Research Statement

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Porous media are ubiquitous in many areas of applied science and engineering including chemical reactors, aquifer contamination, reservoir engineering, CO_2 sequestration and geothermal energy. Porous media are intrinsically highly complex materials with the consequence that transport phenomena generally occur over a broad spectrum of spatial and temporal scales. The mathematical tools used to represent the physics at these different scales may differ significantly.

My work uses fundamental research on fluid flow and transport in porous media to bridge the gap between the scales and to develop relevant mathematical models and simulation tools at different scales. My research follows a rigorous approach to derive large-scale models based on Darcy's law or variants (usually the scale of interest for engineering applications) from pore-scale physics using consistent averaging techniques. I collaborate closely with experimentalists to validate my models, to get more insights of the different mechanisms involved, and to complement experiments with simulation. My research on porous media applies to very different domains such as chemical engineering (adsorption and distillation processes for air separation units and carbon capture), nuclear engineering (cooling of superconductor magnets), and subsurface engineering (water resources management, CO_2 sequestration, acid stimulation, Enhanced Oil Recovery, unconventional resources).

Current research: Modeling of pore-scale processes associated with the injection and sequestration of CO_2 into the subsurface

Capture and geological storage of CO_2 to reduce carbon emission is among the most critical energy technologies of the next century. My current research in the group of Pr. Hamdi Tchelepi in the Department of Energy Resources Engineering at Stanford University, California is supported by the US Department of Energy through the Center for Nanoscale Controls on Geologic CO_2. It aims at improving our fundamental understanding of the pore-scale processes associated with the injection and sequestration of CO_2 into the subsurface and to assess the long-term issues such as the efficiency of CO_2 retention in reservoir rocks resulting from capillary and dissolution trapping, and from the conversion of dissolved CO_2 to solid carbonate. Interfacial properties and dynamics control fluid flow patterns and trapping by their influence on wetting properties, multiphase fluid and chemical transport, and reactivity. I am interested in developing computational tools to simulate these different processes at the pore-scale, and to translate the results to larger scales. The topic is vast, involving complex physics such as multiphase flow with thin films, mass transfer across interfaces, and the evolution of the pore-space morphology due to reactive mass transfer at the mineral surfaces.

We have developed mathematical and numerical models to efficiently represent dynamics of immiscible CO_2-brine systems at the pore scale. The model, implemented in a Computational Fluid Dynamics software, simulates the mass transfer of CO_2 from the supercritical phase to the brine after ganglia of supercritical CO_2 are trapped in the pore space by capillary effects. We proposed a volume averaging method to translate the information (constitutive relations and governing equations) to larger scales. The methodology can be applied to any kind of multicomponent multiphase flow in heterogeneous porous media. In particular, it can complement and replace micromodel experiments where the use of dye to track the concentration may alter significantly the interfacial properties.

In parallel to this computational effort, we have developed in collaboration with experimentalists (Dr. Sophie Roman and Pr. Tony Kovscek from Stanford University), a micro-Particle Image Velocimetry technique to provide direct visualization and high resolution measurements (2×2 microns vector grid) of the velocity profiles in micromodels [1]. This gives us reference data to validate, quantitatively, the simulations of drainage and imbibition. We also observed and measured dissipative events during two-phase flow experiments such as flow oscillations before and after the passage of the interface and recirculations in the trapped ganglia. The observation of these dissipative events opens new lines of research and further experiments and modeling are scheduled to understand fully their behavior and to characterize their consequences at the different scales.

After injection of CO_2 in deep saline aquifers, the brine is acidified and chemical reactions at the minerals surface, such as dissolution and precipitation can completely reorganize the pore space, *i.e.,* the rock permeability, porosity and effective surface area evolve and consequently impact the flow properties at larger scales. It is very important to characterize the evolution of the rock properties to provide accurate models to reservoir simulators. To tackle this problem, I proposed a micro-continuum formulation based on the Darcy-Brinkman-Stokes equation to simulate dissolution phenomena at the pore-scale [2]. The technique has many advantages compared to classic pore-scale models such as Level-Set or Lattice Boltzmann Methods. In particular, the formulation is multi-scale and the same framework is used for both pore- and core-scale which enables us to simulate the dissolution of a single calcite crystal as well as the emergence of wormholes in a core sample [2]. The numerical model has been successfully compared with experimental observations of the dissolution of a calcite crystal in a microchannel (in collaboration with Dr. Sophie Roman and Pr. Tony Kovscek from Stanford University). By upscaling the simulation results, we showed that hydrodynamics has an order one effect on the large scale dissolution rate and we proposed a correlation that relates flow conditions and mineral properties to the large scale dissolution rate. These results are important to assess the potential CO_2 leakage from the storage reservoir, but also to Enhanced Geothermal System which aims to improve the productivity of a geothermal reservoir by increasing the conductivity of reservoir rock. Indeed, the framework we propose can help to find the best injection rate to get the more efficient ramified wormholes. I am currently working on extending this framework to multiphase flow.

I am also interested in Digital Rock Physics, *i.e.* the computation of rock properties from 3D images of the pore space. Together with the group of Pr. Philippe Gouze in Géosciences Montpellier, France we have proposed a filtering approach [3] to compute the absolute permeability including the smallest length scales that are not always resolved in the acquired images. We showed that for a Berea sandstone imaged with synchrotron micro-CT (ESRF, France) containing only 2% of sub-voxel porosity (below the resolution of the instrument, $3.16\,\mu$m/vx), the permeability estimation can be misled by up to 100% when the micro-scale heterogeneities are ignored. It is planned to repeat the work on different carbonate rocks presenting higher microporosity content and to investigate the impact of microporosity in carbonates on non-fickian behaviors.

Past achievements

Modeling of gas-liquid flow in distillation columns

My Ph.D. research at the Institute of Fluid Mechanics of Toulouse (IMFT), supervised by Pr. Michel Quintard and funded by Air Liquide, concerned the modeling of air distillation and CO_2 absorption columns equipped with structured packing. Such structures maximize the exchange surface between gas and liquid while pressure drops remain low. Due to their peculiar structured geometry, the modeling of the multiphase flow from a macroscopic point of view remains a challenging problem that has to be solved to design enhanced devices. My objective was to develop an original and comprehensive physically-motivated model using a multi-scale analysis to simulate gas-liquid flow and mass transport through the distillation columns.

I adopted a rigorous approach using mathematical tools for changing scales such as the volume averaging method to derive column-scale models from the pore-scale physics. Three main points have been investigated. First, a non-Darcean law that includes inertial and turbulence effects has been derived and the large scale parameters were computed from pore-scale simulations. With this methodology, we can predict the pressure drops directly from pore-scale simulations. Then, to model the liquid spreading, both liquid films, one-per-sheet, were treated separately and upscaled as multi-continua. I have identified the mechanisms that lead to the liquid radial dispersion effects: the main part comes from the geometry itself, the other part is due to the capillary effects at the contact points between adjacent sheets that result in a local redistribution of the liquid from one sheet to the other. The numerical model I proposed accounts for these different mechanisms and simulation results of the liquid distribution have shown a very good agreement with experimental data acquired by tomography imaging within a lab-scale column [4] at IFP Energie Nouvelles.

LHC superconducting magnet cooling with helium superfluid

In collaboration with the European Organization for Nuclear Research (CERN), the Institute of Fluid Mechanics of Toulouse (IMFT) and the French Atomic Research Institute (CEA), I developed a numerical tool to simulate helium superfluid flow in porous media at the pore-scale. Below 2.17 K, helium no longer behaves as a classical fluid: it has almost no viscosity and a high effective thermal conductivity that is used to cool superconducting devices. My main objective was to get more insights in the theory of superfluid helium (He II) in porous media to design enhanced cooling devices for the Large Hadron Collider's magnets, the particle accelerator in Geneva.

The code we developed is the first code that solves the full physics of helium superfluid so far [5]. Two important results have been obtained already. First, we were able to reproduce and explain, for the first time, interesting and unexpected experimental observations about thermal counterflow of He II past a cylinder reported ten years ago in *Nature Physics*. Then, in the case of forced flow of He II, we emphasized that the temperature increase was not only due to the Joules-Thomson effect as it is usually accepted in the cryogenics engineering community but that quantum turbulence also generated a temperature increase of the same order of magnitude that can not be neglected. Based on this new argument, we were able to reproduce very accurетly the temperature profiles obtained in published experiments. This code, released in the public domain, is a powerful tool in the He II community to support new experiments and to design new cooling devices for superconducting magnets and for quantum computers.

Future research

My future research will continue to investigate fundamental fluid flow processes (single phase reactive flow and multi-phase flow) in multi-scale heterogeneous systems by developing novel approaches to model various engineering processes from pore to column/reservoir scales.

I wish to integrate my past experience in Enhanced Geothermal System (EGS) to model efficiently soft stimulation treatment of geothermal reservoir and to assess the potential risk of the technique. This will involve research at the different scales to improve our knowledge of fluid/rock interaction that leads to the formation of ramified wormholes and to propose relevant simulation tools to assist engineering processes. I am very interested in the multidisciplinary and complex aspect of flow and transport in porous media and look forward to collaborate with geochemists, geophysicists, and fluid dynamicists to better understand and characterize processes controlling the permeability enhancement during the stimulation. This will include the integration of microtomography imaging of the rock structure, core-to-field scale measurements into the modeling, coupling with solid mechanics and stochastic upscaling.

I also plan to continue my research activity in the field of carbon capture and storage. One particular research area that I would like to work on in the future is the potential contamination of near-surface aquifers by CO_2 leakage.

References

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