Application of GOTHIC to Groundwater Transport Analysis

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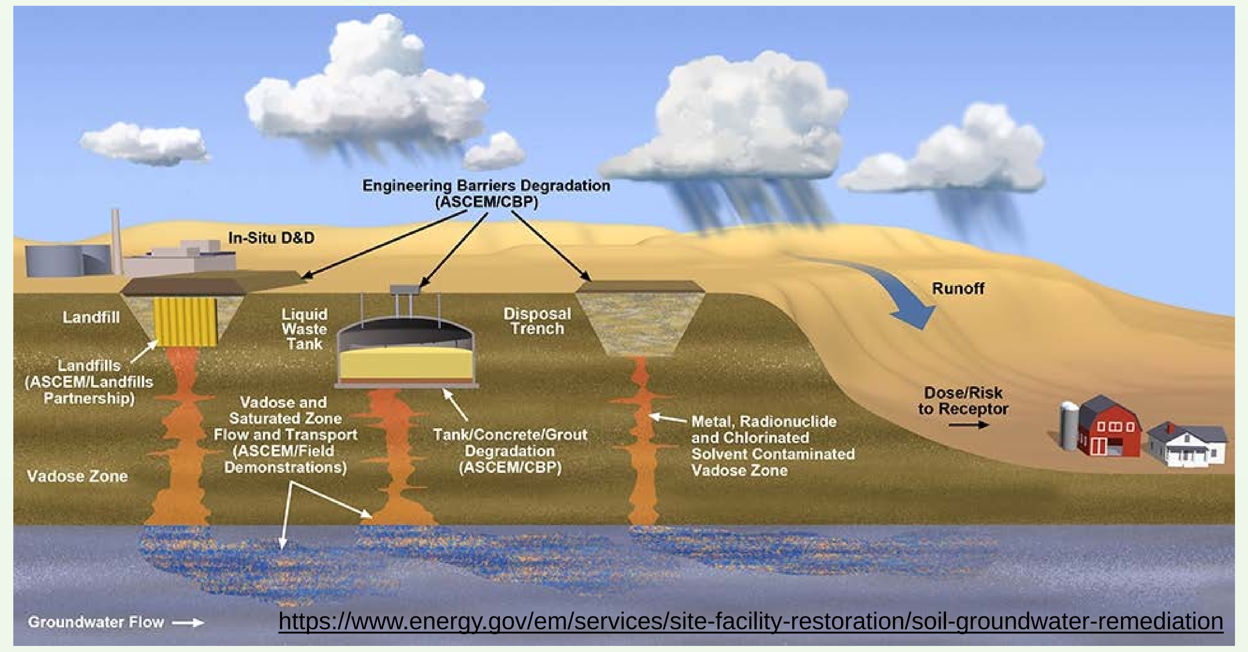
Introduction

Migration of pollutants and hazardous wastes, potentially containing radioactive isotopes, via groundwater transport is a concern at most waste cleanup sites. Predictive analysis tools, such as GOTHIC [1] can be used to evaluate mitigating actions intended to minimize impact on the environment and public exposure.

GOTHIC is a multipurpose thermal hydraulics code that is used extensively in the nuclear industry for design, licensing and operation evaluations. The general porous body modeling approach makes GOTHIC well suited to groundwater transport analysis.

Advantages of using GOTHIC for groundwater transport of nuclear materials:

- Developed and maintained under a Quality Assurance program in compliance with the requirements of 10CFR50 Appendix B [2].
- Tracking of any number of tracer elements for contaminants and other species of interest.
- Radioactive decay and progeny of tracer elements.
- Adsorption/desorption of tracer elements.
- Tracking of any number of dissolved gases.
- Release and absorption of dissolved gases.
- Vapor phase tracking.
- Non-Newtonian fluid modeling.
- Expandable modeling capabilities using custom add-on modules, e.g., groundwater chemistry.



Methods

Adsorption/Desorption: Custom Add-ons can be used to model adsorption and desorption of tracers on surfaces in contact with the groundwater

Chemistry: Custom Add-ons can be used to model groundwater and soil chemistry

Methods – con't

Hydraulic Conductance:

Relationship of flow to pressure field, Darcy's law:

$$q_i = -\sum_{j=1}^{3} K_{ij}\frac{\partial P}{\partial x_j}$$

Average flux velocity components related to average pore velocity:

$$q_i = \varphi_i u_i$$

Assume K_{ij}=0 for i ≠ j ,

$$q_i = -K_i\frac{\partial P}{\partial x_i}$$

q_i = avg. flux velocity, Cartesian direction *i*
K_{ij} = hydraulic conductivity tensor
P = pressure
φ = directionally dependent area porosity

GOTHIC groundwater transport analysis solves for local pore velocity, u_i from momentum balances.

For single phase groundwater flow, effective GOTHIC momentum balance for one direction reduces to:

$$\frac{\partial P}{\partial x_i} = \frac{f(Re_i)}{2D_{h,i}}\rho u_i^2$$

ρ = fluid density
D_h = hydraulic diameter
f(Re) = Reynolds number dependent friction factor

Considering only laminar flow with GOTHIC friction factor add-on:

$$f(Re) = \frac{64\lambda_G}{Re} = \frac{64\lambda_G u}{\rho u D_h}$$

Combining equations:

$$\frac{\partial P}{\partial x_i} = -\frac{64\lambda_G u}{2D_{h,i}^2}u_i = -\frac{32\lambda_G u}{D_{h,i}^2\varphi_i}q_i$$

Which reduces to:

$$K_i = \frac{D_{h,i}^2\varphi_i}{32\lambda_G u}$$

λ_G = specified geometry factor
μ = fluid dynamic viscosity

Diffusion and Dispersion:

Molecular diffusion and mechanical dispersion on flux of contaminant with concentration C can be expressed as:

$$J_i = -\varphi_i(D^m + D_i^M)\frac{\partial C}{\partial x_i}$$

D^m = molecular diffusion coefficient
D_i^M = effective diffusion coefficient for mechanical dispersion in i direction

Contaminants: GOTHIC has two features used to track species:

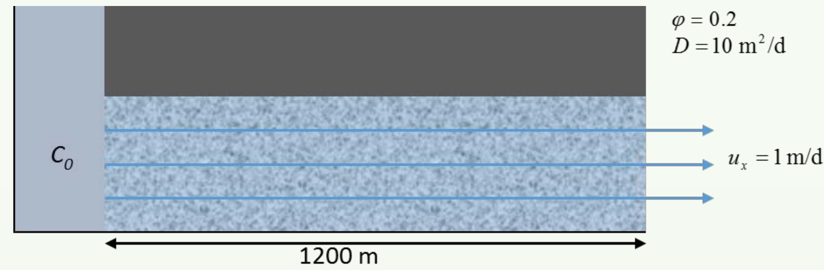
1) Tracers: tracked in liquid and vapor phases and on surfaces, including diffusion, radioactive decay and progeny.
2) Liquid Components: tracked in liquid phase only; component treated as collection of solid particles or dissolved gas.

Verification

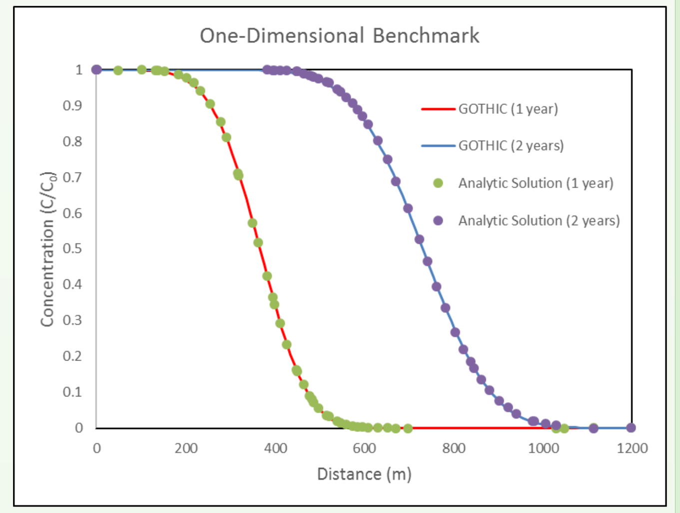
To demonstrate GOTHIC's basic capabilities for groundwater modeling, GOTHIC is benchmarked to one, two and three-dimensional analytic and semi-analytic solutions for contaminant migration:

ONE-DIMENSIONAL BENCHMARK

GOTHIC compared to analytic solution for dispersion of a contaminant in an aquifer from Reference [4] pg 25.



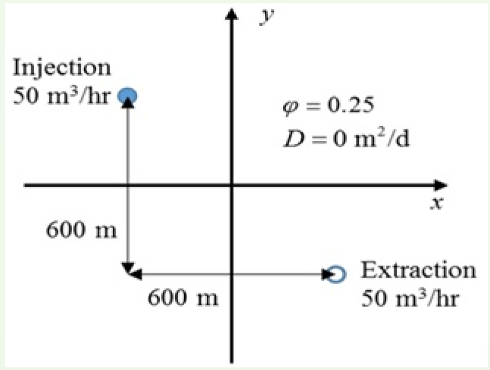
- Aquifer of constant height with a specified constant pore velocity.
- Aquifer initially free of contaminant C and upstream source for groundwater flow has constant contaminant concentration C_0.
- Tracer component specified diffusion coefficient used to model contaminant.
- Groundwater flow modeled using specified inlet and outlet flow boundary conditions.



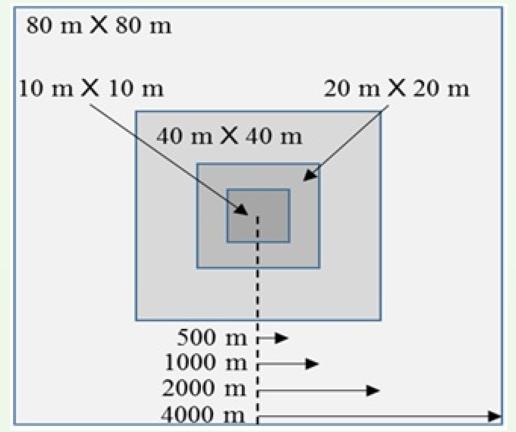
TWO-DIMENSIONAL BENCHMARK

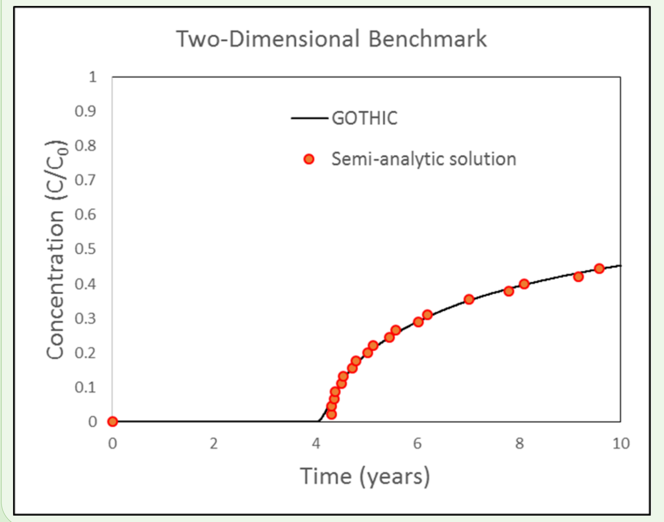
GOTHIC compared to "x-y" aquifer field of constant height with two widely-separated water wells from Reference [4] pg 46.

Problem definition:



GOTHIC Nodalization:





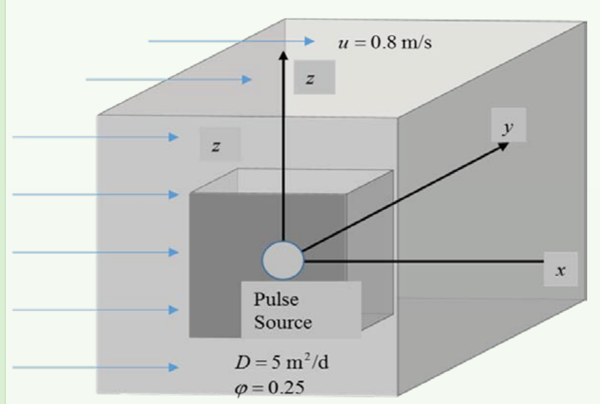
- One well is an injection source of contaminated water and the extraction well removes water at the same volumetric rate as the source.
- Injection and extraction were modeled with inlet and outlet flow boundary conditions.

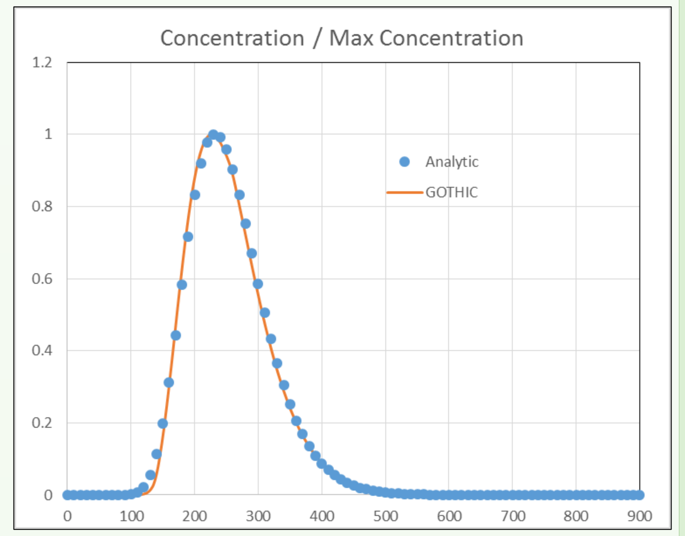
Verification (con't)

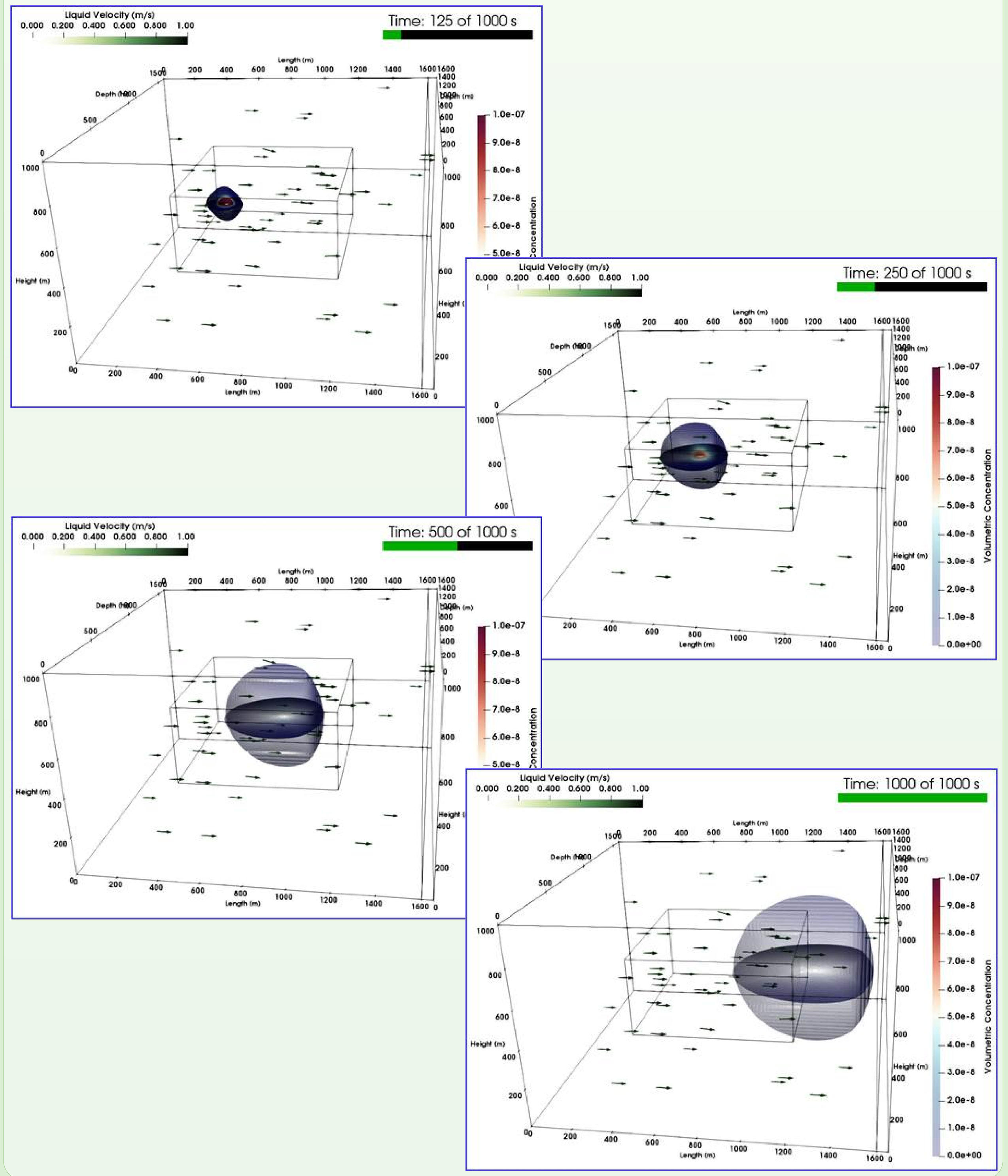
THREE-DIMENSIONAL BENCHMARK

Pulse source in infinite bed with uniform transverse velocity in x-direction from Reference [6].

- Nested grid modeled 1600 m X 1600 m X 1000m region around pulse
- Inner grid has uniform 10 m mesh, outer grid has 20 m mesh.
- Contaminant tracer was injected over a short time interval at beginning of transient.







Conclusions

- GOTHIC results are in good agreement with analytic and semi-analytic solutions.
- The thermal hydraulic modeling software GOTHIC provides extensive modeling capabilities for groundwater transport problems.
- GOTHIC is suited for nuclear industry applications since it is developed, well tested and maintained under a 10CFR Appendix B/NQA-1 Quality Assurance program.
- An add-on feature allows the code to cover situations not directly covered by the base code.
- Incorporating input parameters for diffusion anisotropy factors and direct access to hydrological data sources for setting local media characterization factors (e.g., directionally dependent porosities and diffusion anisotropy factors) enhances usability for additional scenarios.

References

1. GOTHIC Thermal Hydraulic Analysis Package, Version 8.3(QA). EPRI, Palo Alto, CA: 2019.
2. Nuclear Regulatory Commission 10 CFR Part 50, Monitoring the Effectiveness of Maintenance at Nuclear Power Plants, USNRC, 1997.
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4. I. Javandel, et al., Groundwater Transport: Handbook of Mathematical Models, American Geophysical Union, Washington DC, 1984.
5. C.D. Langevin, et al., Documentation for the MODFLOW 6 Groundwater Flow Model: Techniques and Methods 6-A55, U.S. Geological Survey, Reston, VA, 2017.
6. H.F. Hemond and E.J. Fechner-Levy, Chemical Fate and Transport in the Environment, 2nd Ed., Academic Press, San Diego, 2000.

Acknowledgments

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