**Analytical model of three-dimensional multiple** contaminant transport with complex reaction pathways subject to time-dependent source boundary conditions

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## Introduction

Groundwater contamination is an important issue of global concern. Chlorinated solvents such as tetrachloroethene (PCE) and trichloroethene (TCE) have been frequently found as contaminants in groundwater and can produce stepwise degradation compounds, which can be more toxic and mobile. Thus, it is essential to understand the transport processes that affect the contaminant migration in subsurface.

## Motivation

- Mathematical models based on advection-dispersion equations (ADEs) are widely used for understanding plume migration in the subsurface.
- A study of 45 chlorinated solvent sites found that mathematical models were used at 60% of these sites (McGuire et al., 2004).
- The most popular models for coupled multispecies transport is BIOCHLOR (Aziz et al., 2000), however, it only valid for that each contaminant must have the same retardation factor value.
- Recently, Liao et al. (2021) developed exact three dimensional analytical solutions to multi-species transport involving distinct retardation factors.

**Concentration** simulation



## **Mathematical model**



source concentration.



Fig. 1. Development of graphical user interface for three dimensional analytical model.

- Most of multispecies transport analytical models are limited to considering a straight reaction network and a constant source concentration.
- realistic of the behavior • However, transport contaminants may involve both divergent and convergent reactions.



develop analytical model for three-dimensional ΊO reactive transport incorporating the process of complex reaction pathways and time-varying source functions.

solutions and the analytical solutions with a straight chain reaction network.

## Conclusions

This study presents exact analytical solutions to three-dimensional contaminants transport with complex reaction pathway which can provide more realistic for simulating the transport of the contaminants and its degradation-related byproducts. The time-dependent source functions have more practical applicability for matching historical concentration at contaminated sites remediation work. In the future, we will design a friendly graphical user interface (GUI) coupled with the transport and risk assessment models which can greatly enhance the added value of the model and become a popular modeling software.