

Digital Twin of a Carbon Capture Pilot Plant

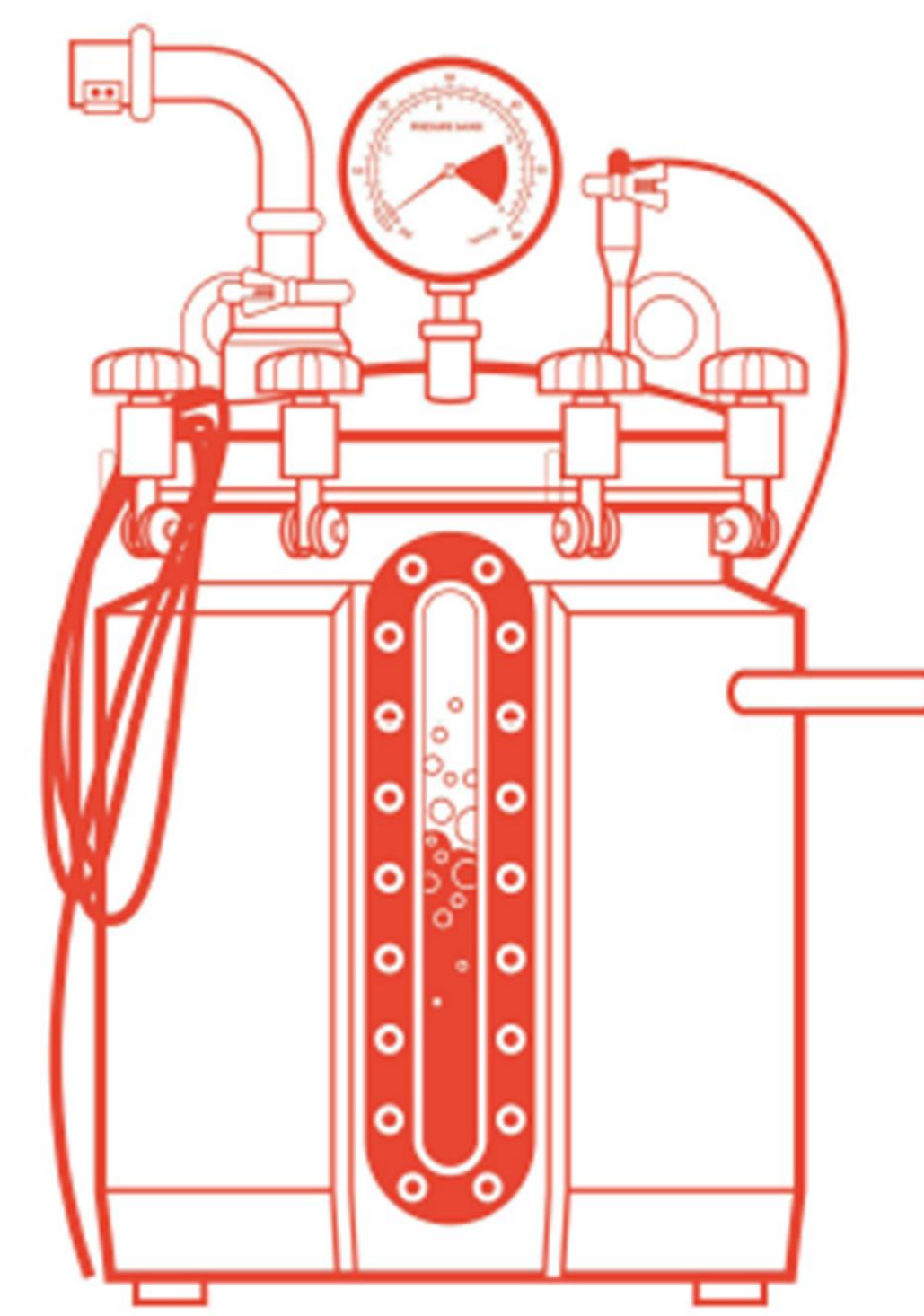
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Master-Thesis, Chemical engineering

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Abstract

A sophisticated model of a carbon capture pilot plant has been developed in MATLAB. The pilot plant is based on the amine scrubbing process and uses the benchmark 30 wt% aqueous monoethanolamine (MEA) solvent to remove the CO₂ out of an Energy-from-Waste flue gas slip stream. Mass transfer is described based on the film theory including enhancement due to chemical reactions in the separation layer. Chemical kinetics in the bulk liquid phase are also considered.

The model predicts the CO₂ capture rate and its concentration in the cleaned flue gas well even for degraded solvent. Validation against AspenHYSYS® found good agreement regarding capture rates. The column profiles show some slight differences between the models.

Introduction

The amine scrubbing process to remove CO₂ from flue gases is a relatively old process first introduced in 1930 mainly intended as a purification process.^[1] Renewed interest started in the early 2000s as a method to reduce carbon emissions. The general process setup of amine scrubbing is as follows:

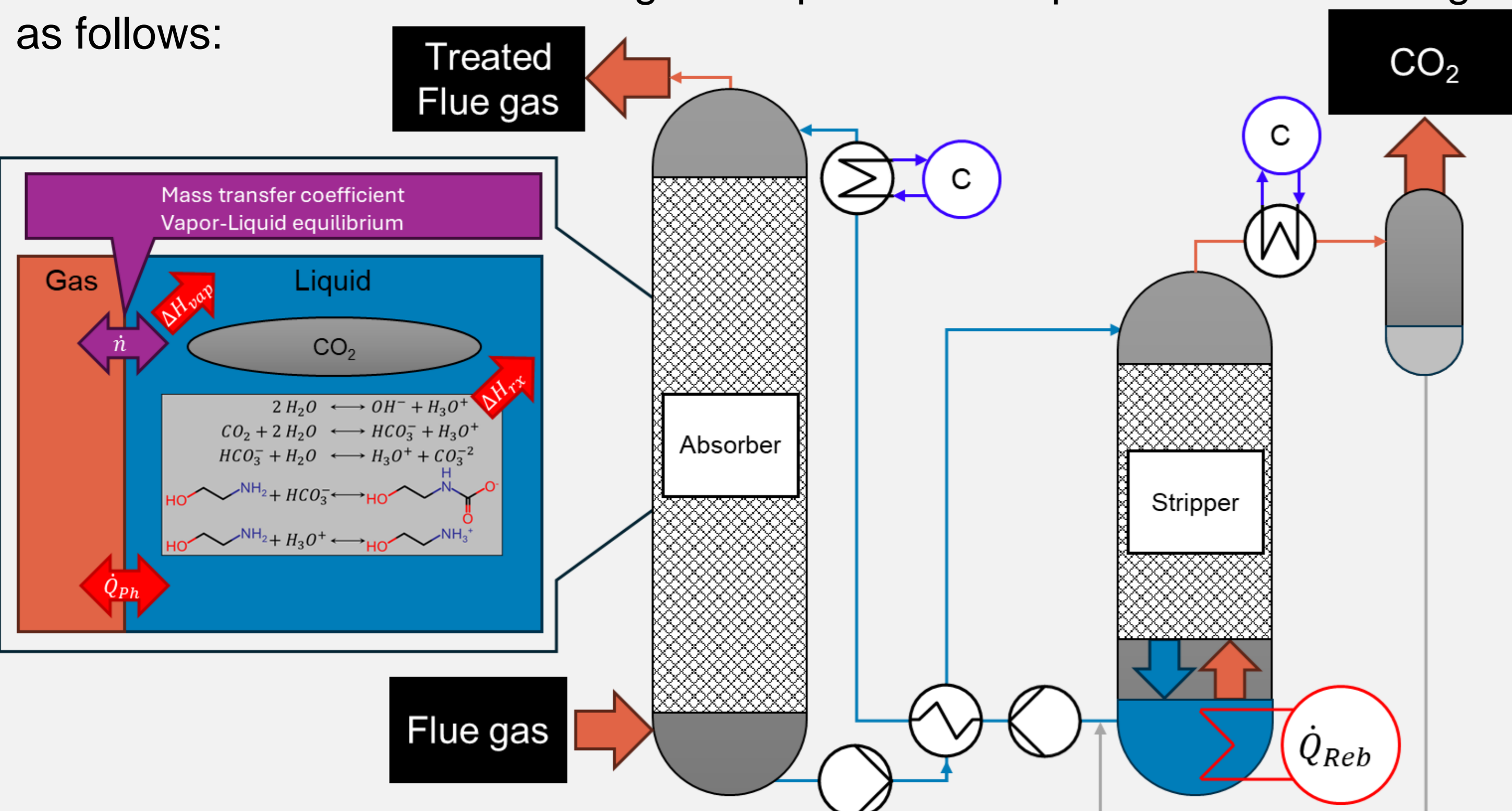


Fig 1 Process flow diagram of the amine scrubbing for flue gas CO₂ removal. Considered flows and reactions in columns also given.

Flue gas is contacted with amine trickling down in the absorber column and CO₂ is absorbed into the liquid phase. Here, CO₂ reversibly reacts with amine and releases considerable heat. The loaded amine is pumped to a stripper column, where the CO₂ is released at elevated temperature and pressure and the solvent is pumped back to the absorber to close the circuit. Interest of Kanadevia Inova AG costumers in carbon capture technology is increasing. To provide the costumers with the best possible solution and to build up in-house knowledge and experience a pilot plant was built. The pilot plant in operated using a flue gas slip stream of a KVI Energy-from-Waste plant in the UK.



Fig 2 Carbon capture pilot plant modeled in this work. Energy-from-Waste plant can be seen in the background.

The experimental plan for the pilot plant was established based on a D-optimal design.^[2] The four considered parameters are flue gas flow, amine flow, lean amine temperature and the stripper conditions as a paired parameter of pressure and temperature.

Sources:

- [1]: Bottoms, R.R. (1930) 'Process for separating acidic gases'. Patent number: US1783901A
[2]: Klein, B. (2014) *Versuchsplanung, DoE: Einführung in die Taguchi-Shainin-Methodik*. 4. Auflage.

Additionally, solvent degradation is investigated by regular repetition of the center point. Besides standard process sensors, FT-IR is used to measure gas compositions and amine samples are regularly taken for extensive analysis.

Results

Model validation against commercial Aspen HYSYS® process simulator shows good agreement for absorber profiles around the inlets, but notable differences in the more dynamic middle sections.

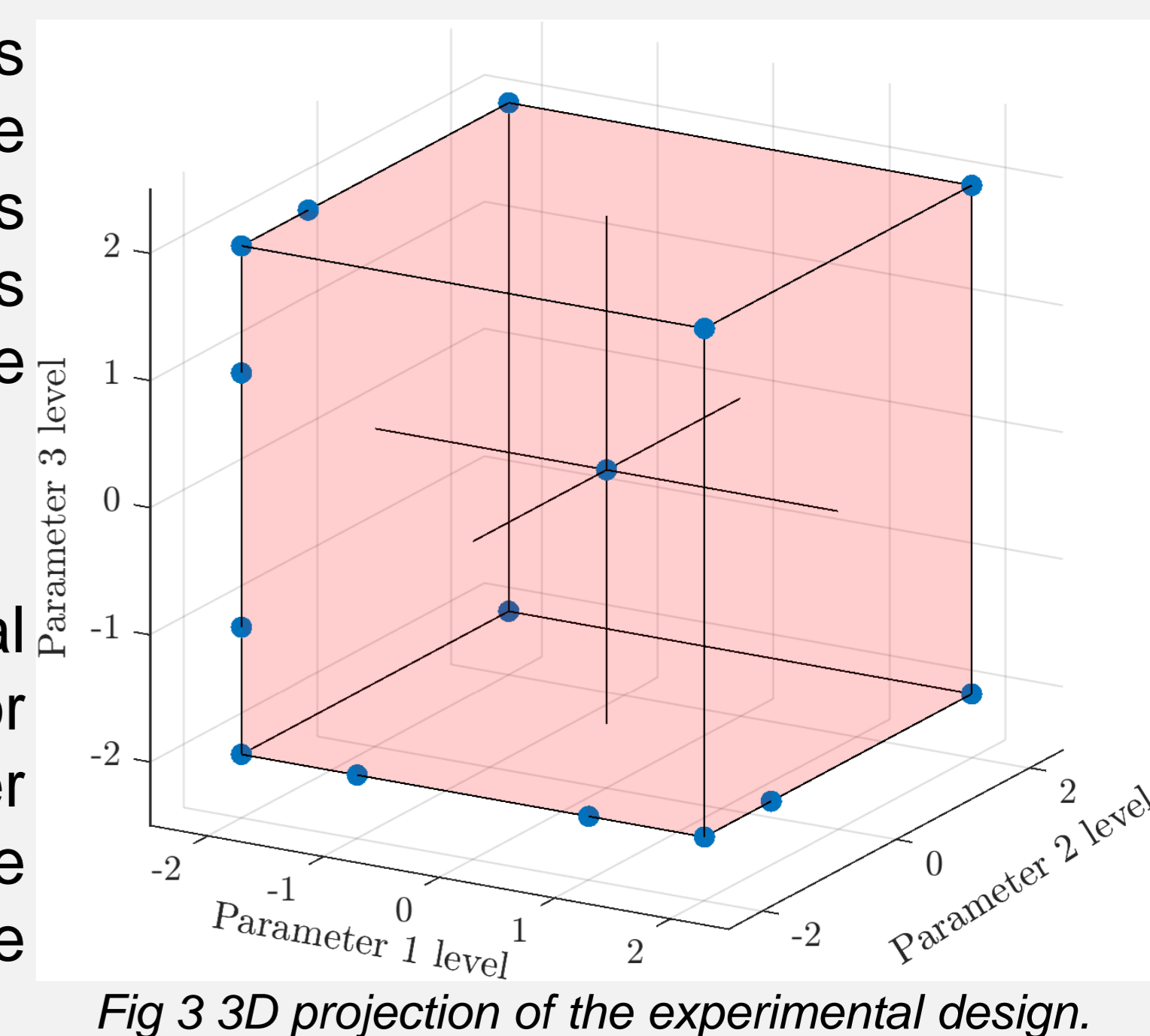


Fig 3 3D projection of the experimental design.

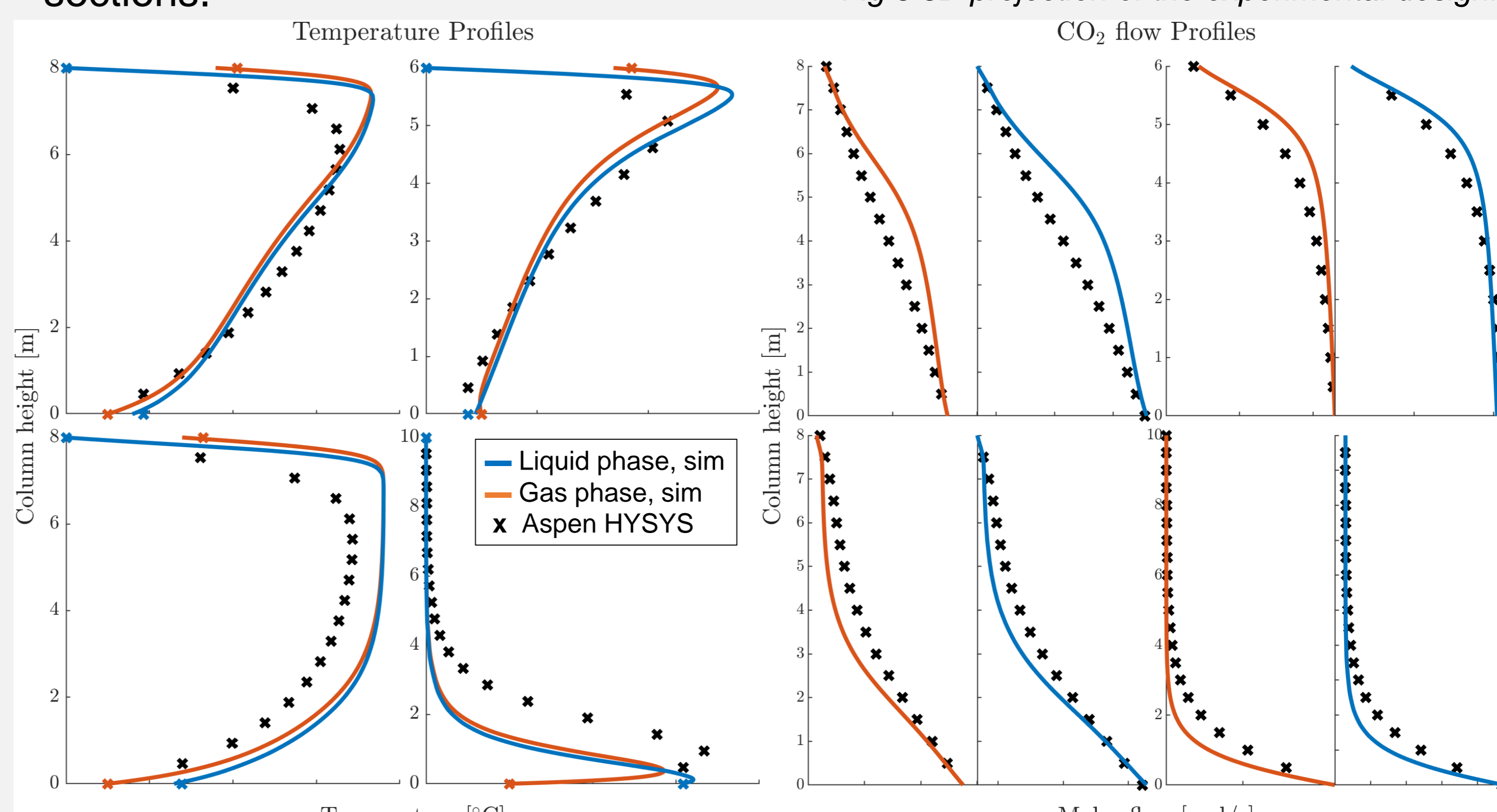


Fig 4 Temperature and CO₂ flow absorber profiles calculated by the established model (— liquid phase, — gas phase) and Aspen HYSYS® using different process parameters and column heights

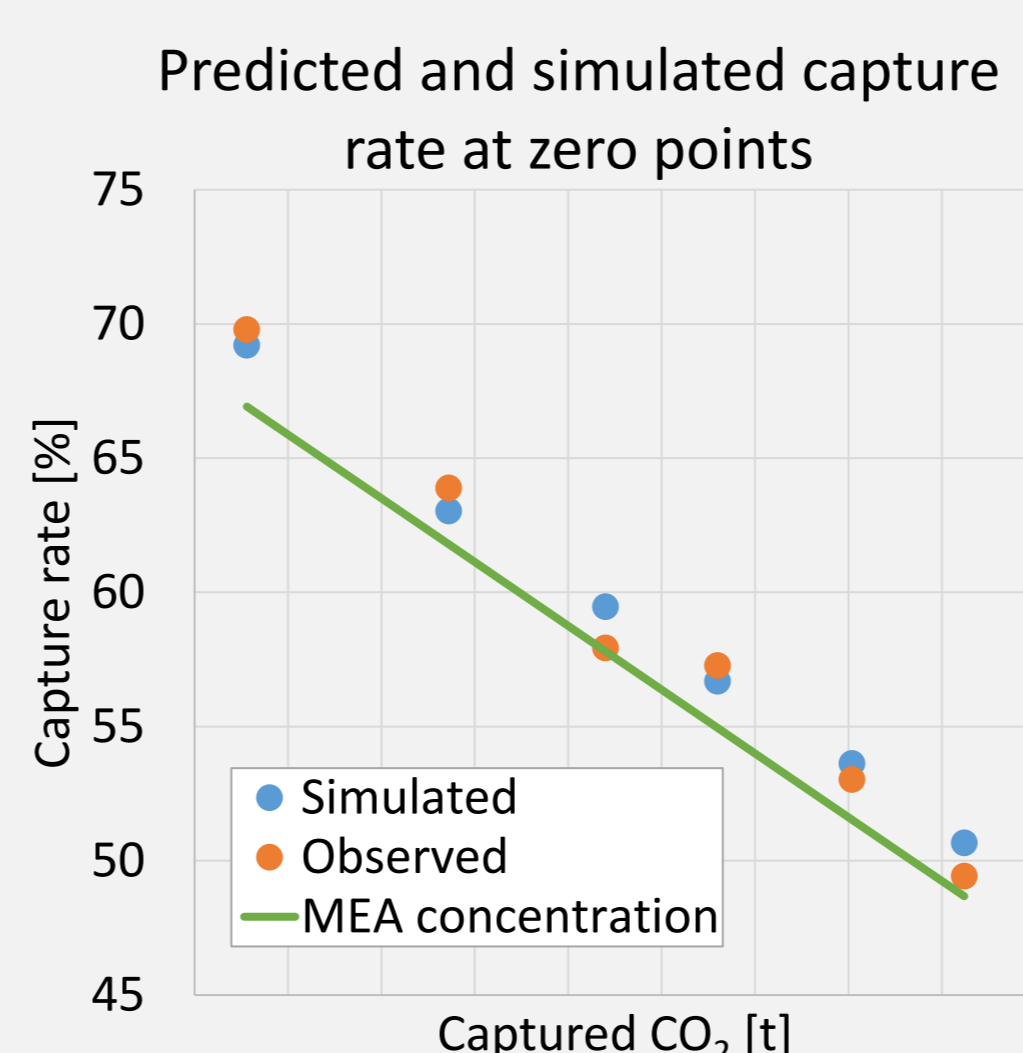


Fig 5 Predicted and simulated capture rate at center points of experimental design

Solvent degradation was observed in periodically drawn liquid samples, as well as in decreasing capture rates over time. A simple linear degradation model as a function of total captured CO₂ was established and applied to predict pilot plant performance.

Validation against pilot plant data shows good agreement in capture rates and CO₂ concentrations in treated flue gas. Some reboiler heat duties are severely underpredicted due to excessive water vapor escaping at the stripper head at certain process conditions.

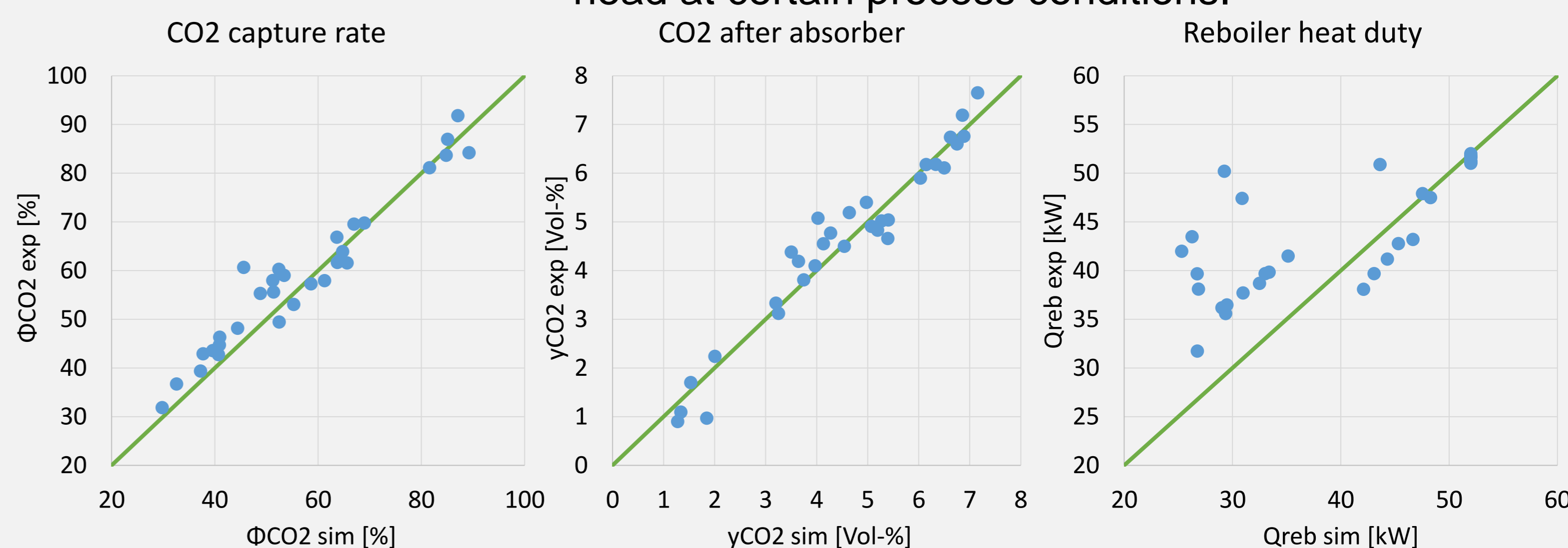


Fig 6 Parity plots of pilot plant data and model predictions for key process parameters. From left to right: CO₂ capture rate, CO₂ concentration in treated flue gas and reboiler heat duty.

Discussion

The MATLAB model established in this work predicts pilot plant performance well, even for advanced solvent degradation. Some model limitations have been identified and approaches to remedy these limitation have been formulated. Future model expansions and improvements are enabled as the source code and documentation is available internally. Thanks to the systematic approach to experimental planning, an invaluable dataset of the carbon capture process was obtained. The data set and the established model are sure to allow for further insight into the carbon capture process, and support future research and development projects.