Application for a TSM-DTC funded PhD studentship

Please complete this form electronically
and submit to Lilian Wanjohi (l.wanjohi@imperial.ac.uk)
by Friday January 8, 2010

1st supervisor
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Please complete the following:

1. Project title
Multiscale simulation of flow and mineralization of CO_2 for Geological Storage

2. Project abstract (≤ 200 words please and please add 1 or 2 key references)

Sequestration in depleted hydrocarbon reservoirs has long been mooted as the most viable method of storing CO_2 for geological timescales. However, if CO_2 is sequestered in the supercritical form, leaking through rock fractures poses an unknown risk (IPCC SRCCS 2005 9). A possible alternative is mineralizing the CO_2 as calcium carbonate or in other forms. This presents significant scientific and technological challenges. Firstly, the flow and reactions occur over length scales ranging from the kilometer scale of the reservoir down to the micron scale of carbonate rock pores through to the nanometer scale nucleation of the solid phase. Secondly, the process is multiphase and reactive with many unknowns in terms of both the reaction thermodynamics and kinetics. This project will use both state of the art simulation and experimental techniques to first determine the critical process steps and then simulate them for optimization of the fine crystal morphology for flow at the pore / fissure level.
The simulation techniques used will be Lattice Boltzmann at the pore scale (see ref. 1) and continuum hydrodynamics at the fissure / rock scale. The Lattice Boltzmann code will be combined with a front tracking technique (phase field) to simulate both reactive flow and calcium carbonate growth. Many of the parameters are unknown, and MD (classical potential and DFT) techniques will be used as required to determine these. The complex, multiscale structures of the reservoir rock will be characterized via multi-scale tomographic techniques: dual beam focused ion beam for the 10's of nanometer scale and X-ray

microtomography for the micron scale (see e.g. ref.2). We will use in situ experiments to quantify the kinetics of crystal growth and dissolution.

References

1. E.S. Boek and M. Venturoli, ”Lattice-Boltzmann studies of fluid flow in porous media with realistic rock geometries”, *Computers and Mathematics with Applications* (2009), doi:10.1016/j.camwa.2009.08.063
2. Fuloria, D. and Lee, P. D., “An X-ray microtomographic and finite element modeling approach for the prediction of semi-solid deformation behaviour in Al–Cu alloys”, Acta Mat. 57 (2009) 5554–5562. doi:10.1016/j.actamat.2009.07.051

3. What is the multi-scale nature of the project? (≤ 100 words please)
The project is inherently multiscale with the simulation techniques scaling from the sub-micron to reservoir scale. It will also combine state of the art in situ experimental observation techniques for model validation.

4. How do the expertises of the supervisors complement each other? (≤ 100 words please)

Boek is an expert on Lattice-Boltzmann techniques applied to pore scale modeling and petroleum engineering problems, with over 15 years experience working at the Schlumberger Research Centre in Cambridge. Lee is an expert on front tracking simulations (and experimental investigations) of crystal formation at the microstructural scale.

5. Is there a self-contained 12-week MSc project that would usefully initiate this PhD project? (If the answer is no the project will not be offered as an MSc project)

Yes. The initial characterization of the porous structure at a micron scale using XMT and flow simulation using Lattice Boltzmann, with preliminary linkage to the front tracking code, is very appropriate as a 12wk MSc.