Master thesis proposal spring 2018

Sustainability of phase-change solvents for CO2 capture: benefits and disadvantages from sustainability perspective

Project description
With the CO₂ concentration hitting the 400ppm record and continuing to grow, the battle against global warming seems to be lost. The need for climate change mitigation technologies has never been so urgent. According to IPPC Carbon Capture and Storage (CSS) is one of the essential technologies to mitigate climate change. However, among all the abatement techniques CO2 capture might be the most debatable one. The necessity of its usage seems to be inevitable while the high cost creates a significant barrier to acceptance and industrial application.

Post-combustion capture of CO2 by chemical absorption is the most mature of CO2 capture technologies. The main obstacle for optimization of the technology is the high energy demand for solvent regeneration. Careful selection of solvents can significantly improve the performance of the system in terms of energy requirement and cost. A new class, the phase-change solvents, seem to be a promising alternative to conventional solvents because they can be partly recovered before the thermal regeneration stripping process, which is the main driver of the cost. Processes utilizing phase -changed solvents were reported to be able to operate with energy demands as low as 2.1 GJ/ton of CO2 [1].

While a significant amount of research focuses on physical and operational properties of phase-change solvents, there is very little work done on safety, health and environmental (SHE) hazard assessment of these.

Task description
- Extensive literature screening to create a knowledge database (or knowledge synthesis) on SHE hazards of phase changing solvents
- Modifying/adjusting existing frameworks for SHE hazards of conventional solvents to a custom tailored one for phase changing solvents
- Incorporate aspects of the framework or the framework as a whole into an existing computer-aided molecular design (CAMD) approach for efficient multicriteria screening of solvents in early design phases.

Required education and potential course requirements
The applicants should have a background in chemistry /chemical engineering with knowledge of sustainability.

Starting time and supervision
Preferable project start is January/February 2018. The duration of the project can be 20 calendar weeks (or decided according to RWTH Aachen conditions). The student(s) can receive support by the IDEA league agreement between Chalmers and RWTH Aachen. The examiner
at RWTH Aachen will be Prof. Alexander Mitsos and the supervisor at Chalmers will be Assoc. Prof. Stavros Papadokonstantakis (Division of Energy Technology).