NERC Centre for Doctoral Training in Oil & Gas (2018 start)

Project Title: Modelling Immersion Enthalpies and Contact Angles for Improved Multiscale Enhanced Oil Recovery Simulation

Host institution: Durham University

Supervisor 1: Prof. H. Chris Greenwell (Earth Sciences)

Supervisor 2: Dr M. Degiacomi (Chemistry)

Additional Supervisors: Dr I. Collins (BP); Dr R. Anderson (STFC); Dr E. Pyzer-Knapp (IBM)

Project description: Understanding enhanced oil recovery using low salinity water floods presents a challenge to multi-scale modelling. While results need to be understood at a field scale, the initial release of oil is governed by nanoscale interactions at mineral surfaces in the reservoir and transport by micron scale interactions. In particular, interactions at the nanoscale are very hard to robustly determine for molecular/atomistic level models. In this research we will determine these interaction parameters using artificial intelligence, algorithms that will iteratively run two different sets of theoretical "experiment" to determine wettability and then use large-scale data processing to refine model parameters until both these experiments give consistent answers for each mineral interface of study. Molecular models will be built of mineral surfaces (kaolinite, quartz, montmorillonite) and both the contact angle of water/oil droplets and the immersion enthalpy calculated in two different sets of simulations. As these quantities can be related to each other, then they provide a way of consistently checking the parameters used to describe the mineral/water/oil interactions. Initially, model surfaces, e.g. mica, will be used where there are abundant experimental data to work from. Having developed a unique parameter set, we will use this to calculate relevant wetting parameters for a range of oilfield relevant mineral surfaces.

CDT Research theme(s): The proposed research mainly falls into the following two research themes: (i) **Extending the life of mature basins:** Enhanced oil recovery (EOR) will allow increased hydrocarbon recovery. Low salinity methods are particularly efficient and environmentally friendly as no further chemicals are added. (ii) **Effective production of unconventional hydrocarbons:** Understanding the parameters controlling immobile oil, vs expelled and mobile oil are critical to understanding the resource in unconventional reservoirs, and hence the production potential.

Research context: The Greenwell group has been working with BP on understanding low salinity enhanced oil recovery for the last 5 years, and has published 5 high impact papers in this to date. This project builds on the work of Dr Tom Underwood, a former PhD student, now at Princeton University, USA. Under an EPSRC IAA award, Dr Underwood developed the proof of concept work for this present PhD application. The applicant will fit within 4 other PhD researchers working on geological/laboratory based experiments on EOR and will have excellent training and collaborative opportunities. In addition, the applicant will gain skills in software development and computational chemistry from the group of Degiacomi, and high performance computing and advanced data analyses from STFC/IBM. The Greenwell group has established collaborations with both to characterize interactions between clay surfaces and soft matter.

Research costs: The student will make extensive use of the Hamilton high performance computer at Durham, as well as computing resources at STFC Hartree Centre. The main costs will be travel and Subsistence for conferences and visits to the Hartree Centre. The £5K per annum RTSG will cover these.

Career routes: The last two PhD students working in this area in the Greenwell Group were offered PDRA posts at prestigious US Universities (Stanford and Princeton) before they had graduated; academia is an obvious route (Physics/Chemistry/Geoscience). BP have expressed in recruiting past PhDs, and data science routes (eg via STFC and IBM), oilfield, stochastic modelling (financial), environmental consultancy and other numerate careers are also possible.