Analytical Solute and Heat Transport Model (ASHTM): Tool to Assist Superfund Oversight

CLU-IN

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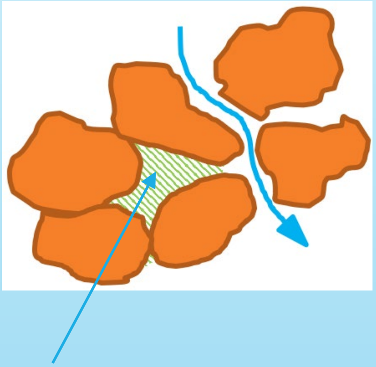
Background

- Oversight of modeling work
  - Limited effort
  - Limited analytical modeling tools available – Stringfellow perchlorate modeling
- Why analytical solute transport model?
  - Exact results for simple geometry
  - Easy to set up
  - Guide selection of transport parameters
  - Simulate general plume behavior (reality check)
  - Verify accuracy of a complex numerical model
  - Simulate smaller scale transport (e.g. tracer tests)

Desired capabilities of analytical solute transport model in oversight role

- Preferably satisfy all:
  - 3D solute transport in aquifer of finite thickness
  - Advection, dispersion, sorption, decay
  - Dual porosity ("effective" porosity = mobile region)
  - Source term with arbitrary time-dependence
  - Sequential decay of multiple species
  - Transport of solute or heat
  - Inverse simulation
- Other capabilities (reactions, heterogeneity) are not easy to include

Dual porosity – groundwater flows through portion of pore space



Stagnant groundwater

New Model

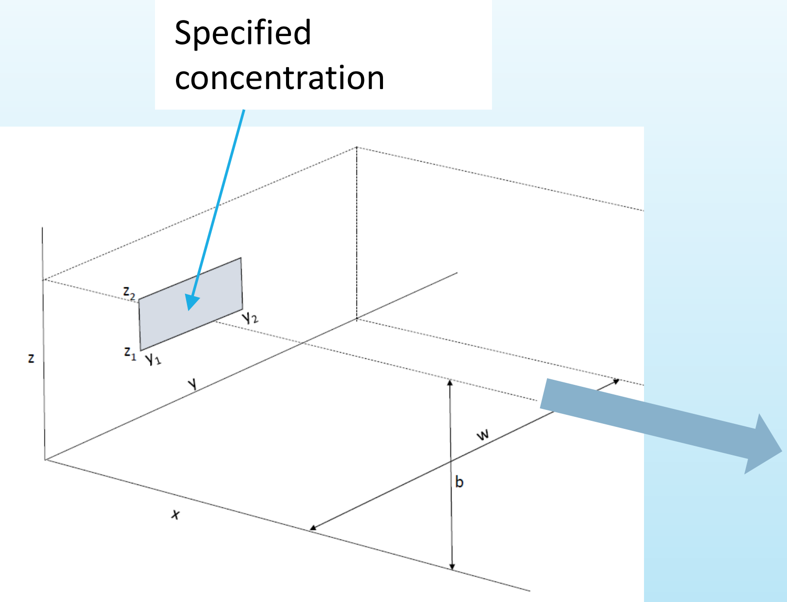
- Governing equations
  - Mobile region $$\frac{\partial}{\partial t}\theta_m C_m + \frac{\partial}{\partial t} f\rho S_m = -\nabla \cdot J_m - (\nabla \cdot \vec{q})\, C_m - \theta_m \lambda_m C_m - f\rho\lambda_{sm} S_m - \alpha\,(C_m - C_i)$$
  - Immobile region $$\frac{\partial}{\partial t}\theta_i C_i + \frac{\partial}{\partial t}(1-f)\,\rho S_i = -\theta_i \lambda_i C_i - (1-f)\,\rho\lambda_{si} S_i + \alpha\,(C_m - C_i)$$
  - Source boundary condition – two different types
  - Sequential decay leads to a system of 2J equations for the J-th species
    - Equations for daughter products have additional terms

Two sorption and four decay coefficients for sorbed/dissolved mass in mobile/immobile domains

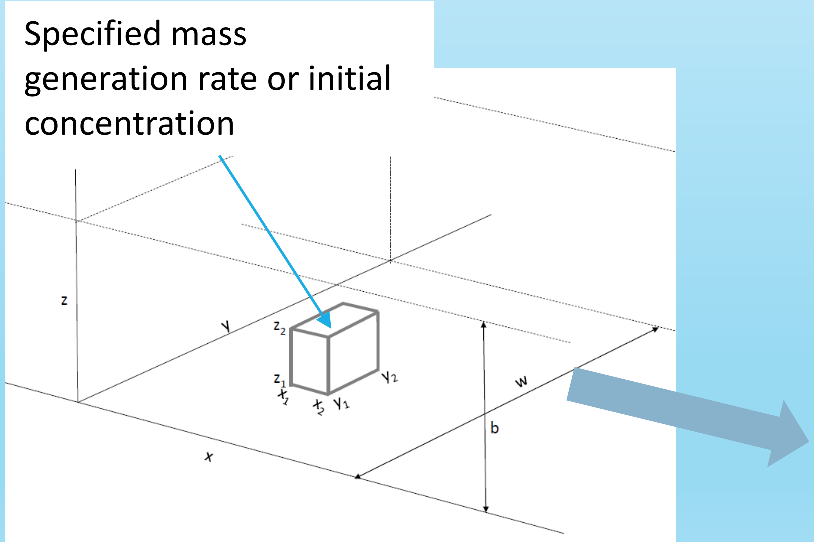
- Solution by integral transforms, numerical inverse Laplace transform
- Heat transport – change of variables
- Special cases – steady state, 1D, single porosity…

Model Domain

- Patch Source
  - Model 1 – Single species
  - Model 3 – Sequentially decaying species

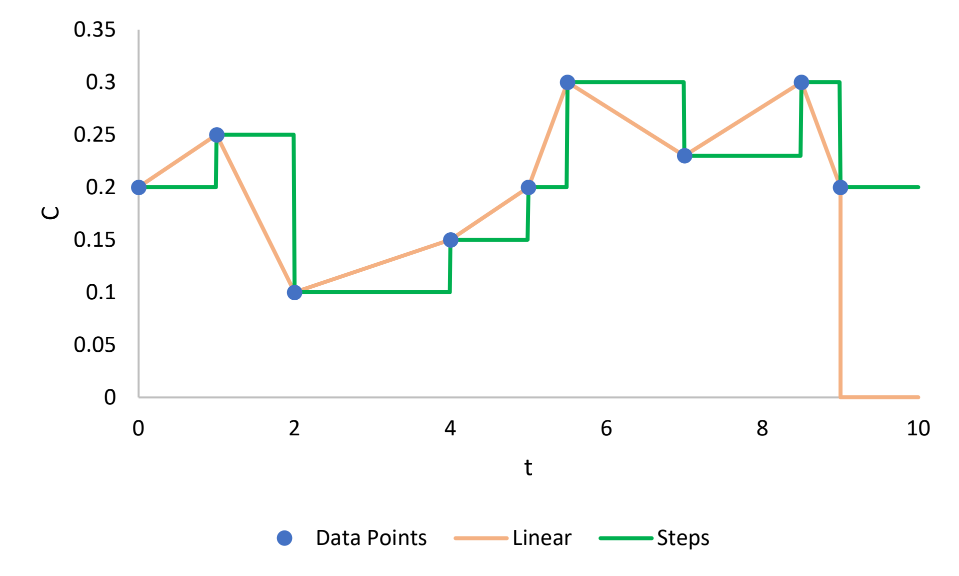


- Volumetric Source
  - Model 2 – Single species
  - Model 4 – Single species, single porosity



Time Dependency of Source Term

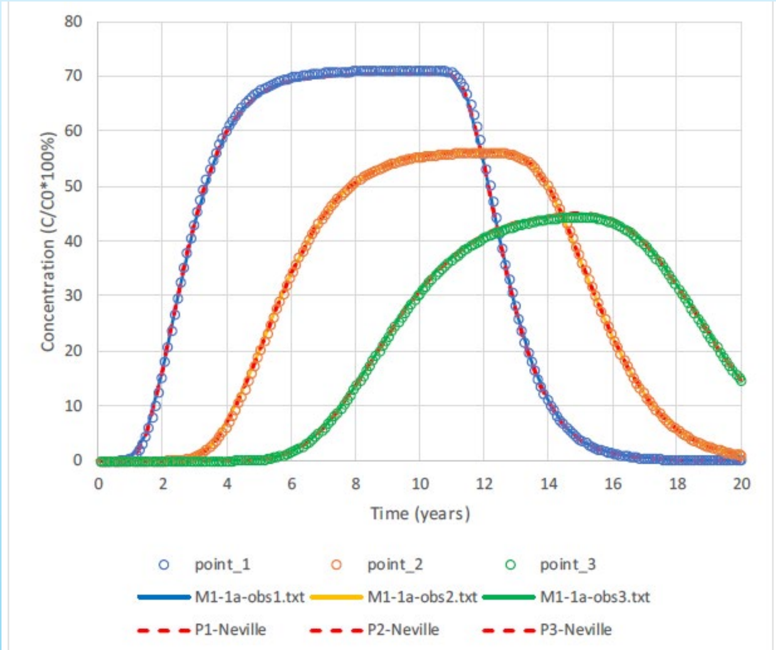
- Constant
- Pulse
- Exponential $C_s(t) = C_0 \exp(\lambda_s t)$
- Shifted sine $C_s(t) = C_0 + C_1 \sin(w_s t - \varphi_s)$
- Line $C_s(t) = a_0 + a_1 t$
- Steps
- Linear interpolation between points



Alternatively: No source and initial concentration/temperature

Benchmark simulations

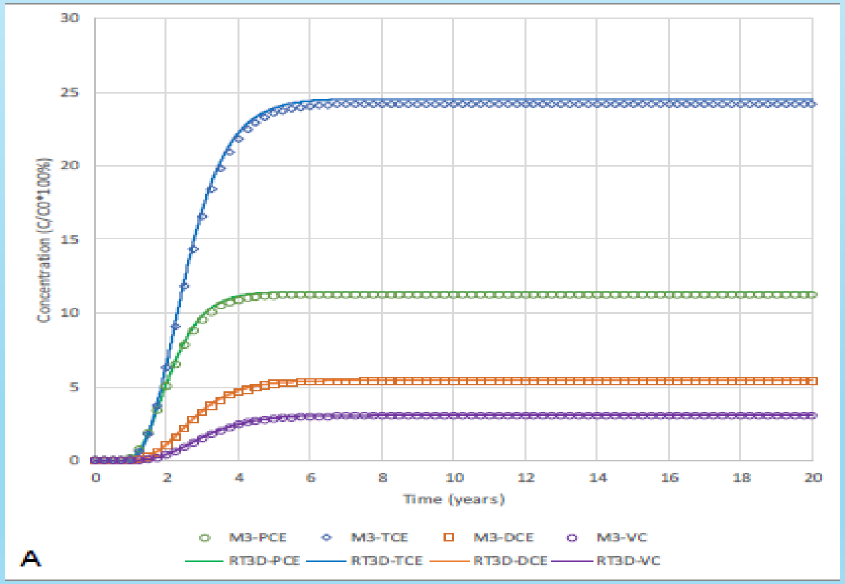
Comparison of Model 1 to MT3DMS, source duration 10 years, dual porosity



Verification simulations - comparison against:

- Existing analytical time-domain models for special cases – Model 1, Model 2
- Numerical models MT3DMS and RT3D – Model 1, 2, 3

Comparison of Model 3 to RT3D for
chain PCE-TCE-DCE-VC with PCE source only



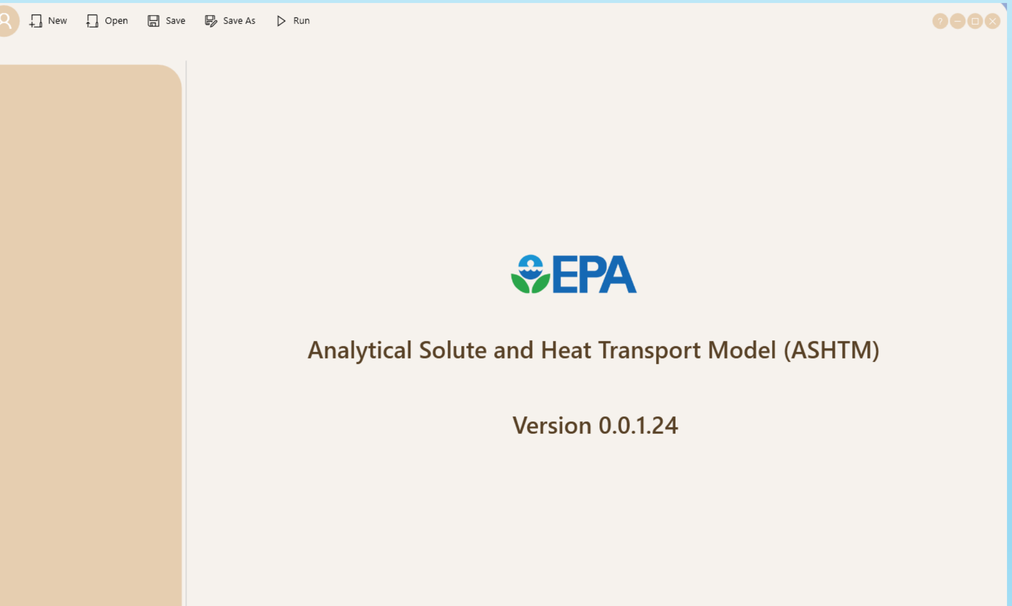
Model publications

- APTIM. 2023. Tracer Test Report Stringfellow Acid Pits Superfund Site Jurupa Valley, California. February.
- APTIM. 2022. Analytical Solute Transport Model Development Report Stringfellow Acid Pits Superfund Site Jurupa Valley, California. May.
- Perina, T. 2022. Semi-analytical model for solute transport in a three-dimensional aquifer with dual porosity and a volumetric source term. Journal of Hydrology 607, 127520. https://doi.org/10.1016/j.jhydrol.2022.127520
- Perina, T. 2021. Semi-analytical three-dimensional solute transport of sequentially decaying species with mobile-immobile regions, sorption, decay, and arbitrary transient source. Mathematical Geosciences, https://doi.org/10.1007/s11004-021-09975-5

Model Execution

GUI

- Create, save, execute, reopen files
- Display output graphically



Standalone executable (*.exe)

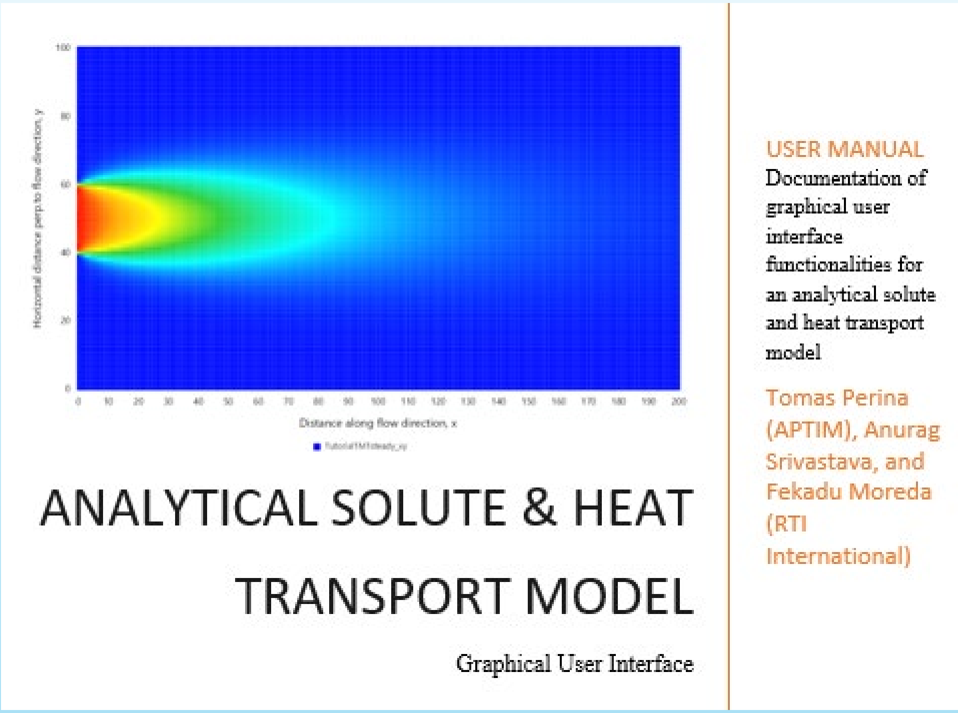
- Command prompt
- Text input/output files
- Template spreadsheet with plots
- Additional models

```
NOTE
Stringfellow Superfund Site - 2022 demonstration tracer test
ENDNOTE

Mode     inverse
INVERSE

AQUIFER
b        29.3
w        10
q        1.0e-6
theta    0.35
phi      0.5
alpha    0.05
Dm       0.00093e-4
ax       1
ay       0.1
az       0.01
lambdai  0.0
lambdais        0.0
lambdam  0.0
lambdams        0.0
Ki       0.0
Km       0.0
```

Model Documentation



- User Manual
  - Instructions for using GUI
  - Instructions for inverse simulation
  - Tutorials
  - Tables
    - Input variables
    - Models, source types
    - Values and units for key input variables
- Analytical Solute Transport Model Development Report, Stringfellow Acid Pits Superfund Site Jurupa Valley, California (APTIM 2022)
  - Detailed derivation of solution
  - Benchmark simulations

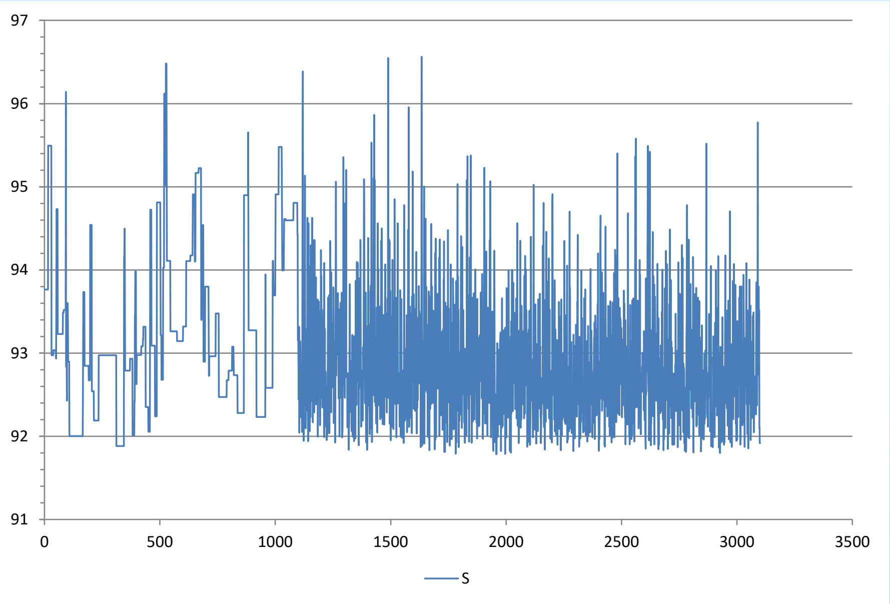
Forward or Inverse Simulation

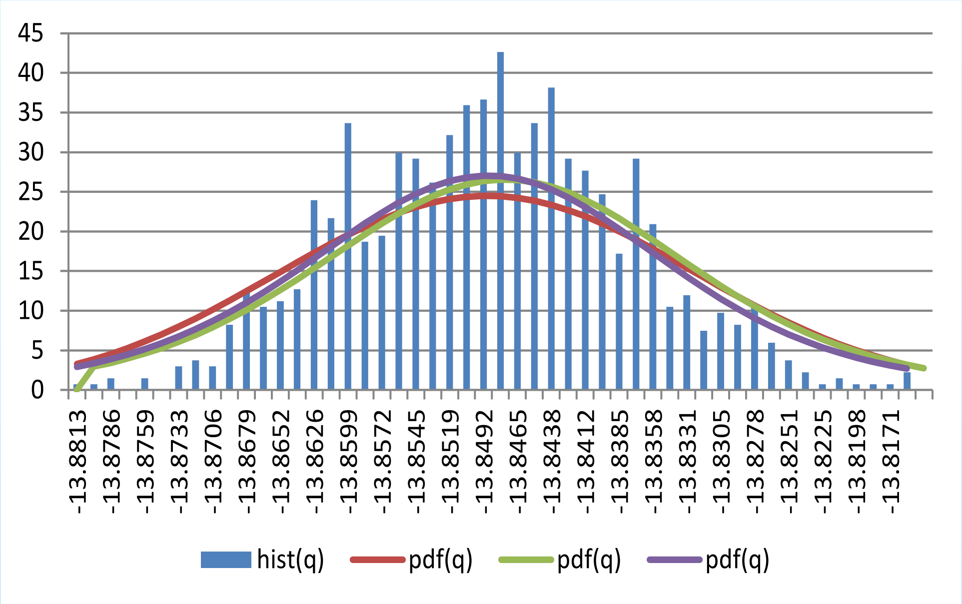
- Forward simulation – all input specified
- Inverse simulation – estimation of selected unknown input variables by matching model computed concentrations to observations
  - Two methods used in sequence:
    - Genetic algorithm
    - Markov Chain Monte Carlo

ASHTM Demo

Inverse simulation – Additional results

Spreadsheet template





Well	Test		N	R2	RMS	ME	AME	ResW
MW6A	MW6A-T		5.00E+01	0.991671	0.017582	0.009363	0.013732	154.567
MW6A	MW6A-C		5.00E+01	0.998844	0.00756	-0.00106	0.004844	28.5796
all data			100	0.995535	0.013533	0.004151	0.009288	183.146

Correlation matrix:			
	q	phi	ax
q	1	0.77954	-5.35E-01
phi	0.77954	1	-0.61761
ax	-0.53525	-0.61761	1

Status and Future Plans

- Finishing GUI and user manual
- Report and beta version executable on CLU-IN website
- Final GUI and manual – August 2024
- Future plans – GUI and code upgrades

Contacts

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