DECOVALEX 2012 – Using Environmental Tracers to Estimate Fracture Network Properties: Bedrichov Tunnel, Czech Republic

Fuel Cycle Research & Development

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Appendix E
FCT Document Cover Sheet

Name/Title of Deliverable/Milestone	Uncertainty Quantification of fractured media flow using Bedrichov Tunnel Experiments (M4FT-12SN0811034)
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This deliverable was prepared in accordance with Sandia National Laboratories
(Participant/National Laboratory Name)

QA program which meets the requirements of
☒ DOE Order 414.1 ☐ NQA-1-2000

This Deliverable was subjected to:

☐ Technical Review	☐ Peer Review
Technical Review (TR)	**Peer Review (PR)**
Review Documentation Provided	**Review Documentation Provided**
☐ Signed TR Report or,	☐ Signed PR Report or,
☐ Signed TR Concurrence Sheet or,	☐ Signed PR Concurrence Sheet or,
☐ Signature of TR Reviewer(s) below	☐ Signature of PR Reviewer(s) below

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N/A

*Note: In some cases there may be a milestone where an item is being fabricated, maintenance is being performed on a facility, or a document is being issued through a formal document control process where it specifically calls out a formal review of the document. In these cases, documentation (e.g., inspection report, maintenance request, work planning package documentation or the documented review of the issued document through the document control process) of the completion of the activity along with the Document Cover Sheet is sufficient to demonstrate achieving the milestone. QRL for such milestones may be also be marked N/A in the work package provided the work package clearly specifies the requirement to use the Document Cover Sheet and provide supporting documentation.

SUMMARY

Environmental tracers are non-applied chemical species present in precipitation with known concentration histories and known decay and production rates in the subsurface. These tracers provide information on the transport characteristics of groundwater systems over a wide range of time scales. The primary goal of this study is to use environmental tracer data from the Bedrichov tunnel experiment to help characterize fracture transport characteristics. Cutting-edge transport theory and computational power will be used to better interpret and utilize environmental tracer information in understanding and predicting fracture network transport. The primary activities accomplish during FY-2012 include attending the DECOVALEX-2012 kick-off meeting and the development of a new set of computational tools for the simulation and utilization environmental tracer data.

DECOVALEX 2012 – USING ENVIRONMENTAL TRACERS TO ESTIMATE FRACTURE NETWORK PROPERTIES: BEDRICHOV TUNNEL, CZECH REPUBLIC

Environmental tracers are non-applied chemical species present in precipitation with known concentration histories and known decay and production rates in the subsurface. These tracers provide information on the transport characteristics of groundwater systems over a wide range of time scales. The primary goal of this study is to use environmental tracer data from the Bedrichov tunnel experiment to help characterize fracture transport characteristics. Cutting-edge transport theory and computational power will be used to better interpret and utilize environmental tracer information in understanding and predicting fracture network transport. The primary activities accomplish during FY-2012 include attending the DECOVALEX-2012 kick-off meeting and the development of a new set of computational tools for the simulation and utilization environmental tracer data.

Methodology:

Interpretation of environmental tracers has proven useful for the conceptualization and parameterization of fracture flow systems. Simplified analytic solutions to the 1-D advection-diffusion models have been used to estimate recharge and fracture spacing [2], and 1-D numerical models have been used to show the effect of matrix diffusion on environmental tracer concentration and groundwater age distribution using parallel fracture networks [3]. However, higher dimensional modeling and or more sophisticated fracture networks have not been used.

Fracture network transport of applied tracers is an area of active research e.g. [5, 1, 4]. However, these studies are concerned with the movement of applied tracers and/or released contamination. Applied tracers have a very limited time range of applicability and even the longest term tracer experiments would be on the order of 10's of years, while travel times in large fracture networks can be over 10^5 years. Making predictions of long term transport over the latter time scale will be highly uncertain using only observations on the former. Improving the interpretation of environmental tracers which can provide information on transport up to 10^8 years will clearly aid when making predictions on the at time scale

The development of massively parallel flow and transport codes has made a new level of computational power available for the simulation and interpretation of fracture network transport, making simulation of multiple environmental tracers in discrete fracture networks possible. In this study information will be extracted from environmental tracers using cutting edge fracture network transport theory and the newest and generation of computational tools.

Results:

The major activities for FY-12 were 1) attendance of the DECOVALEX-2012 workshop and 2) development of the computational framework for simulation and interpretation of environmental tracers. The Bedrichov Tunnel experiment was identified earlier in the year as a possible data set to be utilized for the development of the next generation of tools for interpreting environmental tracer concentration in fractured systems. The DECOVALEX meeting was attended to build connections with the Czech collaborators and assess the quality and availability of the data. The experiment offers a unique ability to sample fracture discharge at depth for many tracers, provide moderate constraints on the fracture network characteristics and there is already data for a suite of environmental tracers. The Bedrichov tunnel data should provide a decent data set for testing the numerical framework.

The majority of the work accomplished during the year was on the development of a high-performance numerical framework for the simulation of multiple environmental tracers and the estimation of groundwater system parameters using environmental tracer data. PFloTran a massively parallel flow and transport code was chosen as the forward simulator. The chemical data base was modified to include the tracers of interest and scripts developed to produce the historical time series of concentration in precipitation for a broad suite of environmental tracers in proper input format. Current tracers included in the framework are ^{3}H, CFC-11, CFC-12, CFC-113, SF_6, ^{3}He and ^{4}He. An example showing modeled concentrations for the year 2012, of the isotopes of helium, ^{3}He and CFC-12 in heterogeneous aquifer discharging to a stream is shown in Figure 1

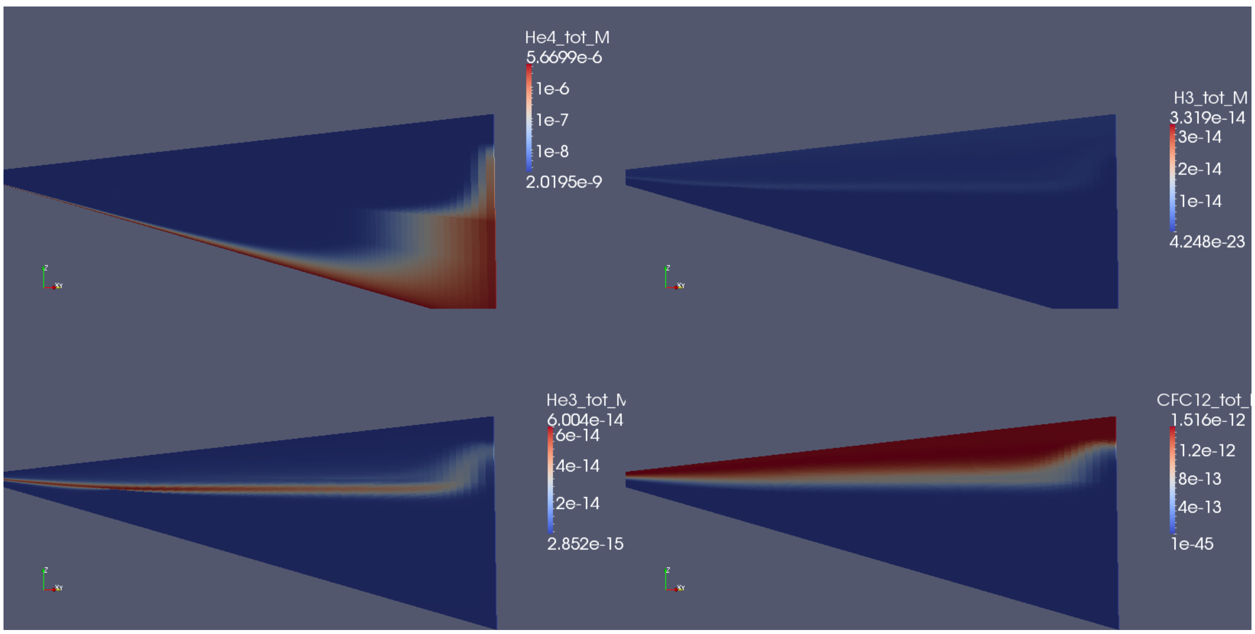

Figure 1 - Modeled helium isotopes, tritium and CFC-12 concentrations for the year 2012 in a heterogeneous aquifer discharging to a stream with recharge across the top.

DAKOTA was coupled to PFloTran to allow estimation of the groundwater system parameters utilizing tracer concentration data. The framework allows for the comparison of a measured time series of tracer concentrations (with a random number of samples and time interval) to the modeled output. In order to fully utilize modern computation power, scripts were developed to use DAKOTA in a nested parallel mode where many concurrent forward simulations PFloTran are called by DAKOTA, while each forward model ran across many processor cores. To date, preliminary inversion tests utilizing synthetic data have shown the ability to determine the hydraulic conductivity of the domain using a time series of tracer data as well as single measurement in time.

While much progress was made in building the fundamental numerical framework, much work remains to be done in order to fully utilize the Bedrichov data. Development of capability for meshing discrete fracture networks is probably the largest task ahead. The development of high quality fracture network meshes and their incorporation into PFloTran is the primary technological hurdle to jump in order to apply the current numerical framework to fractured systems such as the Bedrichov Tunnel. Secondly, a robust parameter and predictive uncertainty methodology must be implemented. Once real data becomes the target of the inversion, smart tools which explore the parameter and resulting predictive uncertainty in a quantitative way are critical to the proper use of the framework. Finally, experimentation with the solute transport modeling paradigm - i.e. full 3-D advection-dispersion vs. Lagrangian particle tracking techniques is another important step. 3-D advection-dispersion is fundamentally more sound, but is much more computational expensive and the trade-offs between the two schemes should be explored.

Conclusion:

The DEVOVALEX Bedrichov Tunnel experiment was identified as a suitable data set to test the use of environmental tracer concentrations in determining fracture network characteristics. These tracers provide powerful information for constraining parameters controlling flow and transport and making better predictions of contaminant transport in fractured network systems. A cutting-edge, powerful numerical framework for extracting information about flow and transport from environmental tracer concentrations was developed. This framework will provide the foundation for the next generation of model development, constraint and transport prediction utilizing environmental tracer concentrations. However, significant technological hurdles remain in place before the current numerical framework can realize its full potential in a fractured system.

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