PhD OPPORTUNITIES

University of Nottingham

Multiscale Modelling and Scientific Computing

School of Mathematical Sciences and GeoEnergy Research Centre

Donald Brown, Matteo Icardi and Bagus Muljadi

Interdisciplinary PhD projects involving state-of-the-art numerics, PDE analysis, physical modelling, data-driven Uncertainty Quantification, and experimental methods are available. The projects will have collaborations with the GeoEnergy Research Centre (GERC), Imperial College London, Warwick Mathematics Institute, Heriot-Watt University, British Geological Survey (BGS) and possible linkages and training with industrial partners and international collaborators (Politecnico di Torino, Virginia Tech, Fraunhofer ITWM Kaiserslautern, KAUST).

1) Multiscale Finite Elements for Reactive Transport in Porous Media: The Impacts of Dissolution, Precipitation, and Clogging at the Pore Scale.

Utilizing *multiscale finite elements* in complex pore geometries has been an area of vivid current research. These methods solve local PDE problems at the sub-grid scale to build in geometric information into the coarse-grid basis. However, these methods suppose a fixed rock microstructure and do not include the effects of dissolution, precipitation, or clogging. The key challenge being that solving fully-resolved *microstructural problems* in each coarse block is expensive. One method of attack is to suppose pore scale geometries are parameterized and reduced basis or empirical interpolation methods can be utilized. Linking these parameterizations to physical processes that govern rock surface evolution will be critical in this project. Thus, making a project that is challenging both numerically, but also in terms of physical modelling. This PhD studentship aims to develop efficient techniques to incorporate these higher order effects into multiscale finite elements at the pore-scale. Then, X-ray micro-tomography and nuclear magnetic resonance imaging technologies can probe reactive transport signatures at the pore and core scales and provide the framework for experimental validations. For this project, candidates with experience with numerical methods as well as ability to program in MATLAB or other programming languages would be at an advantage.

2) Numerical Stochastic Homogenisation for Lithium-Ion batteries: First-principles calculation of physical properties via machine learning

The strong uptake of lithium-ion batteries for energy storage is creating new fundamental challenges for the state-of-the-art (SOA) battery models. These are typically defined by *system identification* techniques and fail to capture the intrinsic functional dependence of the parameters on the material attributes and to predict irreversible and complex non-linear phenomena such as fast (dis)charge and degradation. This has therefore limited the transference of battery system requirements from industry to the design challenge of battery components and limited the design challenge of complex control algorithms for increasingly sophisticated Battery Management Systems (BMS), with fast charging and diagnostic capabilities, that rely on physical models. In this project, we propose new mathematical techniques to develop simple and efficient *reduced order models*, as an alternative to classical equivalent circuit models, to enable the fast, yet accurate, simulation of short and long-term behaviour of lithium-ion cells. Starting from the well-known porous electrode theory and Newman's model, we derive and solve simple differential equations that can retain the interesting features of the full model (e.g., solid diffusion, non-linearities). This model can easily be implemented in online battery management systems and can be coupled with advanced data-assimilation techniques. We also propose a new integrated framework to incorporate both micro- and system scale experimental data into our model.

3) Interfacial dynamics and multiphase flows in porous media: Macroscopic limits for wettability and particulate processes

Multiphase flows in porous media present many interesting mathematical challenges. When the fluids are immiscible, there is a free boundary, or '*wetting front'* between the two phases which must be found as part of the solution with surface tensions acting on both the fluid-fluid and fluid-wall interface. This, not only makes the modelling and simulation particularly challenging, but also give rise to complex dynamics of the front, when observed from a macroscopic point of view, that cannot be captured with simplified Darcy-type equations. Similar problems arise when *non-linear processes* (such as agglomeration or complex reactions) are considered between dispersed droplets or particles in the so-called "population balance model".

Considering representative flow configurations on the pore scale, simulations will allow the development of macroscopic theories for the propagation of interfaces through porous media and for effective population balance models. The stationary or equilibrium configurations (balance between imposed pressure gradient and interfacial forces) can be studied and simulated by solving simple "cell-problems" but more difficulties arise in the dynamic setting when the numerical coupled solution of Navier-Stokes and interface transport equations are affected, for example, by numerical instabilities generating 'spurious currents'. Most numerical methods currently fail for this class of flows. This project will address the possibility of defining new mathematical descriptions of the problem, by using a mixed numerical-analytical approach, to overcome some of these limitations and develop new macroscopic descriptions. Statistical techniques will also be employed to characterise the uncertainty and variability of these models and to feed them into real-world large scale simulation scenarios.

Summary: UK/EU students - Tuition Fees paid, and full Stipend at the RCUK rate, which is £14,296 per annum for 2016/17. There will also be some support available for you to claim for conference attendance. The scholarship length will be 3.5 years and the successful applicant will be part of the Energy Research Accelerator at the University of Nottingham (http://www.era.ac.uk).

Eligibility/Entry Requirements: We require an enthusiastic graduate with a 1st class degree in Applied Mathematics (or other highly mathematical field such as Physics or Chemistry), preferably at MMath/MSc level, or an equivalent overseas degree. The projects can be adapted to students' interest and expertise.

Apply: This studentship will start in October 2017. To apply visit http://www.nottingham.ac.uk/pgstudy/apply, select a PhD in Mathematics with supervisors M. Icardi, D. Brown. Send then copy of your CV and application to matteo.icardi@warwick.ac.uk

For any enquiries please email: matteo.icardi@warwick.ac.uk