LABORATORY FOR CHEMICAL TECHNOLOGY
Technologiepark 125 9052 Gent, Belgium

Coach	**Supervisor(s)**	**Funding**
Afroditi Kourou	Prof. Dr. Ir. Kevin M. Van Geem, Prof. Dr. Ir. Yi Ouyang	N/A

Rate-Based Modeling Toolbox Development for Point-Source CO_2 Capture

Aim

The objective of this work is to develop a modular, rate-based 1-dimensional modeling toolbox for point-source CO_2 capture that predicts key process indicators across absorber-desorber systems for multiple gas–liquid reactor types, including intensified reactors.

Justification

Despite all recent efforts to mitigate climate change, in 2021 the largest annual increase in emissions related to energy ever was recorded [1]. While various emerging technologies strive for zero emissions, this transition will take time, especially for sectors facing significant challenges in decarbonizing. Therefore, it is imperative to develop technologies that can efficiently **capture CO_2 either from the air or from point source gases**. Among different CC technologies, chemical absorption is the most commonly used on an industrial scale. However, substantial barriers are associated with the high capital expenditure (CAPEX) linked to large columns used and high operational expenditure (OPEX) due to the **elevated energy required for solvent regeneration**. At the same time, solvent development (amines, blends, and novel solvents) and reactor/process intensification concepts are advancing rapidly, creating a strong need for a fast, reliable, and reusable engineering model that can compare operating conditions, solvents, and contactor types on a consistent basis.

This thesis addresses that need by developing a rate-based 1D absorber–desorber model that links detailed mass and heat transfer and reaction with process-level indicators, enabling rapid screening and design decisions. The toolbox will support both conventional contactors and process-intensified reactors, allowing identification of operating windows that reduce energy use and equipment size. As a case study, the framework will be extended to the Gas–Liquid Vortex Reactor (GLVR) – a process-intensification reactor developed at LCT (UGent) in which gas is injected tangentially to induce strong swirling flow and enhanced gas-liquid contact and mass transfer [2], demonstrating how reactor-specific hydrodynamics and transfer correlations can be incorporated into the generic modeling structure.

Program

- Literature review on rate-based CO_2 capture models for conventional and intensified reactors.
- Model development of the rate-based absorber and validation based on experimental data.
- Model development of the rate-based desorber including evaporation and heat transfer model and validation based on experimental data.
- Implementation of the gas–liquid vortex reactor as a case study within the toolbox and execution of a parametric comparison across reactor types and operating conditions.

[1] IEA, World energy outlook 2022, IEA Paris, France, 2022.
[2] Y. Ouyang, M.N. Manzano, R. Wetzels, S. Chen, X. Lang, G.J. Heynderickx, K.M. Van Geem, Liquid hydrodynamics in a gas-liquid vortex reactor, Chemical Engineering Science 246 (2021) 116970.

GHENT UNIVERSITY

LCT DRIVING CHEMICAL TECHNOLOGY