Project title: Developing effective macroscopic equations for reactive multiphase flow in porous media using thermodynamic and rigorous mathematical principles

Summary: Important energy technologies such as fuel cells and batteries crucially depend on the complex interplay of multiple phases on different scales. The mathematical optimization of complex multiphase systems, e.g. reducing weight and size, increasing storage capacity and life time, crucially depend on reliable, effective macroscopic equations which we shall systematically and rigorously derive and validate by computational experiments. We will start with well-accepted thermodynamic and physical formulations describing the evolution of immiscible fluids in porous materials on the pore scale. Additionally, we account for the transport of species in the aqueous phase. The non-aqueous phase can be for instance a gas or an oil. Our general formulation shall also account for interfacial reactions (e.g. Butler-Volmer reactions) on the pore walls. A major challenge will be how to reliably include fluid flow into the problem without strong restrictions on the validity of the upscaled equations.

Collaborations: The project will foster national and international collaborations, e.g. with Imperial College [S. Kalliadasis G.A. Pavliotis, (Maths)], University of Edinburgh [Ben Goddard (Maths), Prashant Valluri (School of Eng.)], and University of Alberta -Augustana [Peter Berg (Physics)].

The geological CO2 storage is a formidable complex multiphase problem to which we can extend our results towards the forecast of storage capacity of geological formations and the influence and possible consequences of storing CO2 in deep saline aquifers. In this context, the Carbon Capture & Storage Association (CCSA) and UKCCSRC provides a promising platform for collaborations with industrial partners.

PhD Candidate: We are looking for a PhD candidate with degree in Mathematics (Analysis,Probability), Mathematical Physics, or any other equivalent field. The student should be enthusiastic for learning and understanding new concepts and preferably have a fundamental understanding in one of the following fields: analysis, finite element methods, probability theory, statistical mechanics, quantum mechanics

If you are interested, please contact me, Dr. Markus Schmuck, by email (**M.Schmuck@hw.ac.uk**), and apply via the link **http://www.hw.ac.uk/student-life/how-to-apply/postgraduate.htm** after selecting a Funding scheme under the tab Funding on the website **http://www.macs.hw.ac.uk/research/phd/phd-opportunities.htm** and indicate the appropriate funding scheme on your application. Further additional information on my research see my **Personal Web**. The successful candidate will be based at the Maxwell Institute at Heriot-Watt but will closely collaborate with teams at University of Edinburgh and Imperial College London. The successful candidate is also expected to present results at premier conferences in fluid dynamics like the American Physical Society - Division of Fluid Dynamics and British Applied Mathematical Colloqium and publish in premier journals such as Journal of Fluid Mechanics.