Catalytic conversion of syngas to oxygenates for the efficient upgrading of biogas

- **Supervisors:** Dr Kechagiopoulos
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- **Deadline:** Sunday, April 15, 2018

Project Description

Focus of this PhD project will be on the efficient upgrading of biogas, produced from anaerobic digestion, towards oxygenates. Biogas, consisting of methane and carbon dioxide at roughly 60-40% concentration, is a promising source for oxygenates production via its conversion to syngas by dry reforming, utilising as such the entire biomass carbon-content and resulting in drastically reduced carbon footprint for the overall process. The typically aimed at oxygenate from syngas is methanol using Cu based catalysts, with the product potentially further dehydrated to dimethyl ether (DME) over solid acids. However, using noble metals such as Rh or modified methanol and Fischer–Tropsch synthesis catalysts the targeted production of higher alcohols, namely ethanol, has attracted significant research interest as well.

While methane reforming is a fairly established technology, a variety of challenges still need to be addressed to effectively convert syngas to oxygenates and obtain an energy efficient and modular system that is flexible in its feed. Particularly when the entire anaerobic digestion-to-syngas process is considered, the adaptability of the oxygenates synthesis to the H_2/CO stoichiometry and syngas pressure, determined by the reforming step, are key issues to tackle, while achieving high conversions at low-pressure is critical from an economic feasibility point. More importantly, the ability to selectively produce higher alcohols, minimising the production of hydrocarbons, given the above constrains, remains a challenge that requires a considerable theoretical understanding to be developed.

The project will address these challenges specifically via the development of comprehensive micro-kinetic models for oxygenates synthesis, aiming at the clarification of the role of surface species in the production of the observed products and the discrimination of pathways that predominantly lead to oxygenates versus unselective hydrocarbons. The work will benefit from available existing experimental data, but will further be supported by targeted experimentation where needed. During model development special attention will be devoted on the *a priori* determination of thermodynamic and kinetic parameters using a variety of theoretical methods, such as transition state and collision theories, UBI-QEP calculations and Brønsted–Evans–Polanyi relationships. Through the correlation of model parameters to selected (atomic) chemisorption enthalpies, the elucidation of mechanistic features over different catalysts will be achieved, opening the road towards the selective production of specific oxygenates.

The excellent research facilities and world-class expertise will provide a very attractive opportunity for a highly motivated PhD student looking to progress a career in the exciting field of chemical reaction engineering and heterogeneous catalysis.

Selection will be made on the basis of academic merit. The successful candidate should have, or expect to obtain, a UK Honours degree at 2.1 or above (or equivalent) in Chemical Engineering or other relevant discipline and, preferably, have the below skills:

- Knowledge in reaction kinetics analysis and/or kinetic and reactor modelling.
- Experience in programming using e.g. FORTRAN or MATLAB.
- Experience in the operation of experimental apparatus and/or in the preparation and characterization of catalysts.
- Familiarity with methane conversion processes.

Funding Notes

Leverhulme Doctoral Scholars will receive maintenance costs at Research Council rates and tuition fees at the rate for UK/EU students. In 2017-18 the maintenance grant for full-time students was £14,533 per annum. International applicants who can pay the difference between the Home and International Fees would also be welcome to apply.

APPLICATION PROCEDURE: Formal applications can be completed online: https://www.abdn.ac.uk/pgap/login.php

- Apply for the Degree of Doctor of Philosophy in Chemical Engineering
- State the name of the lead supervisor as the Name of Proposed Supervisor
- State 'Leverhulme CDT in Sustainable Production of Chemicals and Materials' as the Intended Source of Funding
- State the exact project title on the application form