Application of GOTHIC to Groundwater Transport Analysis – 20152

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ABSTRACT

Migration of pollutants and hazardous wastes, potentially containing radioactive isotopes, via groundwater transport is a concern at most waste cleanup sites. Predictive analysis 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. It combines the capabilities of typical one-dimensional system codes and the essential features of CFD codes for three-dimensional analysis. There are other codes that are specifically developed for groundwater transport analysis and the results presented here are consistent with prior analyses. However, GOTHIC has some unique features that offer advantages for applications related to nuclear waste. Most importantly, it has been developed and maintained under a Quality Assurance program in compliance with the requirements of 10CFR50 Appendix B and applicable portions of ASME NQA-1 since 1995. Available GOTHIC capabilities that make the code especially useful for groundwater transport of nuclear materials include:

- 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 for dissolved gases
- Vapor phase tracking
- Non-Newtonian fluid modeling

The general porous body modeling approach makes GOTHIC well suited to groundwater transport analysis. The multi-region modeling approach used by GOTHIC simplifies model construction for regions of varying hydrologic characteristics and focuses the computational effort on regions of particular interest while simultaneously capturing the macroscopic response and any feedback effects across the larger domain.

The applicability of GOTHIC to groundwater transport applications is demonstrated by comparing code results with available analytic or semi-analytic solutions for groundwater behavior.

INTRODUCTION

Migration of pollutants and hazardous wastes, potentially containing radioactive isotopes, via groundwater (GW) transport is a concern at most waste cleanup sites. Predictive analysis 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. GOTHIC has been developed over 30+ years, with lineage tracing back to FATHOMS, COBRA-NC and COBRA-TF. It can perform transient analysis including compressibility effects with heat and mass transfer. Although GOTHIC was not developed specifically for GW transport analysis, the general porous body modeling approach makes GOTHIC well suited to GW transport analysis. The multi-region modeling approach used by GOTHIC simplifies model construction for regions of varying hydrologic characteristics and focuses the computational effort on regions of particular interest while simultaneously capturing the macroscopic response and any feedback effects across the larger domain. The results presented here demonstrate the applicability of GOTHIC to GW transport analysis.

In addition to the computational capabilities, GOTHIC offers several other advantages for nuclear waste applications. Most importantly, GOTHIC has been developed and maintained under a Quality Assurance program in compliance with the requirements of 10CFR50 Appendix B and applicable portions of ASME NQA-1 since 1995. Ongoing support and error reporting comply with 10CFR Part 21 requirements.

Also, GOTHIC has been used for design & licensing of existing plants, small modular reactors (SMR) and next generation plant designs. As such, it has an established pedigree with verification & validation (V&V) covering a wide range of single and two-phase flow situations, which is documented in the Qualification Report that is updated and released with each version of the software. Applications of the software have been reviewed and accepted by the USNRC for a wide range of scenarios, including:

- Containment analysis, room heat-up (FLEX/ELAP) and equipment qualification (EQ)
- Thermal stratification
- Fluid hammer
- Gas transport in piping systems
- Various spent fuel pool (SFP) applications including cooling and hydrodynamic loads,
- Tracking concentration of hazardous gases and chemicals
- Hydrogen management
- Radioisotope transport

The GOTHIC software is still under active development and there is a large user base both within the US and internationally.

Available GOTHIC capabilities that make the code especially useful for GW transport of nuclear materials include:

- 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 for dissolved gases
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The GOTHIC "add-on" feature allows extensions to the code for special applications. For example, the add-on capability can be used to include chemical kinetics for the tracked tracers. This approach has been successfully used for simulating iodine chemistry in post-accident analysis for nuclear power containment. A similar approach could be used to account for chemistry effects in GW transport.

METHODS

GOTHIC solves a set of time dependent mass, energy and momentum balance equations for vapor, liquid and drop phases for three-dimensional pressure, velocity and energy distribution, including interphase mass, energy and momentum exchange. For GW transport analysis, the drop field is typically not involved and is not included in the discussion below. The vapor phase includes steam and any number of noncondensing gases, some of which may be dissolved in the liquid phase, and may or may not be included in GW transport analysis. The general nature of GOTHIC makes it applicable to GW transport analysis once the correspondence between the dominant physical phenomena are aligned with GOTHIC capabilities and terminology as described below.

Hydraulic Conductance

The usual assumption that relates the flow to the pressure field is the generalized form of Darcy's law,

$$q_i = -\sum_{j=1}^{3} K_{ij} \frac{\partial P}{\partial x_j} \qquad \text{(Eq. 1)}$$

where q_i is the average flux velocity in Cartesian coordinate direction i, K_{ij} is the hydraulic conductivity tensor and P is the pressure. The average flux velocity components are related to the average pore velocity components by

$$q_i = \varphi_i u_i \qquad \text{(Eq. 2)}$$

where φ is the directionaly dependent area porosity.

It is typically assumed that $K_{ij} = 0$ for $i \neq j$ (see, e.g., [2]) so that, Eq. 1 becomes

$$q_i = -K_i \frac{\partial P}{\partial x_i} \qquad \text{(Eq. 3)}$$

In GW transport analysis terminology, GOTHIC solves for the local pore velocity, u_i from a momentum balance that includes the stored momentum (inertia), momentum transport, viscous and turbulent shear, gravitational body force, pressure gradient and wall drag. The viscous and turbulent shear can be ignored by user selected options. All of the other terms are always included but for GW transport applications the inertia and momentum transport are typically small relative to the wall drag and pressure gradient, and effects of the gravitational body force are automatically included in the pressure distribution. Therefore, for single phase GW flow, the effective GOTHIC momentum balance for one direction reduces to

$$\frac{\partial P}{\partial x_i} = -\frac{f(\mathrm{Re}_i)}{2D_{h_i}} \rho u_i^2 \qquad \text{(Eq. 4)}$$

where $f(\mathrm{Re})$ is the Reynolds number dependent friction factor, ρ is the fluid density and D_h is the hydraulic diameter. GOTHIC considers both laminar and turbulent flow when calculating the friction factor. However, the linear relationship between velocity and the pressure gradient in the Darcy model is consistent with only laminar flow. To ensure that only the laminar friction factor is applied in the GOTHIC model, a GOTHIC add-on can be used to replace the normal friction function with one that calculates only a laminar friction factor given by

$$f(\mathrm{Re}) = \frac{64\lambda_G}{\mathrm{Re}} = \frac{64\lambda_G \mu}{\rho u D_h} \qquad \text{(Eq. 5)}$$

where λ_G is a user specified geometry factor (normally 1.0 for pipe flow) and μ is the fluid dynamic viscosity. Combining Equations 2, 4 and 5 gives

$$\frac{\partial P}{\partial x_i} = -\frac{64\lambda_G \mu}{2D_{h_i}^2} u_i = -\frac{32\lambda_G \mu}{D_{h_i}^2 \varphi_i} q_i \qquad \text{(Eq. 6)}$$

Comparing Equations 3 and 6 gives

$$K_i = \frac{D_{h_i}^2 \varphi_i}{32\lambda_G \mu} \qquad \text{(Eq. 7)}$$

Thus, given a specific hydraulic conductivity, the equivalent resistance can be realized in GOTHIC by an appropriate combination of the user input parameters for D_{h_x}, φ_x and λ_G. User control of the direction dependent values for D_h and φ allow for modeling of formations with direction dependent hydraulic conduction.

Contaminants

GW transport is typically concerned with the migration of some contaminant or other species of interest through a porous bed. There are two features in GOTHIC that can be used to track such species; tracers and liquid components.

Any number of user defined tracers can be tracked in the liquid and vapor phases and on surfaces. The tracers have no mass or volume and do not affect the fluid properties. Diffusion, radioactive decay and progeny are included. Except for the diffusion, the tracers move at the same velocity as the carrying fluid.

Any number of liquid components can be tracked in the liquid phase only. Each liquid component is treated as either a collection of solid particles or as a dissolved gas. In both cases, diffusion of the liquid components is included and the mass and energy associated with the components are included in the fluid mass and energy balances, assuming that they are in thermal equilibrium with the fluid. Dissolved gases are absorbed or desorbed depending on the concentration in the fluid and the partial pressure in the contacting vapor phase according to Henry's law. Like the tracers and the dissolved gases, solid particles travel at the liquid velocity except that relative motion in the *z* direction due to buoyancy forces is considered and determined by the user specified inputs for the density, characteristic diameter and drag shape factor for the particles.

For both tracers and liquid components, there are provisions for user specification of local sources and the local initial concentration.

Diffusion and Dispersion

Mechanical dispersion of a contaminant due to the tortuous path of the bulk fluid flow though the porous media is typically assumed to be linearly related to the concentration gradient. The combined effects of molecular diffusion and mechanical dispersion on the flux of a contaminant with concentration *C* then can therefore be expressed as

$$J_i = -\varphi_i \left(D^m + D_i^M\right)\frac{\partial C}{\partial x_i} \qquad \text{(Eq. 8)}$$

where D^m is the molecular diffusion coefficient and D_i^M is the effective diffusion coefficient for the mechanical dispersion in *i* direction.

GOTHIC 8.3 and earlier versions allow for user specification of a single fixed value for the combined diffusion coefficient ($D^m + D_i^M$) for each contaminant that is sufficient for the case of isotropic mechanical dispersion. For the more general case an add-on can be used to provide the directional dependence of the dispersion coefficient.

Adsorption/Desorption

GOTHIC can track the concentration of a tracer on surfaces in contact with the fluid. Adsorption/desorption can be accommodated with an add-on that calculates the source and sink terms for the fluid and the surface. This approach can be used to simulate retardation effects in GW transport and has been used, for example, to model interaction of iodine with organic paint.

Chemistry

GOTHIC includes coupling methodology that allows the code to interact with a separate chemistry module. GOTHIC tracks the local concentration of tracers representing various chemicals and the chemistry model provides the necessary source and sink terms corresponding to the reaction rates.

VERIFICATON

To demonstrate GOTHIC's basic capabilities for GW modeling, one, two and three-dimensional benchmarks of GOTHIC against analytic and semi-analytic solutions for contaminant migration are presented here.

For a one-dimensional benchmark, a GOTHIC solution was compared to an analytic solution for dispersion of a contaminant in an aquifer, as described in [1] p 25. The test consists of an aquifer of constant height with a specified constant pore velocity. The aquifer is initially free of contaminant *C* and the upstream source for the GW flow has a constant contaminant concentration of C_0. Relevant parameters are shown in Fig. 1. A tracer component with the specified diffusion coefficient was used to model the contaminant. The GW flow was modeled using specified inlet and outlet flow boundary conditions.

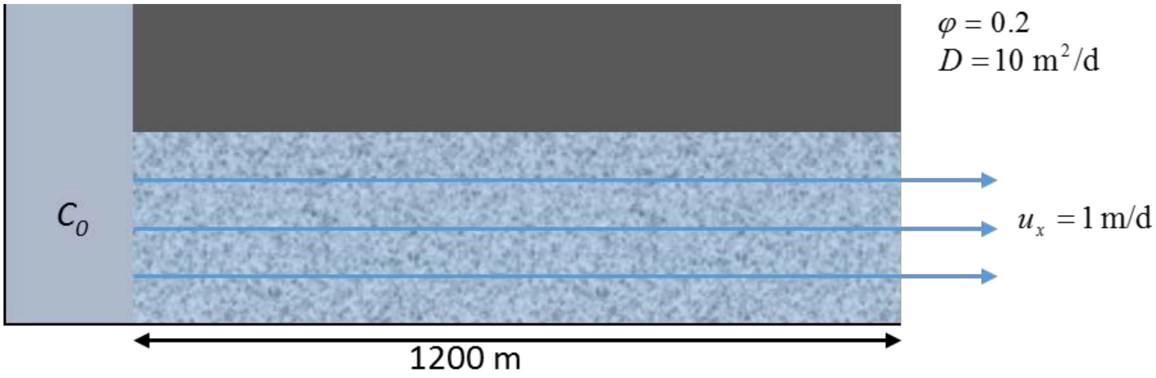

Fig. 1. 1D Dispersion Test

A comparison of the GOTHIC results to the analytic solution is shown in Fig. 2. GOTHIC results are in good agreement with the analytic solution. The uniform grid spacing for this test was 10 m.

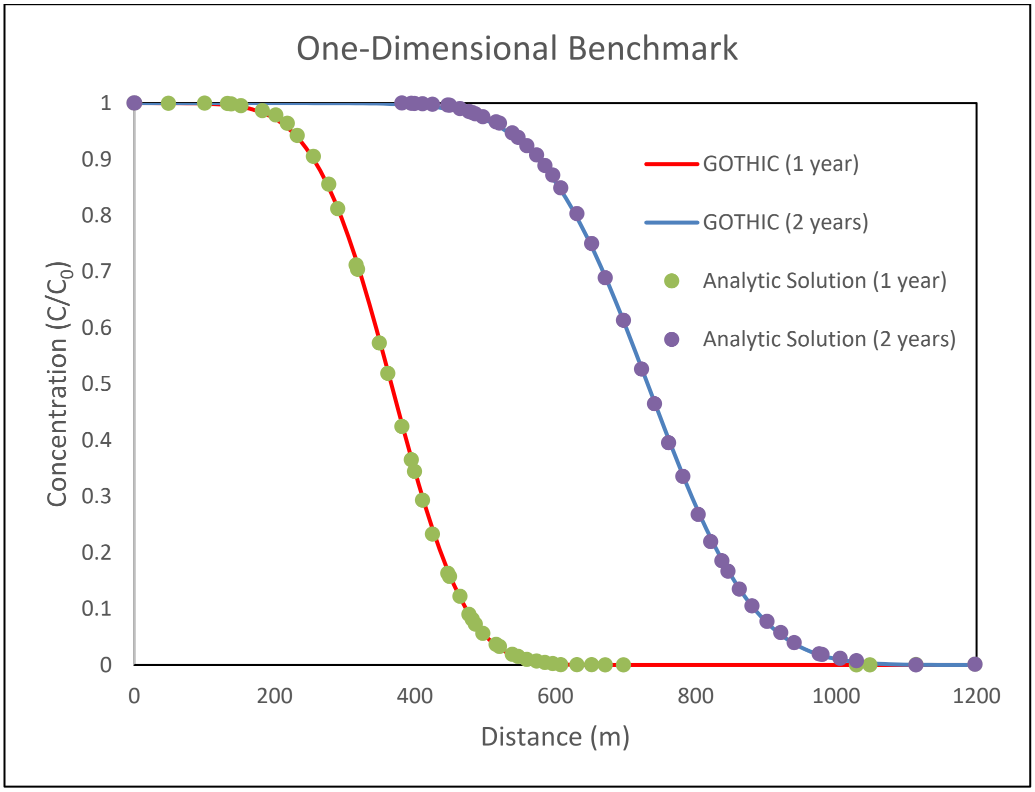

Fig. 2. Comparison of GOTHIC Results with Analytic Solution for 1D Dispersion Test

The two-dimensional test consists of an “x-y” aquifer field of constant height with two widely-separated water wells as described in [1] p 46. One well is an injection source of contaminated water and the extraction well removes water at the same volumetric rate as the source. Relevant parameters are shown in Fig. 3. The injection and extraction were modeled with inlet and outlet flow boundary conditions.

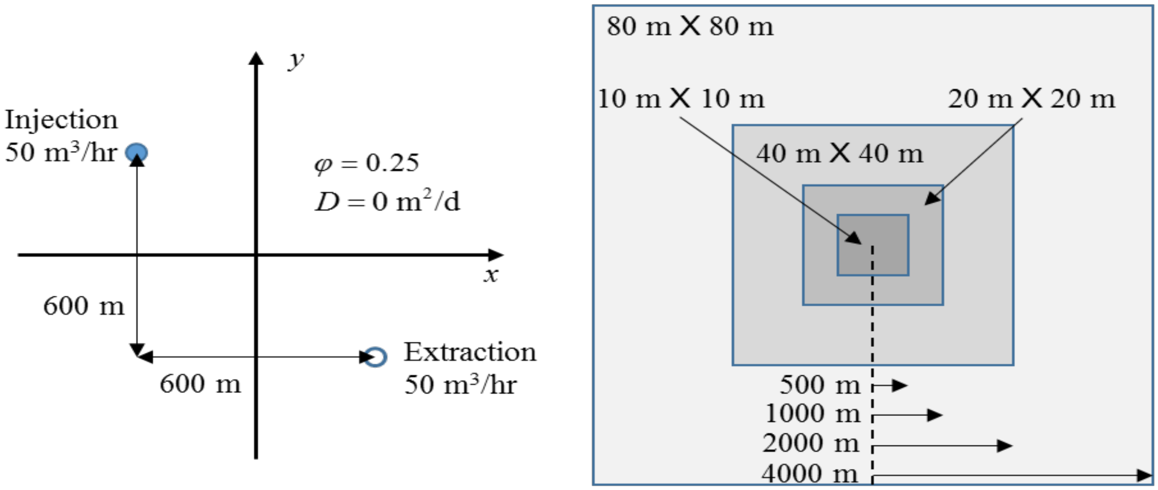

Fig. 3. 2D Injection/Extraction Test

For this analysis a nested grid refinement was used as shown in Fig. 3. A comparison of the GOTHIC results to the semi analytic solution from [1] is shown in Fig. 4. GOTHIC results are in good agreement with the analytic solution. The reported semi-analytic results has some unexpected minor variation, possibly due to nonconvergence of the numerical solution.

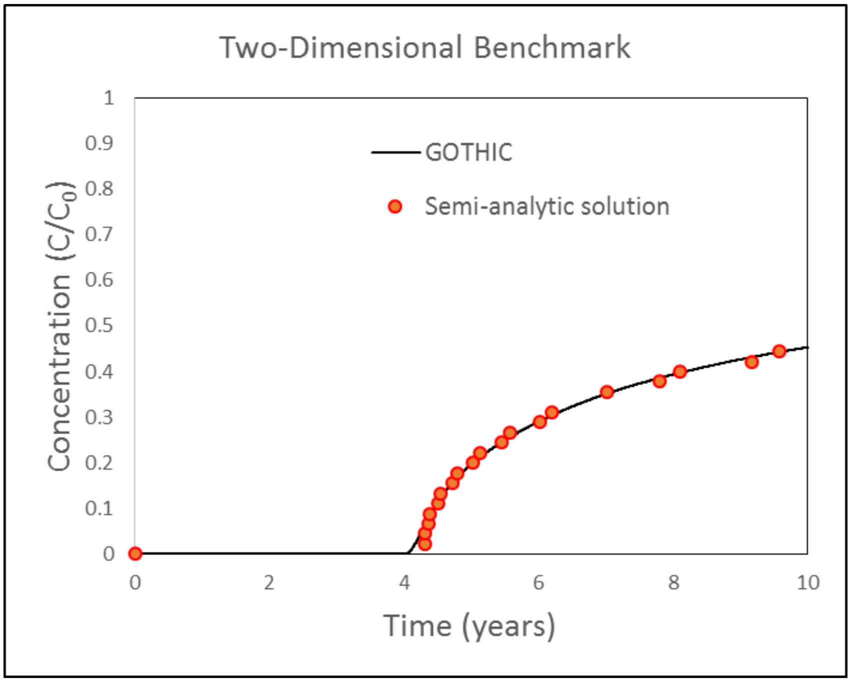

Fig. 4. Comparison of GOTHIC Results with Semi-Analytic Solution for 2D Injection/Extraction Test

The three-dimensional test is for a pulse source in an infinite bed with a uniform transverse velocity in the *x* direction as shown in Fig. 5.

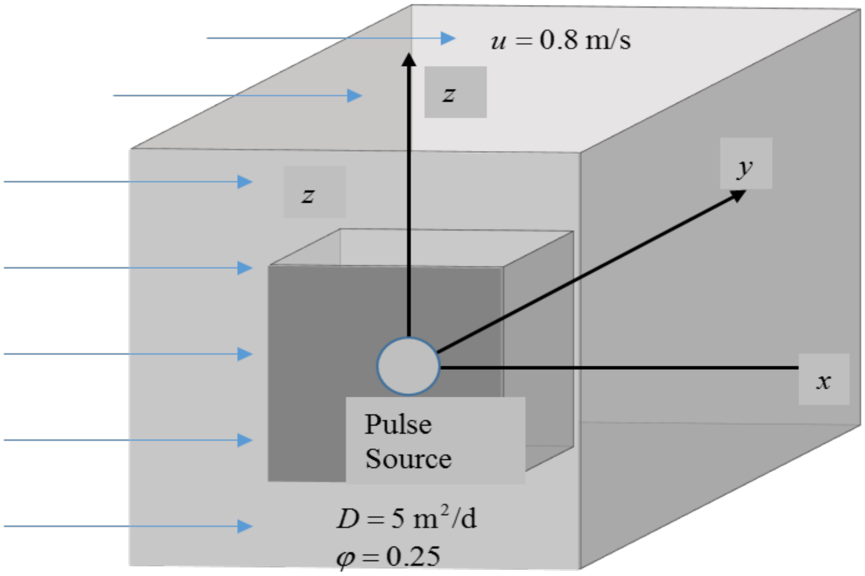

Fig. 5. 3D Pulse Source Test

A nested grid was used to model a 1600 m X 1600 m X 1000 m region around the pulse. The inner grid has a uniform 10 m mesh and outer grid has a 20 m mesh. To simulate the pulse, the contaminant tracer was injected over a short time interval at the beginning of the transient. Results are in good agreement with the analytic solution from [3] as shown in Fig. 6.

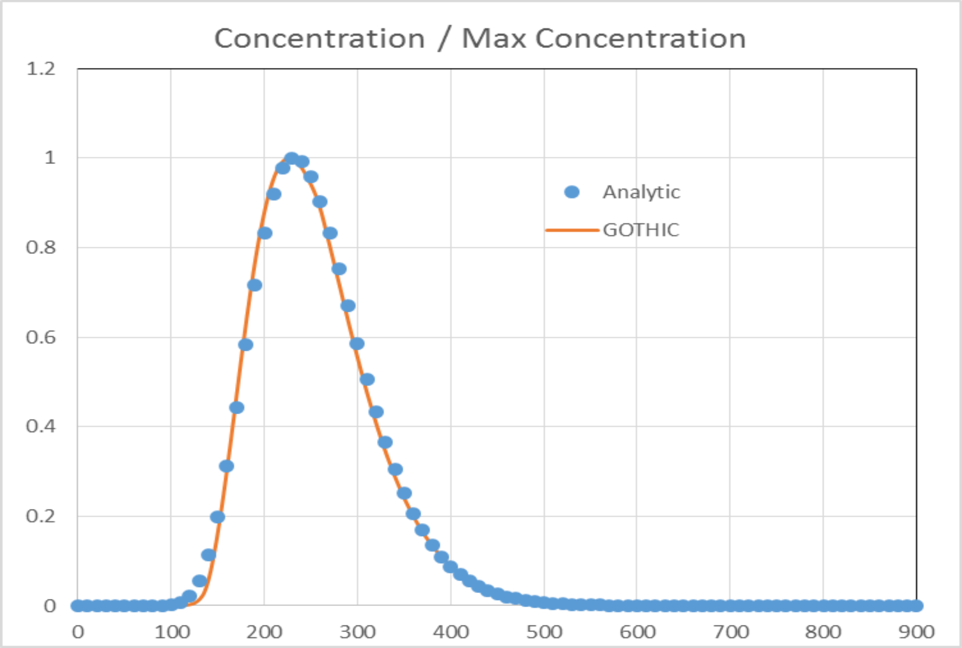

Fig. 6. Comparison of GOTHIC Results with Analytic Solution for a 3D Pulse Source

CONCLUSIONS

The fundamental thermal hydraulic modeling capabilities make GOTHIC applicable to GW transport problems. With development, testing and maintenance under a 10CFR Appendix B/NQA-1 Quality Assurance program, GOTHIC is particularly suited for applications in the nuclear industry. The add-on feature allows extension of the code for situations that are not directly covered by the base code. Usability could be enhanced by 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).

ACKNOWLEDGMENTS

GOTHIC^{TM} incorporates technology developed for the electric power industry under the sponsorship of EPRI, the Electric Power Research Institute.

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