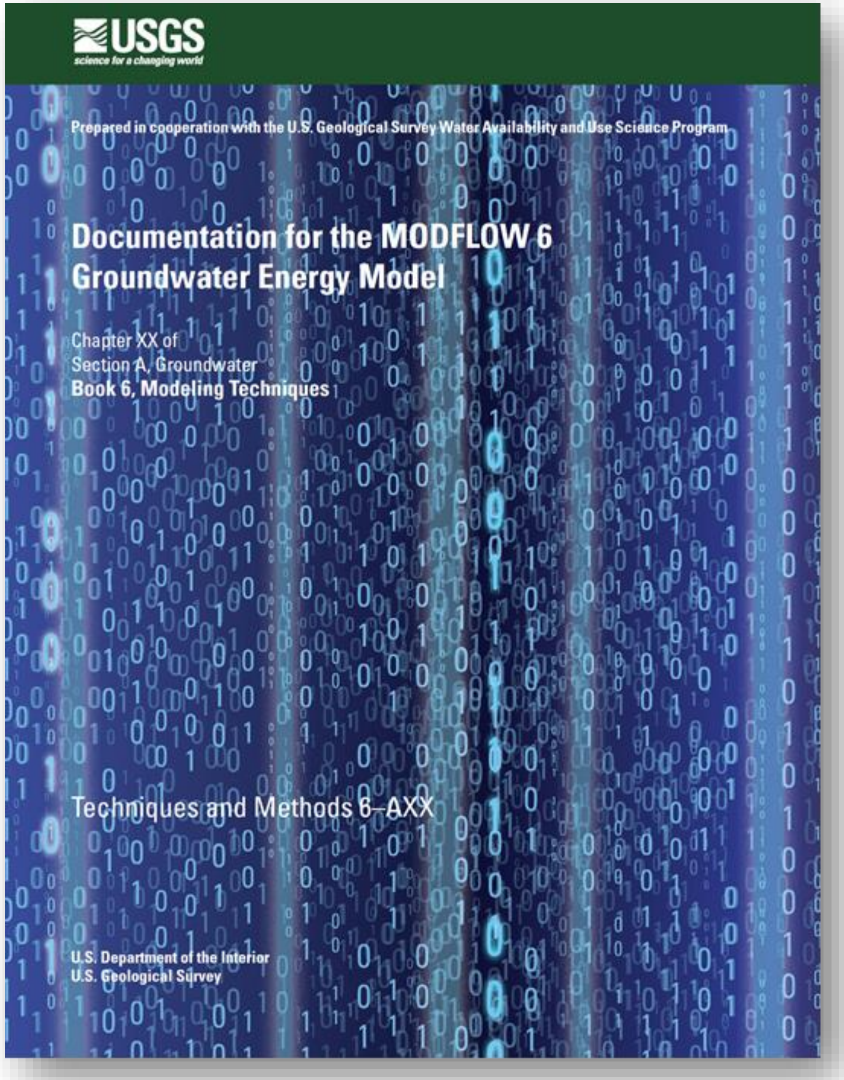
By Christian D. Langevin, Alden M. Provost, Sorab Panday, and Joseph D. Hughes

Chapter 61 of
Section A, Groundwater
Book 6, Modeling Techniques

Techniques and Methods 6–A61

MODFLOW-6

- Capabilities similar to MODFLOW-USG-Transport
- Groundwater Transport Model (GWT)
- Groundwater Energy Model (GWE)



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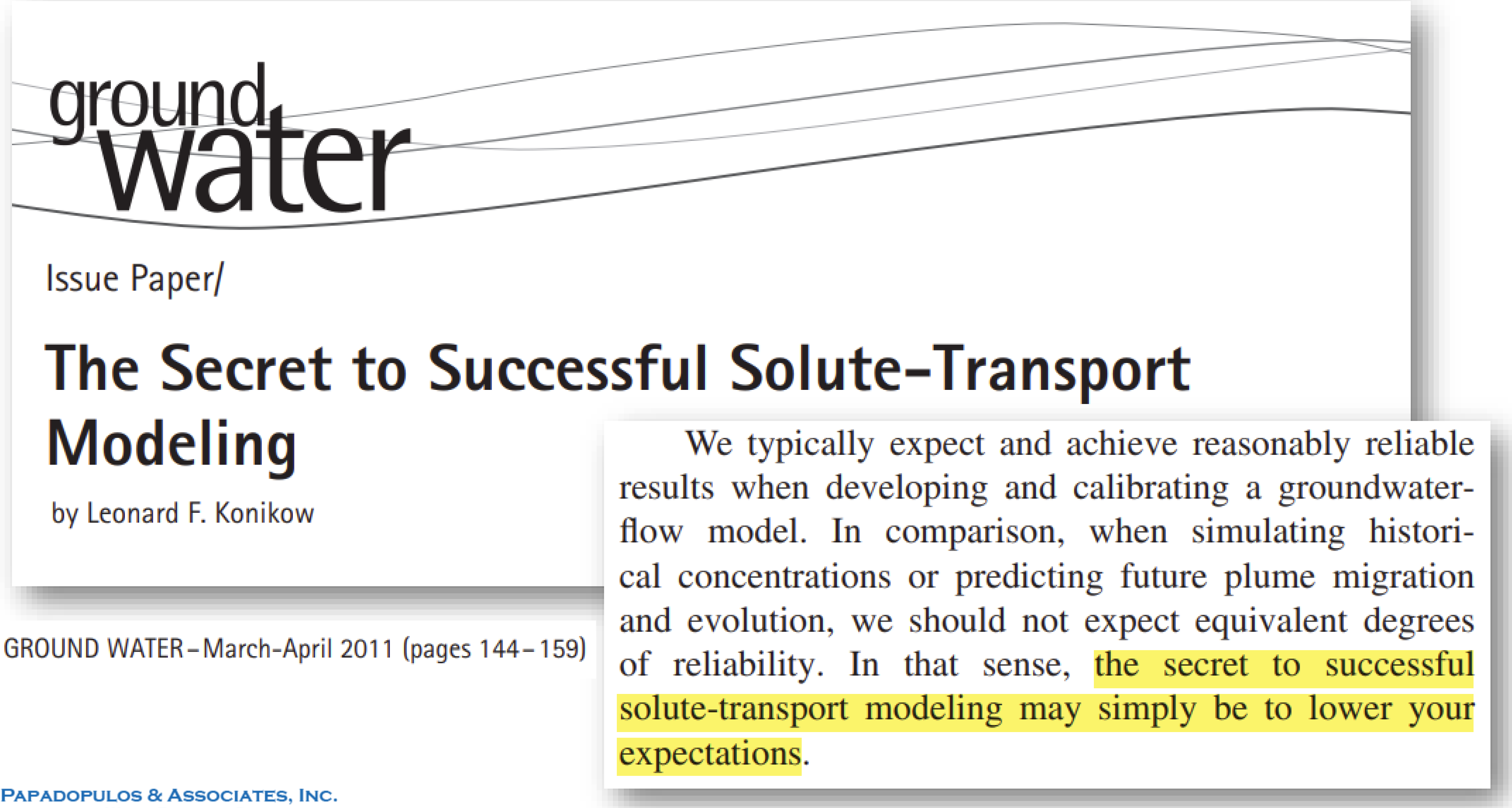
Documentation for the MODFLOW 6 Groundwater Energy Model

Chapter XX of
Section A, Groundwater
Book 6, Modeling Techniques

Techniques and Methods 6–AXX

U.S. Department of the Interior
U.S. Geological Survey

Reflections



ground water

Issue Paper/

The Secret to Successful Solute-Transport Modeling

by Leonard F. Konikow

We typically expect and achieve reasonably reliable results when developing and calibrating a groundwater-flow model. In comparison, when simulating historical concentrations or predicting future plume migration and evolution, we should not expect equivalent degrees of reliability. In that sense, the secret to successful solute-transport modeling may simply be to lower your expectations.

Vol. 49, No. 2–GROUND WATER–March-April 2011 (pages 144–159)

Reflections

ground water

Review Paper/

Lessons Learned from 25 Years of Research at the MADE Site

by Chunmiao Zheng[1,2], Marco Bianchi[3], and Steven M. Gorelick[4]

Abstract

Field studies at well-instrumented research sites have provided extensive data sets and important insights essential for development and testing of transport theories and mathematical models. This paper provides an overview of over 25 years of research and lessons learned at one of such field research sites on the Columbus Air Force Base in Mississippi, commonly known as the Macrodispersion Experiment (MADE) site. Since the mid-1980s, field data from the MADE site have been used extensively by researchers around the world to explore complex contaminant transport phenomena in highly heterogeneous porous media. Results from field investigations and modeling analyses suggested that connected networks of small-scale preferential flow paths and relative flow barriers exert dominant control on solute transport processes. The classical advection-dispersion model was shown to inadequately represent plume-scale transport, while the dual-domain mass transfer model was found to reproduce the primary observed plume characteristics. The MADE site has served as a valuable natural observatory for contaminant transport studies where new observations have led to better understanding and improved models have sprung out analysis of new data.

Vol. 49, No. 5–GROUND WATER–September-October 2011 (pages 649–662)

Figure 14. An outcrop image from a rock quarry in close proximity to the MADE site (Zheng and Gorelick 2003).

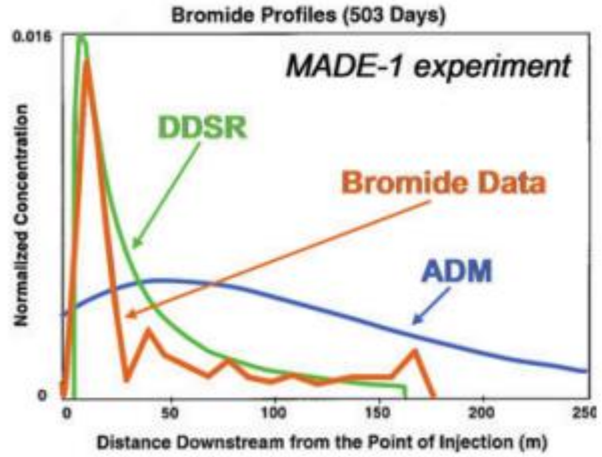
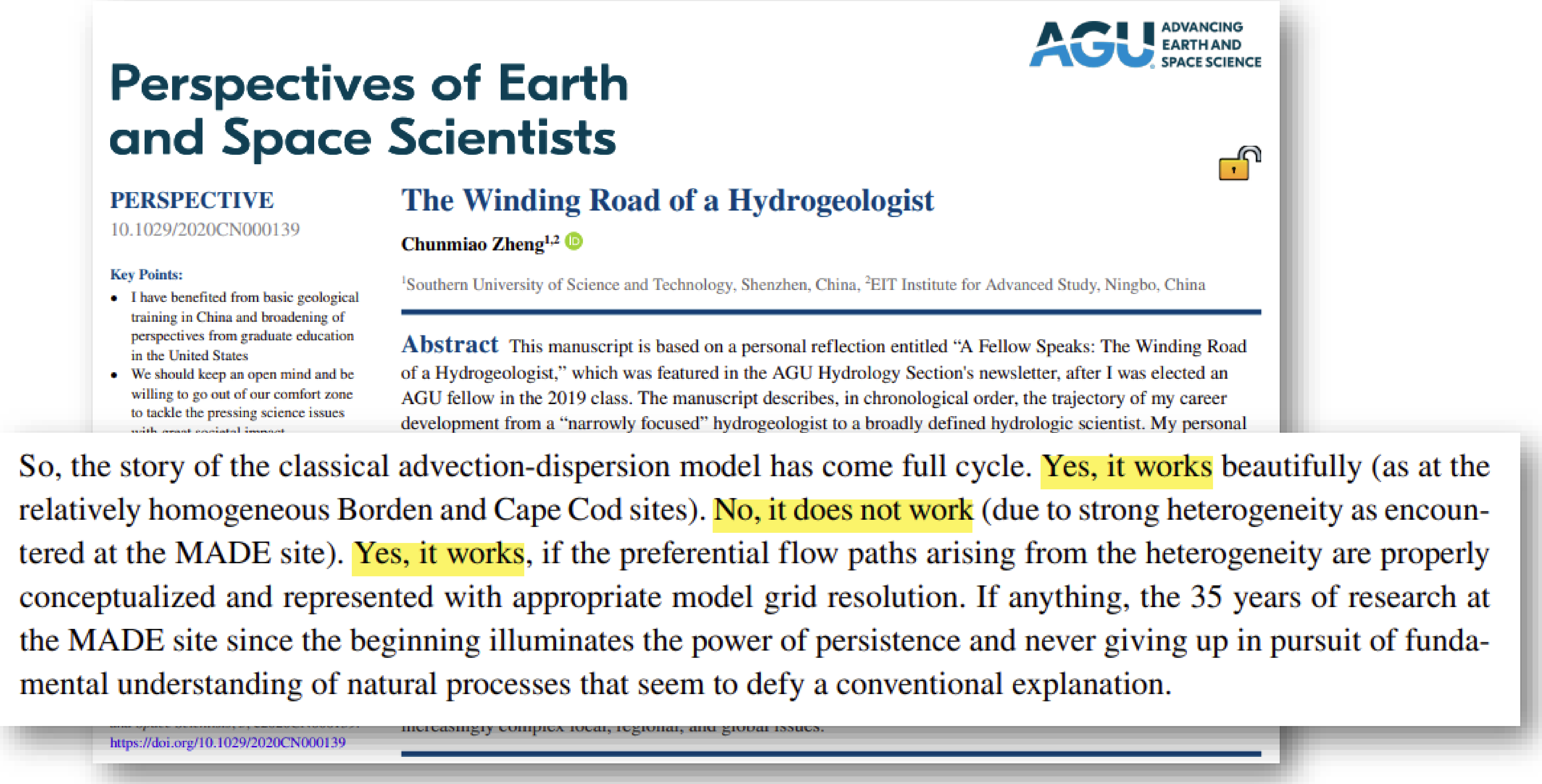


Figure 9. Comparison of model-calculated mass distributions with the field-measured bromide plume for the MADE-1 test at 503 days after the source injection. ADM is the acronym for the classical advection-dispersion model, while DDSR stands for the dual-domain mass transfer model with a single uniform mass transfer rate coefficient.

Reflections



Perspectives of Earth and Space Scientists

AGU ADVANCING EARTH AND SPACE SCIENCE

PERSPECTIVE

10.1029/2020CN000139

Key Points:

- I have benefited from basic geological training in China and broadening of perspectives from graduate education in the United States
- We should keep an open mind and be willing to go out of our comfort zone to tackle the pressing science issues

https://doi.org/10.1029/2020CN000139

The Winding Road of a Hydrogeologist

Chunmiao Zheng[1,2]

[1]Southern University of Science and Technology, Shenzhen, China, [2]EIT Institute for Advanced Study, Ningbo, China

Abstract This manuscript is based on a personal reflection entitled "A Fellow Speaks: The Winding Road of a Hydrogeologist," which was featured in the AGU Hydrology Section's newsletter, after I was elected an AGU fellow in the 2019 class. The manuscript describes, in chronological order, the trajectory of my career development from a "narrowly focused" hydrogeologist to a broadly defined hydrologic scientist. My personal

So, the story of the classical advection-dispersion model has come full cycle. Yes, it works beautifully (as at the relatively homogeneous Borden and Cape Cod sites). No, it does not work (due to strong heterogeneity as encountered at the MADE site). Yes, it works, if the preferential flow paths arising from the heterogeneity are properly conceptualized and represented with appropriate model grid resolution. If anything, the 35 years of research at the MADE site since the beginning illuminates the power of persistence and never giving up in pursuit of fundamental understanding of natural processes that seem to defy a conventional explanation.

Closing Thoughts

- Solute transport codes have evolved to support engineers and practitioners to solve practical problems.
- The role of solute transport codes is anticipated to continue to support remediation challenges, for example, PFAS.
- Solute transport codes are anticipated to adapt to new information and data availability.

Thank you for your time!

Questions?

vivekb@sspa.com