Employing Laguerre Function Bases To Extend Analytic Transport Solutions to Arbitrary Boundary Conditions: Mathematical Underpinnings of a New Modelling Technique for Multi-component Dissolution with Reactive Transport

Organizer: **Scott Hansen**, Queen's University, 613-214-5154, scott.kalev.hansen@gmail.com

Type: **Oral**

Special Session 1: **Subsurface Biogeochemistry and Reactive Transport Modeling**
Special Session 2: **General Session**

Number of Authors: **2**

1. Scott K. Hansen, Queen's University
2. Bernard H. Kueper, Queen's University

Presenter: **1**

File Uploaded: SUBMITTED

A variety of 1D analytic solutions for reactive contaminant transport in the subsurface are solved in the Laplace domain, and inverted (in practice, numerically) to the time domain; an example commonly used for screening calculations being the 1982 Sudicky-Frind solution for transport in fractured porous media. These models make simplifying assumptions about the contaminant source boundary condition, usually assuming a constant, Heaviside step source. This limits their utility in certain screening settings, such as those concerning multi-component dissolution problems or other situations leading to time-varying contaminant source histories.

We present a new computational method that exploits certain properties of the Laguerre functions to allow existing Laplace-domain analytic solutions to be used to predict concentration profiles and breakthrough curves for arbitrary contaminant source histories, and to do so in a way that is much more elegant and computationally efficient than time-domain superposition. This method employs a class of techniques that invert general Laplace transforms as Laguerre series with numerically computed coefficients, a convolution property of the Laguerre functions, and expansion of arbitrary boundary conditions (i.e. source histories) in the same Laguerre basis as the inverted transform. One obstacle to such an approach is this last step: computing the coefficients for the Laguerre expansion of the boundary condition. Since the Laguerre functions are highly oscillatory, with dense zeros, they resist numerical integration. However, we have developed a novel technique employing discrete Fourier transforms to circumvent this difficulty. This new technique can compute thousands of terms in a Laguerre expansion in a matter of seconds on a personal computer, whereas Mathematica 8 has difficulty beyond about 25 terms.

Underscoring the relevance of this work, we have implemented a screening tool in Python that couples a Raoult's Law-based model for dissolution of multi-component DNAPL residual with the Sudicky-Frind solution for transport in parallel fractures in porous rock. This tool enables analysis of the respective effects of nonlinear dissolution as well as reversible sorption and irreversible decay on the fate of the various DNAPL components. In addition, because of the generality of the method we have developed, it can easily be extended to handle single fractures, porous media, and decay chains. By contrast, the only other coupled dissolution and transport screening tool we are aware of is restricted to LNAPL and porous media.