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

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Please complete the following:

1. Project title
Multi-scale simulation of asphaltene aggregation and deposition in oilfield operations.

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

Asphaltenes are known as the 'cholesterol' of crude oil. They form nano-aggregates, precipitate, adhere to surfaces, block rock pores and may alter the wetting characteristics of mineral surfaces within the reservoir, hindering oil recovery efficiency. This is a problem of general importance to the oil industry. For instance, in recovery of heavy oil (without CO2), the production of hydrocarbons is often limited by asphaltenes blocking rock pores. Also, asphaltenes often causes oil pipe lines to be blocked, causing "flow assurance" problems.
One example where asphaltene precipitation gives rise to severe asphaltene deposition is the storage and sequestration of CO2 in depleted oil reservoirs, as the solubility of asphaltenes in CO2 is particularly small. Despite a significant research effort, the structure, aggregation and deposition of asphaltenes under flowing conditions remain poorly understood. For this reason, we propose to investigate asphaltenes, their aggregation in CO2 and deposition in capillary flow using multi-scale simulations and experiments. We already

have successfully applied such a multi-scale model to aggregation from solvents such as heptane,[1,2,3] and here we will extend it to CO2.

In this project the effect of in CO_2 on asphaltene aggregation and deposition in a capillary flow environment will be investigated using multi-scale simulations and experiments. Two elements of the multi-scale model have already been developed for aggregation and deposition from solvents such as heptanes (see ref.1), where a mesoscopic flow model for colloidal asphaltene was coupled to atomistic interactions from classical molecular dynamics (MD) simulations. Here we will extend this model to include quantum chemical methods (Hunt) to develop some of the first accurate CO_2 asphaltene interaction potentials. These will be employed in MD simulations of asphaltenes in a CO_2 rich environment (structures determined using the Quantitative Molecular Representation approach developed by Boek, see ref. 2). The simulations will deliver information on the interactions between asphaltene molecules, which will be upscaled to a coarse-grained model that describes mesoscopic scale colloids. At this level, the thermodynamic phase behaviour of the asphaltenes will be elucidated using SAFT techniques (Muller). Finally, the colloidal asphaltene model will be coupled with a dynamic solvent simulation model providing both hydrodynamic and Brownian motion (Boek) to predict aggregation and deposition in capillary flow. Thus this project will produce a well founded and rich model able to describe and tune asphaltene aggregation and deposition in a (confined and flowing) CO_2 rich environment. The model will be evaluated against capillary flow and Small Angle Neutron Scattering experiments (carried out at the Qatar Carbon Capture Storage Research Centre at ICL) of asphaltene aggregation and deposition in supercritical CO_2.

E.S. Boek, J.T. Padding, T. Headen, ”Multi-scale simulation of asphaltene aggregation and deposition in capillary flow”, *Faraday Discussions* **144**, 271-284 (2010).

E.S. Boek, D.S. Yakovlev, T.Headen, ”Quantitative Molecular Representation of asphaltenes and Molecular Dynamics simulation of their aggregation”, *Energy & Fuels* **23**, 1209-1219 (2009).

3. What is the multi-scale nature of the project? (≤ 100 words please)
The project proposed is inherently multi-scale. We will use mesoscopic methods to describe the flow behavior, atomistic classical MD to describe aggregation and quantum chemical methods to determine accurate interaction potentials. We also extend the current model to thermodynamic phase behavior modeling.

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

Boek: Mesoscopic simulation techniques applied to flow at the pore scale, (including SRD and LB) and over 15 years experience in petroleum engineering problems.
Hunt: Quantum mechanics (electronic structure theory: density functional and higher levels), Classical atomistic and ab-initio molecular dynamics simulations of liquids. Experience in the molecular level chemistry of such systems
Muller is an expert on thermodynamic phase behavior and classical MD simulation.

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 student will be given a "taster" from key stages in the project, applying the relevant techniques to a single very simple model system and comparing their results to those in the established literature. Perform high level quantum chemical calculations studying the interaction of CO_2 with a model asphaltene structure. (3 weeks) These will be used to generate an effective semi-empirical intermolecular potential. (2 weeks) Undertake atomistic MD simulations of aggregation in CO_2 , generation of potential of mean force for a model dimer (5 weeks). Literature evaluation of MD applied to asphaltenes and analysis of the data (2 weeks). The literature evaluation will give the student an appreciation of the current state-of-the-art in this field. The full project implements this process for a larger range of species involving more complex interactions.

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[1] E.S. Boek, H.K. Ladva, J.P. Crawshaw and J.T. Padding, □Deposition of colloidal asphaltene in capillary flow: experiments and mesoscopic simulation□, *Energy & Fuels* **22** 805-813 (2008).
[2] E.S. Boek, A.D. Wilson, J.T. Padding, T.Headen and J.P. Crawshaw □Multi-scale simulation and experimental studies of asphaltene aggregation and deposition in capillary flow□ accepted for publication in *Energy & Fuels* (2009).
[3] E.S. Boek, J.T. Padding, T. Headen, □Multi-scale simulation of asphaltene aggregation and deposition in capillary flow□, *Faraday Discussions* **144**, 271-284 (2010).