Prediction of CO_2 absorption in amine solutions via Machine Learning techniques

Frederik Vandael

Master of Chemical Engineering Technology

Introduction

Global warming is the main challenge that humanity should face in the near future. The warming goes along with an increase of emission in greenhouse gasses, i.e. CO_2 [1]. Carbon capture and storage (CCS) is one way of reducing the amount of CO_2 in the atmosphere [2]. One promising technique of CCS is **CO_2 capture in a spray column using amine solutions**. In order to better understand and upscale the CO_2 capture process a model, that accurately describes the CO_2 capture process, is necessary.

Problem definition

A spray column for CO_2 capture is yet to be applied on a large scale, this mainly due the fact that there is **no accurate model available** that can model the CO_2 capture process in a spray column. **First-principle models**, which really on thermodynamics and reaction, have **failed** to accurately model the process [3]. A possible solution is the **use of Machine Learning (ML) techniques to model the process.** These models can be trained by learning from the patterns in the input data, to create functional relationships between the input and output.

Method

Training data

Data with three different amines were used to train the model:

- 2-amino-2-methyl-1-propanol (**AMP**)
- Monoethanolamine (**MEA**)
- N-Methyldiethanolamine (**MDEA**)

To train the model data was gattered from three different places:

- AMP-MEA data was gattered using a spray column set-up during the experimental part of the thesis.
- MEA data was taken from previous research at CIPT.
- Literature data on AMP-MEA and on MDEA-MEA

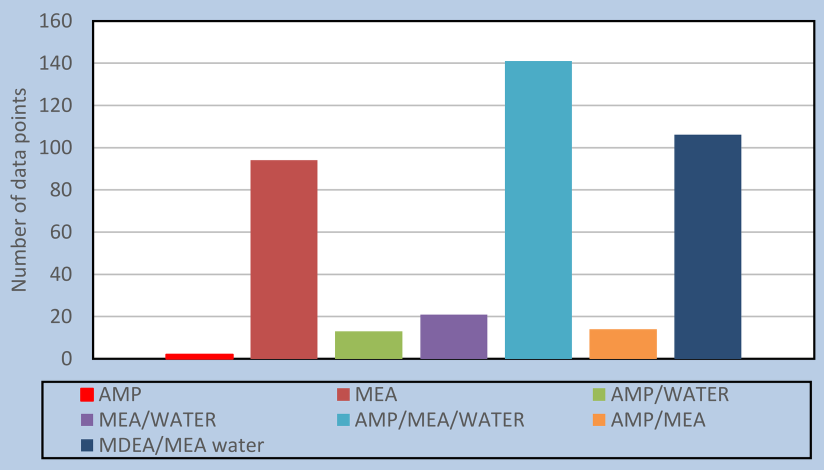

Figure 2: Distribution of training data

Input features

The input features of the model can be divided into three categories: input parameters of the set-up, composition of the amine solution and chemical properties.

Models

Three different types of models were used to model the CO_2 capture process.

Artificial neural network (ANN)

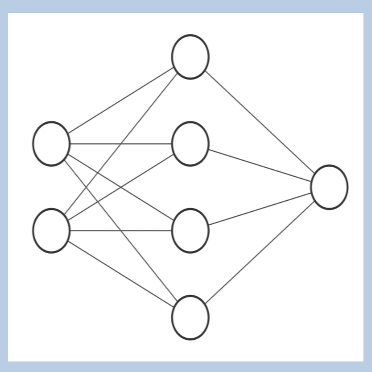

Figure 3: General structure of an ANN

Decision tree regressor (DTR)

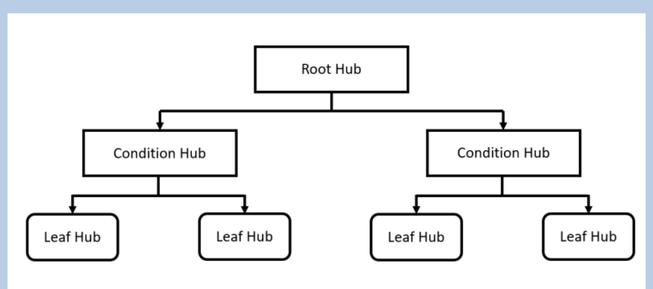

Figure 4: General structure a DTR

Support vector regressor (SVR)

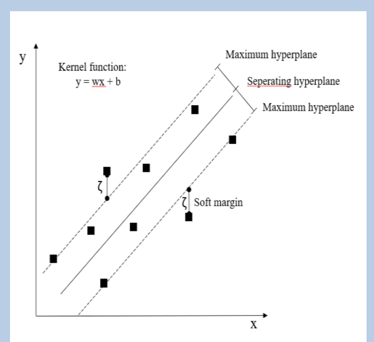

Figure 5: General structure of a SVR

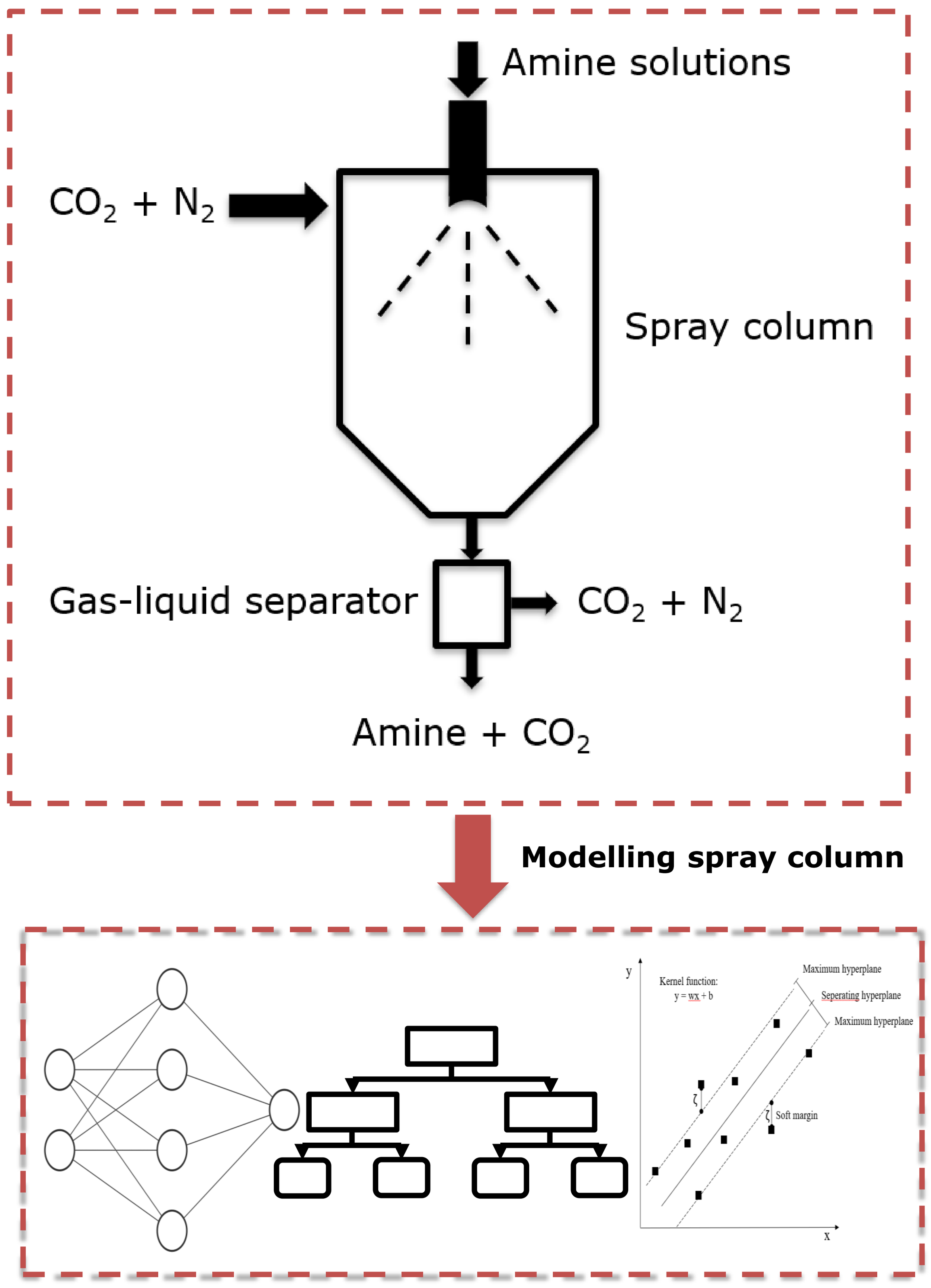

Figure 1: CO_2 capture in a spray column and model types

Results

The output of the five created models is the **K_Ga_e coefficient**, which indicates the performance of the mass transfer during the CO_2 capture.
For each model the modelled K_ga_e versus the experimental K_ga_e is plotted. To compare the models to each other the R² score, MSE and MAE are calculated for each model on validation dataset.

Performance ANN model

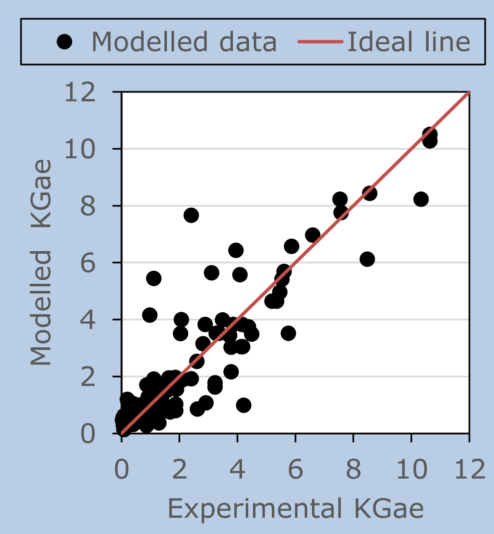

Figure 6: Modelled K_ga_e vs experimental K_ga_e ANN model

Table 1: Performance of ANN model

R² score	0.704
MSE	1.45
MAE	0.738

Performance DTR model

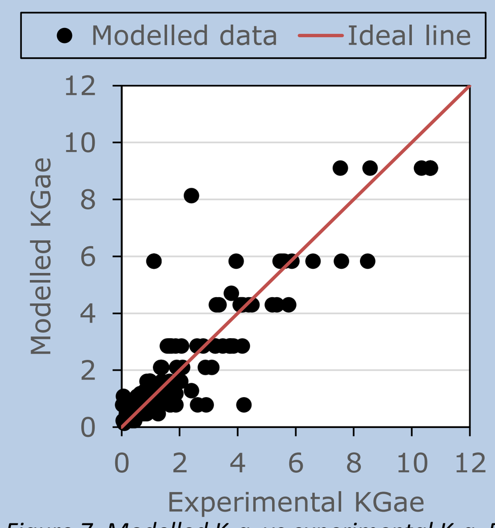

Figure 7: Modelled K_ga_e vs experimental K_ga_e DTR model

Table 2: Performance of DTR model

R² score	0.809
MSE	1.00
MAE	0.648

Performance SVR models

Table 3: Performance of SVR models

SVR-poly			SVR-lin			SVR-rbf		
R² score	MSE	MAE	R² score	MSE	MAE	R² score	MSE	MAE
0.850	0.730	0.291	0.644	1.737	0.881	0.837	0.794	0.330

Polynomial kernel function **Linear kernel function** **Radial basis kernel function**

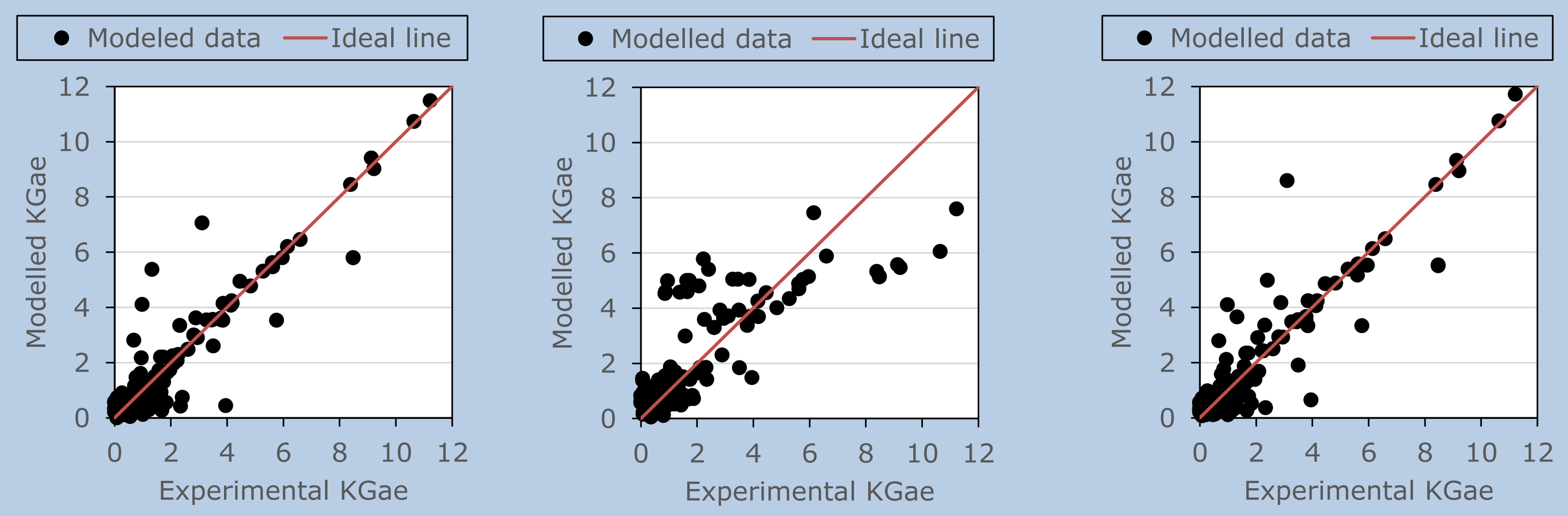

Figure 8 + 9 + 10: Modelled K_ga_e vs experimental K_ga_e for SVR-poly, SVR-lin and SVR-rbf models

Conclusion

- The SVR-ploy and the SVR-rbf can accurately predict the K_ga_e coefficient and were highly flexible both on process condition, spray technology and absorbent.
- The predictions of the ANN model are not accurate, but the model shows potential to further improve. The DTR model and SVR-line are not able to make accurate prediction, the DTR model due to a lack of output variance and the SVR-lin due to the non-linearity relation between input and output.

Supervisors / Co-supervisors / Advisors

Prof. Dr. Ir. Mumin Enis Leblebici
Ulderico Di Caprio

[1] IPCC, *Technical Summary. Contribution of Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change.* 2021.

[2] H. Yang *et al.*, "Progress in carbon dioxide separation and capture: A review," *Journal of Environmental Sciences*, vol. 20, no. 1, pp. 14–27, Jan. 2008, doi: 10.1016/S1001-0742(08)60002-9.

[3] Y. Xu, X. Chen, Y. Zhao, and B. Jin, "Modeling and analysis of CO2 capture by aqueous ammonia + piperazine blended solution in a spray column," *Separation and Purification Technology*, vol. 267, p. 118655, Jul. 2021, doi: 10.1016/J.SEPPUR.2021.118655.

Center for Industrial Process Technology