

A reduced-order model to assist real-time predictions of gas transport in unsaturated fractured media

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Goal: To predict breakthrough of subsurface gas contaminants driven by barometric pumping in fractured media in real-time.

1. Introduction

It is often imperative that we be able to make real-time predictions of gas transport in fractured media. Applications include: shallow CO_2 leakage from carbon sequestration sites, methane leakage from oil and gas operations, radionuclide migration from underground nuclear explosions (UNEs), and remediation of volatile contaminant plumes.

We propose a numerical reduced-order model (ROM) of gas transport in fractured media as a means of reducing computational complexity and allowing quick approximations of gas migration time scales to assist real-time decision-making.

The final product is a software application allowing the user to specify key hydrogeologic parameters and barometric pressure record/forecast to predict gas flux and breakthrough.



Fig. 1: Examples of fractured rock scenarios necessitating gas breakthrough predictions.

2. Barometric Pumping – the driving mechanism

Under certain conditions, barometric pumping enhances gas transport by effectively "ratcheting" the contaminant upwards over multiple atmospheric fluctuation cycles.

Driven by barometric pumping, the time scale of gas transport in fractured media can vary from just days to months or even years. Timescales depend on a variety of hydrogeologic parameters, including: rock type, fracture aperture, matrix permeability, porosity, and saturation. The frequency and amplitude of the barometric signal are also highly important.



3. ROM Development

Our ROM calculates tracer concentration and flux in a 2D single-fracture halfmodel driven by surface pressure fluctuations. We wrap a FEHM (Finite-Element Heat and Mass) multiphase flow and transport simulator within a Python shell, allowing the user to specify key tracer and hydrogeologic parameter values as well as the barometric pressure record.

The code handles mesh generation and domain initialization in addition to solving multiphase gas flow and transport with matrix diffusion and dissolution/volatilization. The code outputs tracer breakthrough as well as molar surface fluxes.



Fig. 2: Conceptual diagram of the barometric pumping mechanism "ratcheting" contaminants upwards over time via advection and multiple micro-scale processes that aid temporary storage.

4. Solution Verification

Two relevant analytical solutions exist from Nilson *et al.* (1991) that we use to validate model performance, and these are included in the software package as benchmark problems.

Flow Verification





Fig. 3: Conceptual diagram of our ROM/tool's workflow.

Early iterations attempted to represent the problem using a statistical ROM such as a MARS/"Earth" model and an artificial neural network. This was done by running a suite of simulations with parameters varied in Latin Hypercube Space, using surface arrival time as a response parameter. Several issues arose:

- Complex, nonlinear correlation among parameters and responses.
- Poor resulting precision of arrival estimates (± 25 days).
- Inability to use real barometric pressure records (had to be simplified to sinusoidal signals).

5. Results

Our numerical ROM can predict gas transport in fractured media on the order of seconds to minutes of simulation time. The model is simplified, but provides valuable end-members for arrival time predictions and assist real-time decision making. The ability to include actual barometric records or forecasts is a significant advantage over a statistical ROM, as the exact timing and duration





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