

## Modelling, Simulation and Risk Assessment for Fractured Geological Media Workshop *March 27-29, 2019*

### **Monica Riva (Politecnico di Milano)**

#### **Sensitivity Analysis and Uncertainty Quantification in Hydrogeology**

We focus on concepts of Sensitivity Analysis (SA) and the ensuing characterization of the way model parameter uncertainties propagate to outputs in the context of hydrogeological modeling. In this sense, we start by recognizing that models can be perceived as (intentionally) streamlined representations of reality and are subject to uncertainty. The latter stems from incomplete knowledge of the physics controlling the evolution of a real subsurface system and their transposition into mathematical formulations, as well as from difficulties of properly defining and characterizing input parameters embedded in such mathematical models.

In this broad context, identifying priorities for the characterization of model parameters and optimizing data acquisition during sampling campaigns for model application should be considered as key elements associated with modern model developments and engineering within an application-oriented framework. Robust sensitivity analyses and uncertainty quantification for a given model are key to accomplish these objectives.

Even as the objectives of a given SA approach can be varied, its most common purpose is the identification of the parameters in a model which are most important/influential. Importance of a parameter can be quantified considering the extent at which perturbations to the parameter affect the magnitude and dynamics of a target model response. Within the broad spectrum of SA techniques, we focus on selected local and global sensitivity analysis approaches. We analyze the way the implementation of a variety of sensitivity analysis tools (local and global) can assist quantification of (a) the relative importance of uncertain model parameters and (b) the ensuing uncertainty of model outputs in the context of relevant environmental scenarios.

## **Gianluca Boccardo (Politecnico di Torino)**

### **Reactive transport in porous media: role of immobile zones, and surface reaction**

A common way to describe transport in porous media is via the classical advection-diffusion equation (ADE), defining the macroscopic dispersion term as Fickian, following the Taylor-Aris model. Nonetheless, data demonstrate that this assumption is not suitable to describe systems subject to tailing effects, nor systems for

which the time scales of interest are much shorter than the characteristic diffusive time (i.e. preasymptotic effects have to be taken into account). Thus, in this work the influence of pore space geometry on solute transport in porous media is investigated performing computational fluid dynamics pore-scale simulations of fluid flow and solute transport. The three-dimensional periodic domains are obtained from three different pore structure configurations, namely, face-centered-cubic (FCC), body-centered-cubic (BCC), and sphere-in-cube (SIC) arrangements of spherical grains. Although transport simulations are performed with media having the same grain size and the same porosity (in FCC and BCC configurations), the resulting breakthrough curves present noteworthy differences, such as enhanced tailing. The cause of such differences is ascribed to the presence of recirculation zones, even at low Reynolds numbers. Various methods to readily identify recirculation zones and quantify their magnitude using pore-scale data are proposed. The information gained from this analysis is then used to define macroscale models able to provide an appropriate description of the observed anomalous transport, and estimate relevant macroscale parameters (hydrodynamic dispersion above all) and their spatial variation in the medium.

Another issue in the definition of macroscopic source terms arises when dealing with particle deposition (i.e. surface reaction). Several computational and semi-analytical models have been studied in the field of colloid filtration to describe this problem, relying on several simplifications regarding both the pore-scale flow complexity and the advection-diffusion interplay, leading to significant errors when used in macroscopic transport equations. In this work we propose an approach clearly separating pore-scale and surface processes, valid when colloidal particles are small enough, and we study Brownian and gravity-driven deposition on a fcc arrangement of spherical grains, and define a robust upscaling based on a linear effective reaction rate.

## **Piotr Łętkowski (Oil and Gas Institute, Krakow)**

### **Coupling geomechanics and reservoir flow models: application to study geomechanical effects upon reservoir performance**

The presentation is devoted to the use of geomechanical - flow coupling to model the impact of geomechanical effects on the behavior of the reservoir. The outline of the presentation incorporates: theoretical remarks, coupling implementation procedure on the example of selected commercial software, preparation of flow and geomechanical models, case study discussion.

## **Hossein Fazeli (University of Nottingham)**

### **CO<sub>2</sub>-Water-Rock interactions in fractured seals**

Fractures are the main flow path in the rocks with very low permeability and their hydrodynamic properties might change due to interaction with the pore fluid or injected fluid. Existence of minerals with different reactivities and along with their spatial distribution can affect the fracture geometry evolution and correspondingly its physical and hydrodynamic properties such as porosity and permeability. In this talk we present results from a series of experimental and numerical studies which investigate the fracture dissolution and fracture sealing in different fractured caprock samples which could be potential caprocks for CO<sub>2</sub> storage sites. The fracture dissolution is triggered by dissolution of minerals with different reactivities which creates altered layer around the fracture which subsequently affect the bulk mineral dissolution rate. For the fracture sealing part, we show results of microfluidic experiments studying the effect of CO<sub>2</sub> phase states on Halite precipitation and how they clog the fractures.

## **Reuben O'Dea (University of Nottingham)**

### **Multiphase and morpho-elastic multiscale models of growing porous media**

The derivation of so-called 'effective descriptions' that explicitly incorporate microscale physics into a macroscopic model has garnered much attention, with popular applications in poroelasticity, and models of the subsurface in particular. More recently, such approaches have been applied to describe the physics of biological tissue. In such applications, a key feature is that the material is active, undergoing both elastic deformation and growth in response to local biophysical/chemical cues. Here, two new macroscale descriptions of drug/nutrient-limited tissue growth are introduced, obtained by means of two-scale asymptotics. First [1,2], a multiphase viscous fluid model is employed to describe the dynamics of a growing tissue within a porous scaffold (of the kind employed in tissue engineering applications) at the microscale. Secondly [3], the coupling between growth and elastic deformation is considered, employing a morpho-elastic description of a growing poroelastic medium. Importantly, in this work, the restrictive assumptions typically made on the underlying model to permit a more straightforward multiscale analysis are relaxed, by considering finite growth and deformation at the pore scale.

[1] Holden, Collis, Brook and O'Dea. A multiphase multiscale model for nutrient limited tissue growth, ANZIAM Journal Volume 59(4) 499-532, 2018

[2] Holden, Chapman, Brook and O'Dea. A simplified multiphase multiscale model for tissue growth. arXiv:1806.09388 , 2018

[3] Collis, Brown, Hubbard and O'Dea. Effective Equations Governing an Active Poroelastic Medium, Proceedings of the Royal Society A. 473, 20160755, 2017

## Eugenio Pescimoro, Deltares

### Modeling Influence of Sediment Heterogeneity on Nutrient Cycling in Streambeds

Rivers and their hyporheic zones play an important role in nutrient cycling. The fate of dissolved inorganic nitrogen is governed by reactions that occur in the water column and streambed sediments. Sediments are heterogeneous both in terms of physical (e.g., hydraulic conductivity) and chemical (e.g., organic carbon content) properties, which influence water residence times and biogeochemical reactions. Yet few modeling studies have explored the effects of both physical and chemical heterogeneity on nutrient transport in the hyporheic zone. In this study, we simulated hyporheic exchange in physically and chemically heterogeneous sediments with binary distributions of sand and silt in a low-gradient meandering river. We analyzed the impact of different silt/sand patterns on dissolved organic carbon, oxygen, nitrate, and ammonium. Our results show that streambeds with a higher volume proportion of silt exhibit lower hyporheic exchange rates but more efficient nitrate removal along flow paths compared to predominantly sandy streambeds. The implication is that hyporheic zones with a mixture of inorganic sands and organic silts have a high capacity to remove nitrate, despite their moderate permeabilities.

## **Chris McDermott, University of Edinburgh**

### **GeoMechanics: Flow Coupling, De-risking the use of Geo-reservoirs**

Coupled processes need to be taken into account in predictive modelling and risk assessment for the exploitation of geo-reservoirs. The geomechanical facies concept offers an approach addressing these challenges by creating a framework facilitating the inclusion of multiple scales of characterisation data, a nested numerical modelling approach, and addressing computationally multi-physics problems in efficient ways. Case study examples are presented including HM coupling at an experimental scale through to reservoir scale, numerical modelling and field data for the KTB site in Germany, and the use of statistical and novel modelling approaches to solve HM(C) problems under laboratory conditions. The relevance of these approaches in terms of risk assessment using FEP approach & surrogate surface concept is demonstrated on hand of a case study for THM stability analysis of CO<sub>2</sub> Storage in the Captain Aquifer, North Sea. This leads to the consideration that the right balance of information is required to improve confidence building in models. Finally new unique state of the art experimental equipment for the investigation of coupled processes under reservoir conditions is presented, with a focus on fluid driven hydraulic fracturing, shear and permeability changes under true triaxial conditions.

## **Florian Doster, Heriot Watt University**

### **Multi-continuum Modelling of Fractured Porous Media**

Fractured porous media play an important role in many different applications. Connected fractures dominate flow-patterns, and their representation is therefore a critical part in model design. The unfractured rock matrix contributes the majority of the pore space and cannot be ignored either.

The explicit representation of fractures in numerical simulators has received significant attention over the last two decades and substantial progress has been achieved. However, for most subsurface applications the explicit representation is still unpractical for two main reasons. The length and time-scales are still too large to allow for a full representation. Reservoir simulation typically relies on 10m size grid blocks. Fracture widths are on the order of mm and smaller and even fracture spacing and lengths on dm to m are important. Second, the detailed properties of fractures such as position, orientation as well as hydromechanical properties are not known. At best, statistical properties and topological structures can be determined from outcrops.

Implicit representations of fractures through multi-continuum approaches therefor remain the gold standard in industry. These approaches represent the fractured porous medium by superimposed porous media that represent fractures and the rock matrix as separate continua that are able to exchange mass through transfer terms. The optimal representation, i.e. when is it possible, how many continua should be used, which fractures should be represented explicitly, what are suitable representations of the transfer processes etc., remains an open question.

In this paper, I will discuss recent achievements with respect to the development of transfer functions and criteria to identify optimal representations of fractures. The developments are based on detailed fine-scaled simulations as well as analytical and quasi-analytical representations. Further, approaches to incorporate additional physics such as poro-elasticity will be discussed.

## **Marco Dentz, Spanish National Research Council**

### **Stable Laws for First Passage Times in Random Fracture Networks**

We study the first passage behavior in the flow through 3-dimensional random fracture networks. Network topology and heterogeneity control the emergence of heavy tailed first passage time distributions. First passage times are constructed as the sum of transition times over hydrodynamically independent network features, and converge toward stable densities with distance from the inlet boundary. Trapping in immobile domains are quantified by a compound Poisson process for the total trapping time. We analyze the preasymptotic first passage behaviors and the evolution toward stable distributions, which are quantified in a systematic way by an unsteady continuous time random walk approach.

## **Xavier Raynaud, SINTEF Digital**

### **Coupled geomechanical simulations in MRST**

In this talk, we will present geomechanical simulations coupled with realistic reservoir flow simulations and filtering processes in fractured porous media. The discretization method of the geomechanical equations is based on Virtual Element Methods (VEM) as we want to handle directly the polyhedral grids that are common in subsurface models. We will briefly review the implementation in MRST and present coupled simulation with black-oil flow models. After a short presentation of our modeling approach for filtering processes and fractured media flow, we will give some details about the implementation framework that has been used in MRST in this context and show 2D and 3D examples on simplified geometries.

## **Marco Iglesias, University of Nottingham**

### **Applications of Ensemble Kalman Inversion: from subsurface environments to composite materials**

The Ensemble Kalman filter (EnKF) developed by Evensen and co-workers in the 1990s has had enormous impact in the geosciences and various engineering disciplines. EnKF has been historically used for data assimilation problems, where the objective is to infer the state of a partially observed dynamic system from observational data. More recently, algorithmic ideas from EnKF have been adapted to solve PDE-constrained inverse problems (i.e. to infer inputs from output of a PDE model) in a derivative-free fashion. In this talk I will discuss recent parameterisations of EKI which enable to infer geometric features of the underlying (unknown) field. I will show the potential advantages of these parameterisations for new application areas which include the non-destructive evaluation of composite materials, the thermal characterisation of building walls, as well as the geological characterisation of the subsurface from geodetic data.