University of South-Eastern Norway
Faculty of Technology, Natural sciences, and Maritime Science
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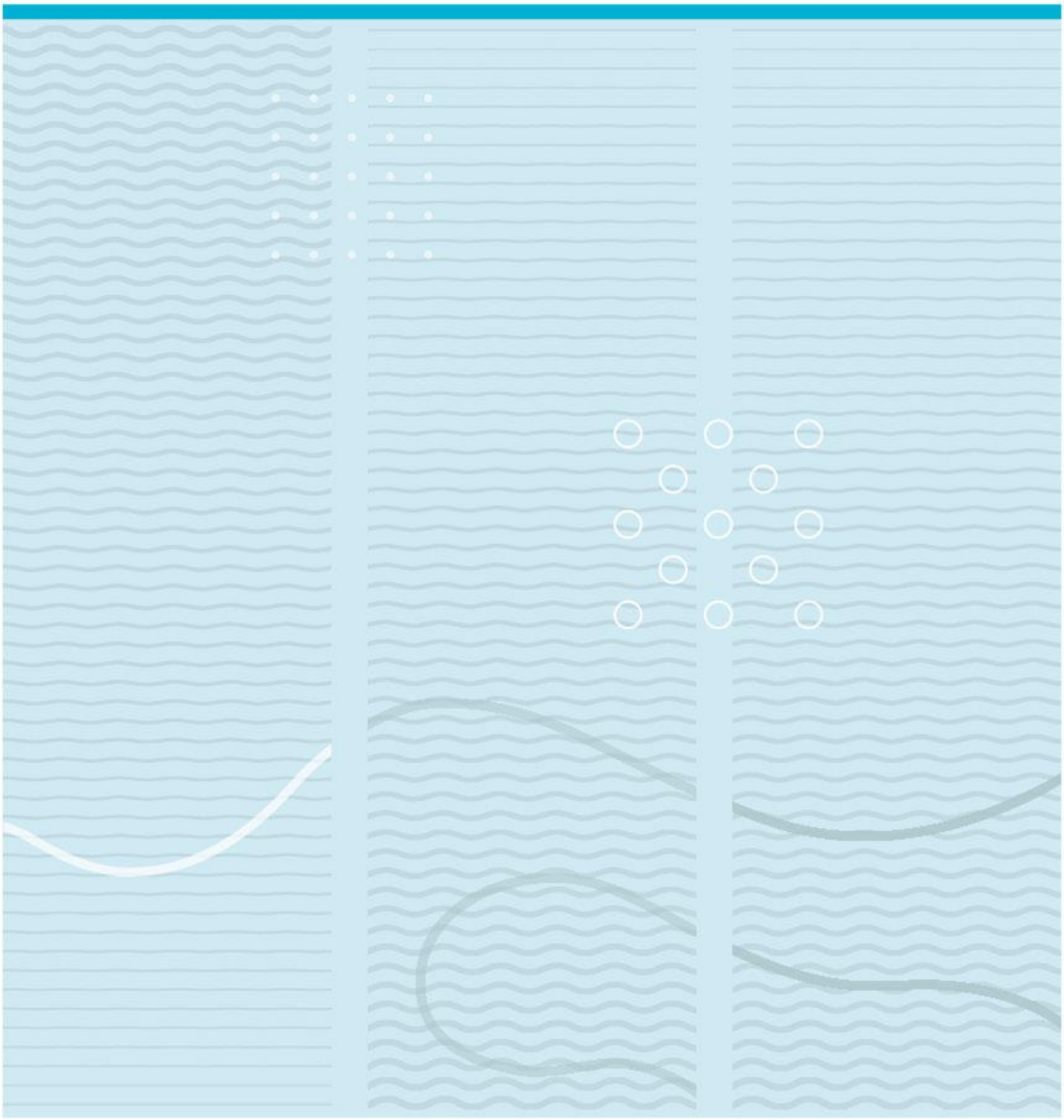
Master's Thesis
Energy and Environmental Technology
Spring 2021

Njål Sæter

Process simulation of CO_2 absorption data fitted to performance efficiency at TCM Mongstad



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Summary

Ambitions and demands to reduce the CO_2 emissions may mean that many CO_2 removal plants will be installed in the coming years. Process simulations are important for safe design and energy optimal solutions.

In this work, models of the absorber at the Technology Centre Mongstad (TCM) have been developed in Aspen HYSYS (V.11) and Aspen Plus (V. 11). It has been studied how well the models manage to reproduce test results. The models have different features and may complement each other.

The Aspen HYSYS models have been developed with user defined Murphree stage efficiencies. Previous student work has shown that the model can easily be updated from one test case to another by utilising a factor, which have been named the Murphree efficiency factor, E_m. This work confirms that the approach is useful, also when the flue gas has much higher CO_2 content than in previous work. The challenge is to determine the Murphree efficiency factor when the absorber removal efficiency is unknown.

A rate-based model has been further developed as a part of the work. The model calculates most of the considered cases quite well, some very well, without case specific tuning. Comparison with test results from four cases from the Esbjerg pilot test facilities was also made, to see the effect of different parameters. The calculations matched well with test results.

There are three cases from TCM, with high lean amine flowrates, where the deviations from test results are large. Two of these cases were specifically selected for comparison. It is important to be aware of the input validity ranges for the model. More comparison with test data is proposed. It is also suggested to perform tests with high removal efficiencies to document calculations when above 90% removal.

The possibility of using a rate-based model in Aspen Plus, together with test results, to produce absorber efficiency data that can be utilised for simulations with Aspen HYSYS, has been specifically considered. A simple correlation was developed which used data generated

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by the rate-based model to calculate absorber efficiencies. The results were quite accurate. Model development work would eventually be required for more extensive use.

It is recommended to continue the work with both the equilibrium based and rate-based models. Test conditions can generally be fitted with only one adjustment factor.

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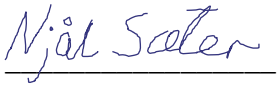
Foreword

This Master's thesis was done during the spring semester 2021 as part of the master program in Energy and Environmental technology at the Department of Process, Energy and Environment at the University of South-Eastern Norway (USN).

I want to thank my supervisor, Professor Lars Erik Øi, for his important guidance and suggestions. Also, many thanks to Neda Razi and Sumudu Karunarathne for their help and support.

Lørenskog, 12.05.2021



Njål Sæter

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Nomenclature

Acid Gas	Fluid property package for amines in Aspen HYSYS
AMP	Amine-2-methyl-1-propanol
CCS	Carbon capture and storage
CHP	Combined Heat and Power plant
DCC	Direct-Contact Cooler
DEA	Diethanolamine
EM	Murphree Efficency
ELECNRTL	Electrolyte non-random two-liquid property package
IAF	Interfacial area factor
MDEA	Methyl diethanolamine
MEA	Monoethanol amine
MEA-4	MEA test campaign no. 4 at TCM
LHUF	Liquid holdup factor
RCC / RFCC	Refinery Residue Fluid Catalytic Cracker
RK-ENRTL	ELECNRTL using Redlich Kwong (RK) for gas properties
SRD	Specific Reboiler Duty
TCM	Technology Centre Mongstad
USN	University of South-Eastern Norway,
Lean amine	The CO2 low amine entering the absorber
Lean amine loading	Mole ratio of CO2 over MEA in lean amine
Rich amine	The CO2 rich amine exiting the absorber
Rich amine loading	Mole ratio of CO2 over MEA in rich amine

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1 Introduction

Carbon dioxide emissions must be reduced to slow down global warming. According to the BP's Statistical review of world energy, the fossil fuel share of primary energy consumption in 2019 was 84% (BP 2020). Wind and solar power are important means to reduce the emissions. However, in average, manufacturing of products like solar panels still depend heavily on the use of fossil fuels.

The carbon market price in EU's Emission Trading System (ETS) is expected to increase significantly in the next 10 years (Platts 202). Gas and coal power plant can ensure sufficient availability when power from solar and wind is fluctuating. Hydrogen production from electrolysers may be used to allow high annual utilisation of power plant capacities. The Nordic Lights project will provide storage of CO_2 from year 2024. (Northern Lights 2021). These are some important reasons why carbon capture and storage (CCS) is assumed important to significantly reduce global emissions within year 2050 (Bellona 2021).

The Technology Centre Mongstad (TCM) started 2012. The facilities are equipped for testing of two different CO_2 capture technologies (Norsk Petroleum 2021):

- Amine technology, in which CO_2 is captured by scrubbing flue gas with a water-based solution of amines.
- Ammonia technology, which uses chilled ammonia as the solvent for absorbing CO_2 from the flue gas.

With dimensions and capacity approaching industrial full scale, the TCM facilities are the largest test facilities in the world.

Researchers and students at the University of South East Norway (USN) have contributed in studies and benefited from results from TCM in their project work. Since 2013, several master theses have included simulations of absorption of CO_2 using monoethanol amine (MEA) as solvent.

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2 Background and task description

Common carbon capture technologies are briefly described. Post combustion carbon capture using amines as solvent are presented with basic process principles. More specific details are included for the TCM facilities. The scope of the thesis is elaborated with comments to earlier student work and relevant publications.

2.1 Carbon capture technologies

There are three groups of technologies within carbon capture:

- Oxy-fuel combustion
- Pre-combustion removal
- Post-combustion removal

In oxy-fuel combustion the fuel is burned with almost pure oxygen. As a result of combustion, the carbon dioxide content of the flue gas is very high, thus significantly reducing the flue gas flowrate and the processing need. More capex is required than for conventional combustion and produces lower net power output because of the oxygen plant (Hou et al 2020). However, hydrogen (H_2) production by electrolysis may mean future availability of larger volumes of oxygen. An integrated process solution including H_2 and O_2 from electrolysis and power production with CCS has been described (NEBB 2021).

The CO_2 capture technology prior to the combustion process is used to produce a synthesis gas (syngas). The syngas is components are mainly H_2, CO_2 and CO, but also some impurities as sulphur compounds. The syngas is produced in connection with gasification of coal, liquid hydrocarbon fuels, or from natural gas. The syngas is cleaned and processed. The final products are H_2 and CO_2. The partial pressure of CO_2 is high in the product gas, so for example physical absorption (alcohols or water as solvent) can be used to capture CO_2. The H_2 can be used as fuel. If the process is integrated in a power plant the efficiency of the electricity generation will be in the order of 11% reduced because of the carbon capture (Martiellia et al 2009)

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Post combustion technology is used to capture the CO_2 in the flue gas when hydrocarbon fuels are burned with air. There are several different methods for post-combustion carbon capture. These methods include chemical and physical absorption and adsorption. There are also various films and membranes that can be used to improve the separation process.

Chemical absorption includes several types of solvents as amines and cooled ammonia. Among the most common amines used in addition to MEA are diethanolamine (DEA), methyldiethanolamine (MDEA) and amine-2-methyl-1-propanol (AMP) (Brickett 2015). Their properties vary. MEA has a relatively large absorption capacity but the total process is energy intensive. The chemical reaction between CO_2 and the amine makes it possible to use at low pressure. The solvent is a mixture of amine and water. For MEA the concentration is normally 30% - 40% on weight basis (30 -40 wt%). Process equipment must be manufactured with corrosion resistant material, usually stainless steel.

2.2 The amine carbon capture process and process optimisation

The flue gas to be treated may be the exhaust gas from a gas or power plant. The source may also be and industrial process as cement manufacturing. The chemical absorption system consists of an absorber, a stripper, heat exchangers and pumps. The figure 2.1 shows the main equipment and the basic principles for a CO_2 removal process with use of an amine. Before the flue gas enters this process, harmful components like NO_x and SO_x, and particles, must be removed. And the flue gas must be cooled to achieve the required temperature at inlet to the absorber.

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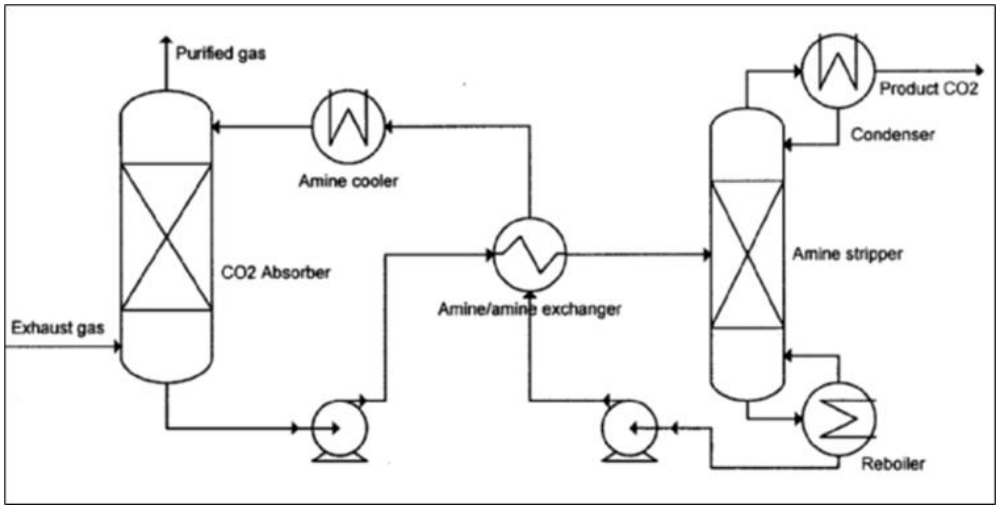

Figure 2-1: Principles for CO_2 removal process based on absorption in amine solution (Øi 2012)

The amine absorbs the CO_2 in the absorber. The lean amine entering at the top of the absorber while the flue gas, or exhaust gas, is entering at the bottom. The rich amine leaving at the bottom, is piped to another process column, called desorber or stripper. The CO_2 is removed by steam in the stripper so that the liquid solvent can be re-used in the absorber as lean amine. The steam is condensed to water, gaseous CO_2 is separated, and the water is recycled to the stripper.

Packed columns are often used for absorption and desorption. The packing material gives a large surface on which the liquid solvent flows and absorbs the CO_2. Various types of packing material are used (Arachchige 2012).

There are different alternatives and options for process optimisation. Energy use is the main cost component. Cost optimisation is often about reducing the energy consumption. Given the process in figure 2-1 examples of options are design of heat exchangers. Increasing the investments in these and the energy used in the splitter process can be reduced. A process alternative example is the lean vapour compression (LVC). The result may vary between the type of amine. Significant energy reductions can be obtained with LVC when using MEA (Aromada and Øi 2017). The lean amine from the stripper bottom is flashed at lower pressure than the stripper pressure. The gas from the flash is compressed and recycled to the stripper. The CO_2 loading (mole CO_2/mole MEA) in lean amine will decrease, thus reducing the

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required amin flowrate, or alternatively increasing the CO_2 removal efficiency in the absorber. The absorber calculations should accurately describe these changes. Intercooled absorber (ICA) is an example of an investment on the absorber itself. Part of the liquid flow in the absorber is modified by removing, cooling, and injecting, to reduce the temperature and increase solvent absorption capacity. The accuracy of the absorber calculations is important to ensure a good basis for investment decision.

2.3 The MEA carbon capture process chemistry

When there is contact between the CO_2 in the flue gas and the MEA solvent in the liquid phase, a set of reactions happens. The basic reactions can be expressed as listed as in equation R2.1 – R2.5 (Liu et al 1999)

Ionization of water

$$2H_2 \leftrightarrow H_3O^+ + OH^- \quad \text{(R2.1)}$$

Hydrolysis and ionization of dissolved CO2

$$CO_2 + 2H_2O \leftrightarrow H_3O^+ + HCO_3^- \quad \text{(R2.2)}$$

Bicarbonate dissociation

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{2-} \quad \text{(R2.3)}$$

MEAH + dissociation

$$C_2H_8NO^+(MEAH^+) + H_2O \leftrightarrow H_3O^+ + C_2H_7NO(MEAH) \quad \text{(R2.4)}$$

Reaction of MEACOO- (carbamate) to bicarbonate

$$C_3H_6NO_3^-(MEACOO^-) + H_2O \leftrightarrow C_2H_7NO(MEAH) + HCO_3^- \quad \text{(R2.5)}$$

Energy is released when the reactions occur, and CO_2 is absorbed. Some water is evaporated but the net effect is a temperature increase in liquid and gas. The temperature profile for the absorber is case dependent. Bulged temperatures can occur both in bottom, top and in the middle of the column (Kvamsdal and Rochelle 2008). The solubility of CO_2 in the solvent is reduced when the temperature increases. Inlet temperatures to the absorber are often tuned to give best absorber efficiency. Liquid gathering and recirculating plates can be used to ensure that the solvent absorption capacity is utilized.

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2.4 The TCM amine facilities

The TCM test facilities includes two test plants. One is built for testing of amines. The other is for testing chilled ammonia technology, which is not presented here.

It is possible to use two types of flue gas qualities. The exhaust gas from the Mongstad combined heat and power plant (CHP) contains between 3.5 and 4.0 mol% CO2. The other flue gas quality with a CO_2 content of 13 – 15 mol% is supplied from the Mongstad refinery residue fluid catalytic cracker (RCC). The figure 2-2 shows the main fluid flows and equipment. Both types of flue gases are considered in this work.

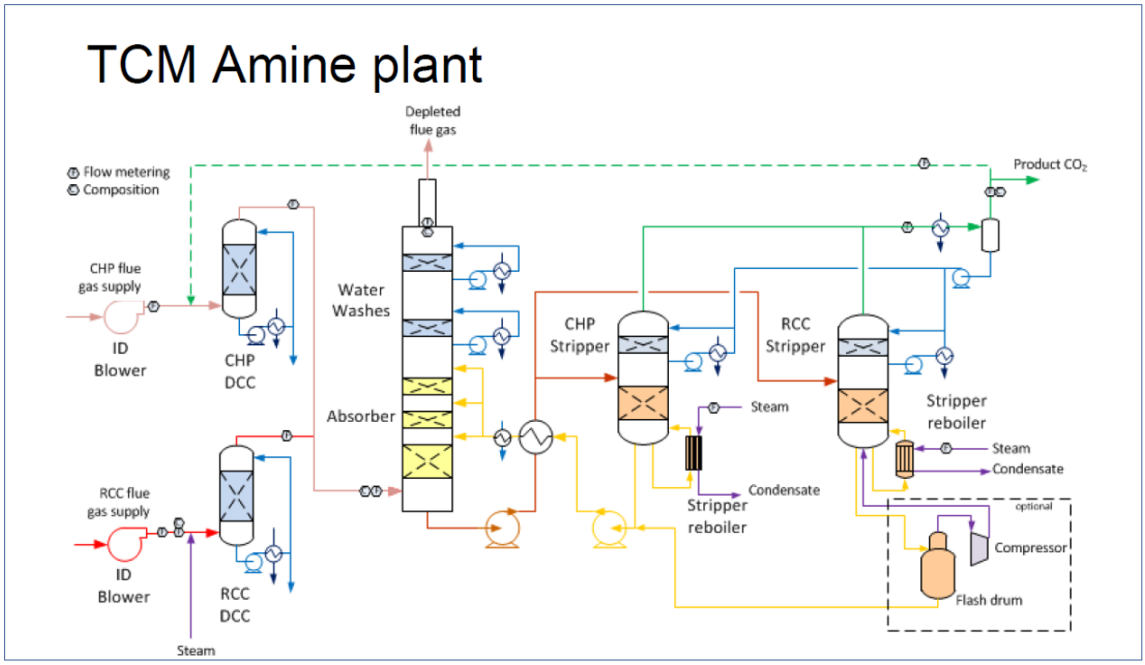

Figure 2-2: TCM amine plant with main items and fluid flows (Hamborg, et al. 2015)

Some main dimensions for the absorber are:

- Total height is 62 meters
- The cross-sectional area is 3.55m x 2m = 7.1m^2, corresponds to a diameter of 3.0 m
- Total of 24 meters absorption height in 3 sections; 12m + 6m + 6 m. It is possible to use 24 m, 18 m, or 12 m in the tests
- Two water wash sections; 3m + 3m
- Koch Glitsch structured stainless-steel packing
- Collector trays and redistributors

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There are 4 temperature sensors in radial plane at regular intervals along the total packed height. In both inlets there is a direct cooler (DCC) where water is in direct contact with the flue gas. In addition to temperature control, the DCC also remove particles in the flue gas.

Test campaigns with MEA have been performed in periods from 2013 to 2018 (TCM 2021). The earliest campaign used gas from the CHP and 24 meters absorption packing height. Data from five of those test cases are used. In 2017 and 2018 there were test campaigns using the higher CO_2 content RCC gas and 18 meters packing height. This work uses data from ten of those cases.

2.5 Mass transfer calculations

Murphree stage efficiency and rate-based models are two different approaches to calculate absorbers and desorbers CO_2 removal efficiencies.

2.5.1 Murphree efficiency

Equilibrium is never reached in a CO_2 absorber. Equilibrium stage efficiency models often use the Murphree stage efficiency (E_m) to describe the difference from equilibrium. An E_m model is referred to as equilibriums model since the mathematical approach is to calculate equilibrium concentrations of CO_2 in gas and liquid. Calculations assume that vapor and liquid is well mixed, and CO_2 has been transferred from vapor to liquid according to equilibrium conditions. E_m tells how well the separation is performed. It is defined as the ratio of the actual change of concentrations to the change that would have been according to equilibrium [Øi 2007]. The Murphree efficiencies are component specific.

The model uses the user defined E_m values to calculate the CO_2 content in the gas and liquid at each stage. The deviation from equilibrium is according to the user defined E_m values.

2.5.2 The two-film model

Rate-based models uses the two-film theory to calculate the mass transfer. The theory considers the interface between gas and the liquid. In a packed column there will be a large

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surface area wetted with the liquid solvent. The mass transfer is assumed by molecular diffusion. In the two-film model by Lewis and Whitman (Kohl Nielsen 1997), Figure 3-1, the gas film and the liquid film has a constant thickness. The figure 2-3 illustrates concentration gradients.

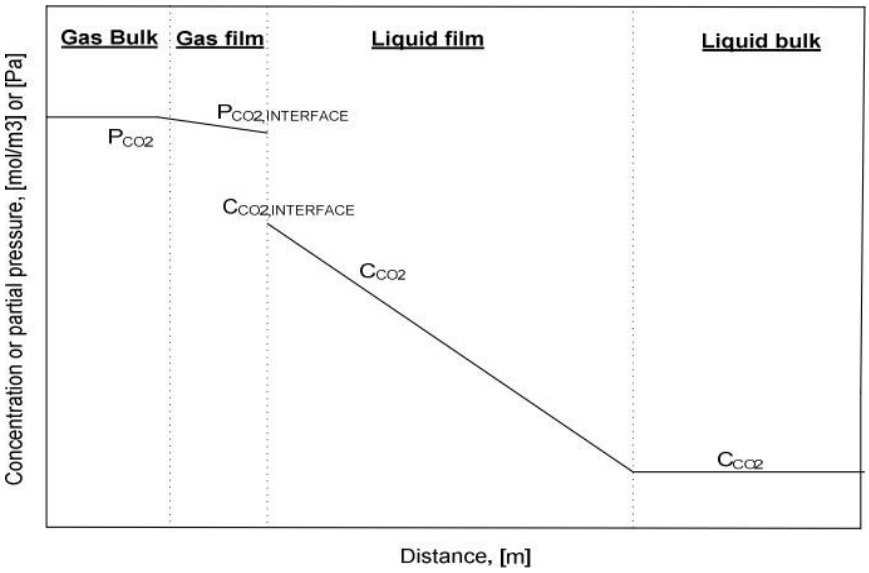

Figure 2-3: Lewis and Whitman two film model, from Lars Erik Øi Ph.D. (Øi 2012)

The system is assumed to be in steady state. The liquid and gas bulk zones assume turbulent flow with no differences in concentration within the bulk. There is equilibrium concentration at the interface between the gas and liquid. The concentration difference between the bulk compositions and the interface compositions represents the driving force for the mass transfer. Laminar flow is assumed in the film zones.

Henry's law with appropriate coefficients is used to calculate equilibrium concentrations for CO_2 at the liquid gas interface. The diffusion mass transfer in the film is calculated by mass transfer correlations. Fick's law states that the mass transfer by diffusion is proportional to the concentration difference. The proportionality factor is called the mass transfer coefficient. Several correlations have been developed to calculate the mass transfer (Razi et al 2012).] It is not a general recommendation on which correlation to be used.

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The mass transfer is enhanced by the fast reaction between CO_2 and MEA [Razi 2013]. An enhancement factor can be included to accommodate this effect.

2.6 Absorption process simulations

Different Aspen Plus rate-based models have been used in several studies to reproduce test results for absorbers and desorbers, for TCM and other facilities. Some of the work includes adjustments of factors used in the model to better fit the experiments. Kvamsdal and Rochelle studied the temperature bulge for MEA systems, varying the liquid – gas ratios in 2008. They used Aspen Plus rate-based model to compare with test data from the pilot plant in Austin, Texas. The work resulted in changes in the model (Kvamsdal and Rochelle 2008). Kvamsdal has also described that dynamical modelling of the process system is important since there are operational issues that will not be sufficiently described in steady-state analysis (Kvamsdal et al 2009). A dynamical model has been developed for the TCM facilities and used to demonstrate flexible operations. The software used, called gCCS, is advertised as "a tool for support of design and operating decisions across the CCS chain" (PSE 2021).

Putta used the Aspen Plus V.8.6 RK-ENERTL model in a study assessing the impact on mass transfer predictions of correlations and models for equilibrium calculations. Even though sub-models were validated against experimental data, the prediction accuracy could vary considerably when used for other experimental data. They concluded that no single kinetic model was able to predict the data from all sources better than the base case kinetic model (Putta et al 2017).

In 2018, Øi compared four sets of test data from TCM, with equilibrium-based models in Aspen HYSYS and Aspen Plus, and a rate-based model in Aspen Plus. It was concluded that equilibrium and rate-based models perform equally well in both fitting performance data and in predicting performance at changed conditions (Øi et al 2018).
The use of equilibrium stage efficiency model in Aspen HYSYS to simulate a removal process by an iterative process with user defined Murphree stage efficiencies, was demonstrated by Øi in 2007 (Øi, 2007). The user defined stage efficiency values was highlighted as the main

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uncertainty. The model was concluded useful for evaluating effects absorber dimensions, amine flowrates, absorption temperature and reboiler temperature.

The Aspen HYSYS E_m model has been used to perform advanced analysis of energy consumption for alternative process configurations. In 2017 Aromada and Øi presented energy and economic optimisation with 4 alternative process configurations for CO_2 capture (Aromada and Øi 2017). In 2017, Rehan studied the performance and energy savings of installing an intercooler (Rehan et al 2017). In 2018, Ali performed simulation with Aspen HYSYS used in economic optimization of amine-based CO2 Capture using excess heat at a cement plant, showing sensitivities to criteria used (Ali et al. 2018). In 2020 Aromoda included the CO2 export compressors in the assumed process and concluded substantial cost differences with different heat exchangers design strategies (Aromoda et al 2020).

2.7 Earlier student work

Simulations of the absorber and of the absorption process, including energy efficiency analysis, have been carried out in master's studies by USN students. Also, students at other universities have been supervised by USN professor. Earlier work has been well summed up in previous thesis reports. A table 2-1 is made to maintain this history, and to include new work in the overview. Each work is briefly commented. Some work that has been of specific importance for this work, is commented below.

- Ye Zhu, USN thesis 2015: HYSYS model was used to simulate TCM test data from 2013. Ye Zhu adjusted the Murphree stage efficiencies to fit the measured temperatures. The stage efficiency profile that he developed have been used
- Kai Arne Sætre, USN thesis 2016: Sætre documented and simulated 7 test cases with both HYSYS and a rate-based model. Data from 5 of these cases have been used
- Sofie Fagerheim, USN thesis 2019: Fagerheim used the stage efficiency profile developed by Zhu, developed other profiles, and showed how the profiles could be fitted to different tests by using a multiplication factor. The factor was named Murphree efficiency factor, E_m. Five of the cases documented by Kai Arne Sætre were used. She also compared the result with rate-based model simulations.

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Table 2-1: Overview earlier student work

Yr - Name	Report name	Description
2011 - Espen Hansen	Comparison of Process simulation programs for CO_2 removal, Master Thesis USN	Aspen HYSYS, Aspen Plus and ProMAX simulations of CO_2 capture with MEA. ProMAX deviated from the Aspen tools.Kent-Eisenberg model in Aspen HYSYS similar to the Aspen Plus equilibrium-based model for the absorber, but significant difference in the reboiler duties. (Hansen 2011)
2012 - Jostein Tvete Bergstrøm	Equilibrium based and rate-based simulation of CO_2 absorption in monoethanolamine, Master Thesis USN	Comparing Aspen HYSYS (Kent-Esienberg and Li-Mather), Aspen Plus (Rate-based and equilibrium) and ProMAX simulations of CO_2 capture with MEA. Equilibrium-based model in Aspen Plus and Kent-Eisenberg model in Aspen HYSYS gave coinciding results. (Bergstrøm 2012)
2013 - Stian Holst P. Kvam	Vapor recompression in absorption and desorption process for CO_2 capture, Master Thesis USN	Comparing calculated energy consumption of a standard MEA process, a process with vapour recompression and a vapour recompression with split stream, using Aspen Plus (rate-based and equilibrium) and Aspen HYSYS (Kent-Eisenberg and Li-mather) (Kvam 2013)
2013 - Even Solnes Birkelund	CO_2 Absorption and Desorption Simulation with Aspen HYSYS, Master Thesis UIT	Comparing a standard absorption process, a vapour recompression process and a lean split with vapour recompression process, using Aspen HYSYS and used (Kent-Eisenberg, Peng-Robinson). All configurations were evaluated due to the energy cost. The lean split vapour recompression and vapour recompression had much lower energy cost than standard process. (Birkelund 2013)
2014 - Inga S. Larsen	Simulation and validation of CO_2 mass transfer processes in aqueous MES solution w, Master Thesis, USN	Simulation and validation of CO_2 mass transfer processes in aqueous MES solution with Aspen Plus at TCM, including comparison of mass transfer correlations in Aspen Plus. (Larsen 2014)
2015 - Coarlie Desvignes	Simulation of Post-combustion CO_2 capture process with amines at CO_2 Technology Centre Mongstad, Master Thesis, CPE Lyon	Evaluating the performance of the TCM flowsheet model in Aspen Plus and compared with the data obtained in the 2013 and 2014 test campaign at TCM. The Aspen Plus model TCM used performed quite well for 30 and 40wt% MEA, but not for higher flue gas temperature and solvent flowrate.(Desvignes 2015).
2015 - Ye Zhu	Simulation of CO_2 capture at Mongstad using Aspen HYSYS. Master Thesis, USN	Based on the data from TCM 2013 campaign published in Hamborg et al [7]. Zhu adjusted the Murphree Efficiency to fit the CO_2 removal grade and temperature profile from the experimental results. (Zhu 2015)
2016 - Kai Arne Sætre	Evaluation of process simulation tools at TCM	Simulation of seven sets of experimental data from the amine based CO2 capture process at TCM, with Aspen HYSYS (Kent-Eisenberg and Li-Mather) and Aspen Plus (rate-based and equilibrium), adjusting rate-based model by the IAF and equilibrium-based model by adjusting the Em profile.(Sætre 2016)
2017 - Erik Sundbø	Partial CO2 capture simulation and cost estimation	Simulating different absorber height with Aspen HYSYS, varying between 5 and 15 m. Although lowest cost with 5 m, 15 m with vapor recompression was comparable (Sundbø 2017)
2018 - Ole Røsvik	Process simulation of CO_2 capture at Mongstad	Simulated the TCM data from the test campaign in 2013, published by Hamborg et al [7]. And the data from TCM's test campaign in 2015, published by Faramarzi et al [32] in Aspen HYSYS and Aspen Plus (equilibrium and rate-based). (Røsvik 2018)
2019 - Sofie Fagerheim	Process simulation of CO_2 absorption at TCM Mongstad, Master Thesis, USN	Development and use of different stage efficiency profiles with HYSYS, including Zhu's, showing how the profiles could be fitted to different tests by using a multiplication factor. The factor was named Murphree efficiency factor. Five of the cases documented by Kai Arne Sætre was used. She also compared the result with rate-based model simulations. (Fagerheim 2019)

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2.8 Problem description

TCM has performed MEA test campaigns from year 2013 to 2018. Test results from year 2013 - 2015 have been utilised in several projects at USN. Process simulations have been performed with Aspen HYSYS and Aspen Plus. The results from test data have been compared with simulated results. The rate-based model used was provided by TCM.

The TCM campaigns performed in 2017 and 2018 with RCC flue gas type and 18 meters absorber packing height, have not been used in the previous students projects, comparing simulations and test results.

Approach

A rate-based model was made using Aspen Plus v. 11 software. Fifteen TCM test cases were simulated. Five of the test cases, with the CHP type of flue gas and 24 meters absorber packing height, have been utilised in earlier student work. The other ten cases with RCC type of flue gas and 18 meters packing height have not been used before. In addition, four cases from the Esbjerg pilot plant were simulated to see how well the model predicted when dimensions and packing type was changed.

The same fifteen TCM cases were calculated with Aspen HYSYS v. 11, with user defined Murphree stage efficiencies. The results were compared with the rate-based model and test results.

The simulations were performed to evaluate how well the models managed to reproduce test data with and without specific tuning. Some of the test cases used in earlier student work were also repeated. These tests include a different flue gas quality. The flue gas CO2 content is important. And earlier simulation results could be used for comparison.

In addition, sensitivity calculations were performed with both models, and another Aspen HYSYS model using model default stage efficiency values. These calculations were done to

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better understand differences observed when comparing model results. These calculations did not consider system capacity limits at TCM.

Aim of project

The aim is to contribute to develop models that are easy to use and calculates reasonably accurately, without case specific tuning. The complexity in the use of the Aspen HYSYS E_m model is to determine appropriate stage efficiencies, which determines the accuracy. One goal was to evaluate further the use of a generic stage efficiency profile. Another goal was to make a rate-based model from available Aspen Plus software. The use of the two models have been compared and discussed. Finally, it was considered if the rate-based model together with test results, can provide a basis to determine stage efficiencies for Aspen HYSYS E_m models.

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3 Methods

The chapter describes how the calculations are performed and model choices and options.

3.1 Model independent assumptions

Calculations are performed for the absorber only.

Absorber efficiency

The CO_2 removal efficiency was calculated by the CO_2 balance over the absorber. There is no alternative when only the absorber is included. During a test, the measured mass balance over the absorber will not correspond exactly to the CO_2 exported from the top of the stripper. The system is never steady state, although as stable as possible, and there are some inaccuracies in measurements.

$$CO_2\ removal\ efficency = \frac{CO_2 inlet\ absorber - CO_2 outlet\ absorber}{CO_2 inlet\ absorber} \quad (3.1)$$

Flowrate unit conversions

Gas flowrates has been converted from Sm3 to kmol by ideal gas law formula:

$$V_m = \frac{RT}{P} = \frac{\frac{8.314kJ}{kmolK} * 288.15K}{101.325kPa} = \quad 23.64 Sm^3/kmol \quad (3.2)$$

The assumed component mol weights, and reference density of air, are given in table 3-1

Table 3-1: Mol weights (MW) and reference density of air

Mol weights MW (g/mol)						Ref. density air at 15 °C & 1atm
N_2	O_2	CO_2	MEA	H_2O	Air	(kg/m^3)
28.0	32.0	44.0	61.1	18.0	28.97	1.225

The reference density of air was used when converting to mass flows.

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Lean amine composition

The mol% in the lean amine was tuned in Excel, by manually varying the MEA mol%, to obtain the given values for the MEA wt% and the lean amine loading.

3.2 Fluid properties in Aspen HYSYS and Aspen Plus

In Aspen Plus the ElecNRTL thermodynamic package was chosen, including the Redlich-Kwong equation of state (RK) for generation of gas properties. The option is called RK-ENERTL in Aspen Plus. By default, the RK choice generated new values for coefficients used, compared to ELECNRTL with ideal gas assumptions.

In Aspen HYSYS the Acid gas package is used for property generation. The Acid gas package is based on the Electrolyte NRTL model (ElecNRTL) and uses Peng-Robinson for gas properties (Watanasiri et al. 2016).

3.3 Calculations with the Aspen HYSYS Em model

Much work has been performed and reported in earlier master thesis on tuning of models to fit the test results for the CHP flue gas type. Some work has been repeated as it represents an important basis. The attention has been on potential use and further development of the E_m factor. The ambition has not been to improve reproduction of the individual test case results. Comparisons with some earlier results are included. A few updates from earlier work were made on some input assumptions in accordance with given information from TCM.

The RCC flue gas type test cases has not been simulated in the earlier work. As for the CHP flue gas type cases, the attention on potential use and further development of the E_m factor.

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3.3.1 Murphree efficiency profiles

The absorber packing height in the CHP and RCC flue gas tests was 24 and 18 meters respectively. Previous work has shown that the absorber can be well modelled by assuming one meter pr stage. The figure 3.1 shows some of the efficiency profiles that have been used earlier to reproduce the TCM temperature test data. The profiles start with relatively high values at the top of the absorber packing height and then reduces.

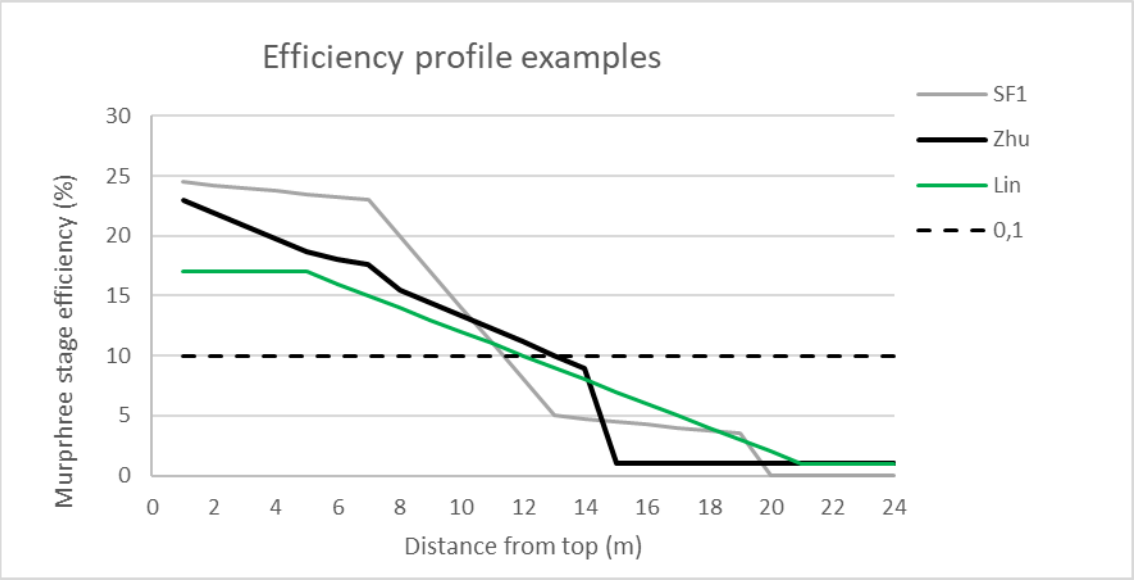

Figure 3-1: Examples of Murphree efficiency stage profiles (Fagerheim 2019)

The efficiency profile named "Zhu" was chosen as a basis in this work. Earlier results show that it described the temperature profiles well. In addition, constant value profiles are used. In the figure this is illustrated with the dotted 10% line

The 18-meter absorber column was modelled as 18 stages. The stage efficiency profile assuming the constant value of 0.1 (10%) was maintained. The Zhu profile has been modified by deleting the 6 last stages and multiply the remaining stage efficiencies by the factor 0.785. The reason for this is to have an average stage efficiency value of 0.1 for this profile also. The modified profile was named Zhu_M.

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Table 3-2: Assumed stage efficiency profiles

Stage	Zhu	Zhu_M	0.1 (24 meter)	0.1 (18 meter)
1	0.23	0.1805	0.1	0.1
2	0.2192	0.1720	0.1	0.1
3	0.2085	0.1636	0.1	0.1
4	0.1977	0.1551	0.1	0.1
5	0.1869	0.1466	0.1	0.1
6	0.18	0.1412	0.1	0.1
7	0.1762	0.1382	0.1	0.1
8	0.1546	0.1213	0.1	0.1
9	0.1438	0.1128	0.1	0.1
10	0.1331	0.1044	0.1	0.1
11	0.1223	0.0960	0.1	0.1
12	0.1115	0.0875	0.1	0.1
13	0.1007	0.0790	0.1	0.1
14	0.09	0.0706	0.1	0.1
15	0.01	0.0078	0.1	0.1
16	0.01	0.0078	0.1	0.1
17	0.01	0.0078	0.1	0.1
18	0.01	0.0078	0.1	0.1
19	0.01		0.1	
20	0.01		0.1	
21	0.01		0.1	
22	0.01		0.1	
23	0.01		0.1	
24	0.01		0.1	

3.3.2 Using the Murphree stage efficiency factor E_m

The model is tuned to match the test results CO_2 removals by manual tuning with the E_m factor. The E_m factor is multiplied with the assumed stage efficiency profile. As an example, referring to the constant 0.1 stage efficiency profile, an E_m factor of 2.0, means that the constant stage efficiency used has been 0.2. Similarly for the Zhu profile, E_m factor of 2.0 means that each stage efficiency is multiplied with 2.0.

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When using the constant 0.1 stage profile, the calculated temperatures deviate substantially from measured temperatures. The reason to include the profile was to see the sensitivity of the E_m factor to the assumed profile.

3.4 Calculations with the Aspen Plus rate-based model

The Aspen Plus rate-based model used is based on a model available through the search in the Aspen Plus software (Aspentech 2019). It is a model of the pilot test plant in Austin, Texas (Rochelle 2012). In this work the model is limited to model the absorber only. The column type used in Aspen Plus is within the column group "Rad frac". It is a distillation column which can also be used for absorption. It is the same as used in the Texas model. An alternative column named absorber was tested. It gave similar results, but it had more user challenges.

Dimensions and packing type

Dimensions and packing material for TCM are used. Aspen Plus has pre-made assumptions for the TCM packing. The number of segments, or stages, was increased from 20 to 50, since the TCM absorber is higher than in Texas. Some calculations were done with 96 stages, without difference in the results from 50 stages. Calculations with 20 stages gave different results from 50 stages.

Fluid properties, mass transfer, interface area and liquid hold-up correlations

In addition to dimensions, packing type, and the number of stages, two other important changes were made to the Texas MEA model:

- The property generations were changed from "ELECNRTL" to "RK-ENRTL". The absorber pressure is just above atmospheric. The use of Redlich-Kwong (RK) for the gas phase instead of ideal gas assumptions, should not matter much. However, by default, the model generated some new kinetic constants, which gave results that matched better with the measured values, when used together with the BRF-1992 (Bravo-Rocha-Fair) (Rocha et al. 1996) correlations for mass transfer and interface area.
- BRF-1992 correlations were used. The temperature calculations were better than alternative correlations. The mass transfer and interface area correlations by

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Onda , which is used in the Texas model, is not a suggested option in Aspen Plus for the TCM packing material.

Model differences between CHP and RCC flue gas

All the main inputs are listed in the table 3-3 for the simulations of the CHP flue gas and the RCC flue gas, showing the common input and the differences. The differences between the two is the column heights of 24 and 18 meters. One model change was done by specifying the film discretization ratio to 2. The value 1 was used for the CHP flue gas. The factor is the ratio of the thickness of the adjacent discretization regions. A value greater than one means thinner thickness at the liquid gas interface. The reason why it was changed was better fit with measurements.

Model tuning

The model was tuned to test data with the liquid hold-up factor. For the RCC cases it is suggested to use the factor 0.72 as a general assumption. The assumption is included in the table 3-3.

Previous work has used the interfacial area factor for tuning. For the options used, mainly related to the BRF-1992 correlations, the comparison of calculated and measured temperatures did not support the use of the interfacial area for tuning to the measured CO_2 removal efficiency.

Flow model

There are four flow models options in Aspen Plus which consider the calculations of bulk properties:

- Mixed, the bulk properties for each phase are the same as the outlet conditions for each phase leaving the stage.
- Countercurrent, the bulk properties are an average of the inlet and outlet properties for each phase.
- VPlug, the bulk properties are calculated by averaging the vapor, and using outlet conditions for the liquid and outlet pressure.
- VPlugP, same as VPlug, but with average pressure instead of outlet pressure

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“Mixed” was used in the Texas-model. The TCM model used in earlier student work, used “VPLUG”. “VPLUG” is included as the assumption in the tables 3-3. The observed difference between “Mixed” and “VPLUG” was very small.

Esbjerg pilot test cases

The same model was used as for the TCM RCC cases but changes to represent the dimensions and packing material. The diameter is 1.1 meter and packed column height 17 meter. The packing material is Sulzer Mellapak 2X (Neda, et al. 2013a). The main model input is given in the table 3-3 together with the TCM models.

Table 3-3: Main input rate-based model

Common input			
Calculation type	Rate-based		
Fluid properties	RK-ENERTL		
Reaction ID	MEA		
Mass transfer coeff method	BRF-1992 (Bravo-Rocha-Fair)		
Interfacial area method	BRF-1992 (Bravo-Rocha-Fair)		
Holdup method	BRF-1992 (Bravo-Rocha-Fair)		
Number of stages	50		
Film Liquid phase	Discrxn		
No. of discr. points liquid	5		
Film Vapor phase	Film		
Reaction conduction factor	0.9		
Flow model	VPLUG		
Interfacial area factor	1		
Heat transfer coeff method	Chilton and Colburn		
Campaign specific input			
	TCM CHP flue gas	TCM CHP flue gas	Esbjerg cases
Packed height [m]	24	18	17
Packed diameter	3	3	1.1
Packing type	Koch metal 2x	Koch metal 2x	Sulzer Mellapak 2X
Liquid hold-up factor	1.0 & tuning	0.72 & tuning	0.72 & tuning
Film discretization ratio	1	2	2

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4 Results - CHP flue gas cases

The work in previous master thesis is important. The work has shown how stage efficiencies can be profiled to give accurate absorber temperature profiles with predicted CO_2 removal according to test results. The possibility to use an efficiency profile developed for one test case also for other test cases, by introducing a correction factor, as demonstrated by Fagerheim, is of special importance for this work. The correction factor has been called "Murphree efficiency correction factor" and has been named E_m.

Calculations with the rate-based model is performed with and without case specific tuning to match test results. A model that calculates reasonably well without tuning can be possible to use for predictions. Case specific tuning is performed with the liquid hold-up factor. Tuning with the interface area factor is discussed.

4.1 CHP flue gas test cases main input data

The flue gas CO_2 content was approximately 3.6 mole%. The table 4-1 shows the flue gas compositions from the test data and used in the calculations.

Table 4-1: Gas compositions (mol%) in the CHP flue gas cases

	Case				
Component	F17	Goal1	H14	2B5	6w
CO2	3.70	3.62	3.70	3.57	3.57
H2O	3.70	3.10	2.95	3.70	3.00
O2	14.60	14.30	13.60	14.60	13.60
N2	78.00	79.00	79.75	78.08	79.83

For four of the cases the flue gas flowrates where almost equal, but for the case 17F it was higher. The input data and the measured CO2 removal are shown in table 4-2.

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Table 4-2: Input data from test cases and measured CO_2 removal

Case	17F	Goal1	H14	2B5	6w
Input					
Lean amin loading (mole CO_2/mole MEA)	0.20	0.20	0.23	0.23	0.25
Lean amin flowrate (kg/hr)	57434	44391	54900	49485	54915
MEA wt% (without CO_2)	31.0	32.3	30.0	31.6	30.4
Flue gas flowrate (kg/hr)	72389	57157	57300	57193	56788
Flue gas pressure (bara)	1.0313	1.0313	1.0313	1.0313	1.0313
Lean amine pressure (bara)	1.0630	1.0630	1.0630	1.0630	1.0630
Flue gas temperature (°C)	29.8	25.0	25.0	28.2	25.0
Lean amin temperature (°C)	37.0	28.6	36.5	36.8	36.9
CO_2 removal (%)					
Test result	*83.5*	*90.1*	*90*	*87.3*	*79*

The lean amin compositions used are based on the lean amin loading and the MEA wt%. They are shown in the table 4-3.

Table 4-3: Lean amine compositions (mol%) in the CHP flue gas cases

	Case				
Component	F17	Goal1	H14	2B5	6w
MEA	11.44	12.04	10.94	11.67	11.09
H2O	86.27	85.55	86.54	85.65	86.14
CO2	2.29	2.41	2.52	2.68	2.77

4.1.1 Measured temperatures

Absorber temperature profiles have been provided by TCM for all the test cases in the previous student work (Fagerheim 2019). Temperature are measurements at 15 different heights of the packed column. At each height, the temperature is measured at 4 points. There are significant differences between the measurements in the radial planes, as shown in the figure 4-1. The assumed reason is difference in gas and liquid temperatures. The average values of the measured temperatures are used as the value for the measured temperature profiles.

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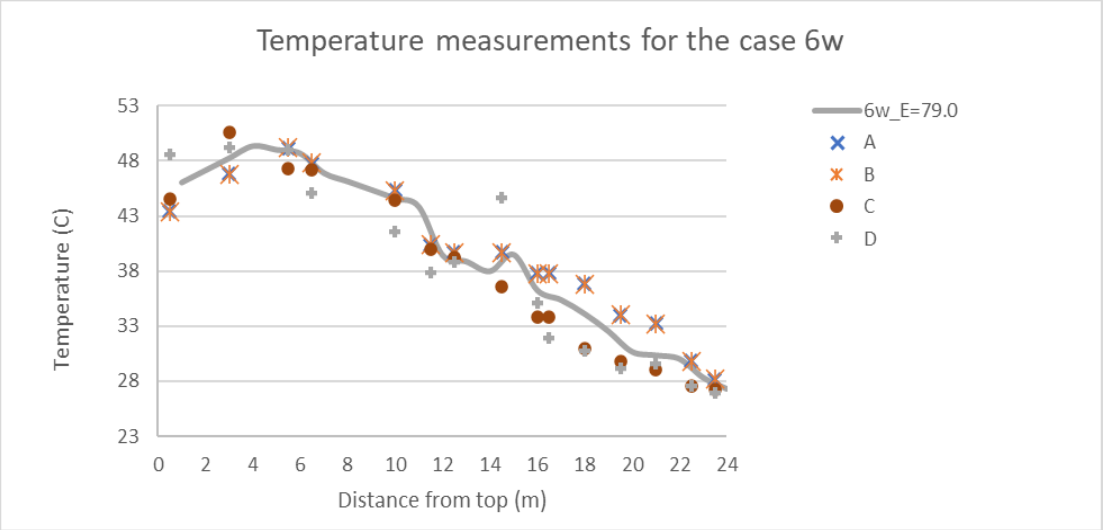

Figure 4-1: Measured and average absorber temperatures for case 6w

The figure 4-2 shows the average of the measured temperatures for the six test cases.

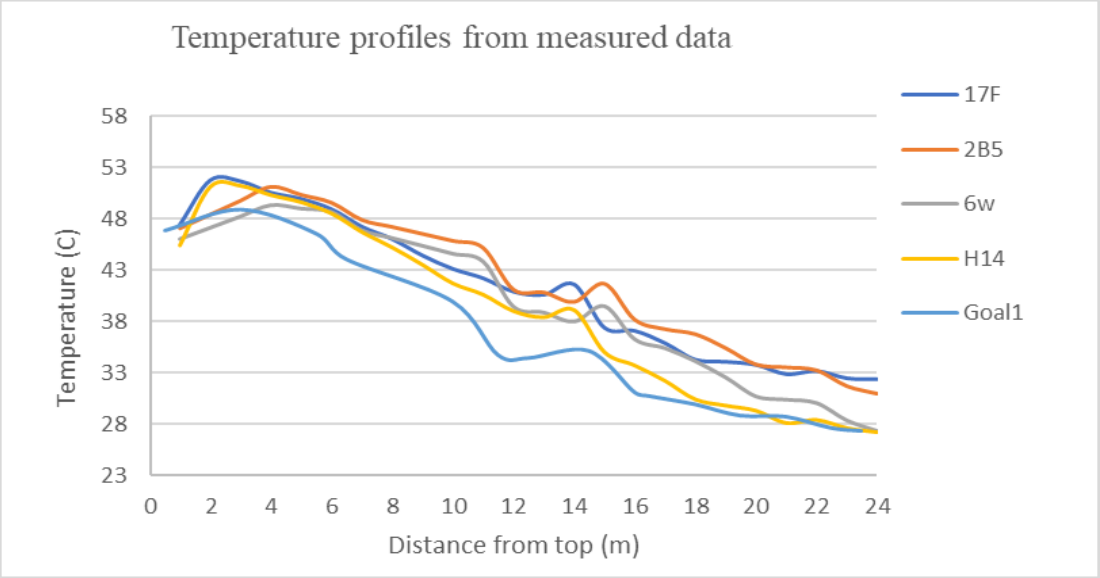

Figure 4-2: Absorber temperature profiles based on the test case measurements

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4.2 Calculations with the Aspen HYSYS Em model

4.2.1 CO_2 removal and calculated E_m factors with the Aspen HYSYS model

The test cases assumptions are presented in chapter 4.1. Key assumptions are repeated in the table 4-2 for an easier overview, together with the tuned E_m factors.

Table 4-4: Key input data from test cases and predicted E_m factors

Case	17F	Goal1	H14	2B5	6w
Key input:					
- Lean amin loading (mole CO_2/mole MEA)	0.20	0.20	0.23	0.23	0.25
- Lean amin / flue gas flow ratio	0.793	0.777	0.958	0.865	0.967
- MEA wt% (without CO_2)	31.0	32.3	30.0	31.6	30.4
CO_2 removal (%)					
Test result	*83.5*	*90.1*	*90*	*87.3*	*79*
E_m factors calculated					
HYSYS_Zhu	0.78	0.96	1.0	0.88	0.68
HYSYS_0.1	0.76	0.96	1.0	0.89	0.66

The Zhu and the constant stage efficiency profiles give approximately the same E_m factors.

It was observed that if an E_m factor equal to one was used for all the cases, the calculated removal efficiencies were close to 90% for all cases. And if the E_m factor according to case 17F were used (E_m =0.78), the removal efficiencies were approximately 83% for all cases.

4.2.2 Comparison of Aspen HYSYS Em model with earlier work

Earlier work has used the Kent-Eisenberg correlation for fluid properties and not the Acid gas correlation that is used in this work. (The Kent-Eisenberg Is not included in this version Aspen HYSYS V11). Table 4-1 shows that an E_m factor of 1.0 was calculated for the case H14. The Zhu profile and the constant 0.1 stage efficiencies calculates the measured CO2 removal of 90%. The corresponding removal efficiency calculated by Fagerheim was 88.4%. Fagerheim calculated the case Goal1 to the measured CO_2 removal while in this work an Em factor of

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0.96 is estimated. Thus, the Acid Gas correlation used calculates slightly higher CO_2 removal efficiencies than previous work. But the difference is not large.

The figure 4-4 shows a comparison of calculated temperatures for the H14 cases with Fagerheim. The temperature profiles are close to identical.

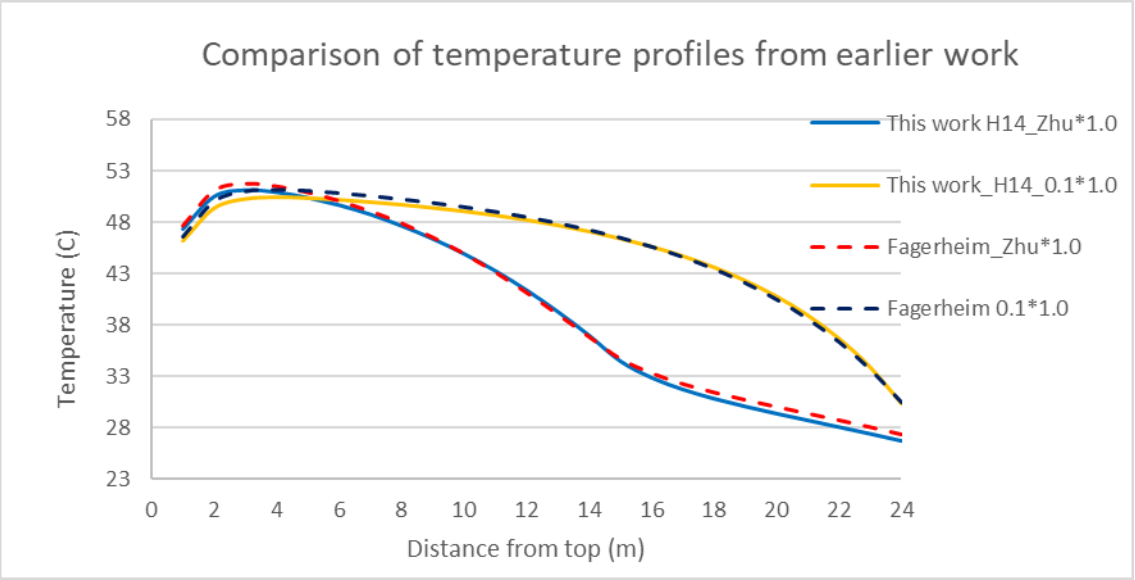

Figure 4-4: Comparing H-14 temperature calculations with earlier work

4.2.3 Temperature calculations with the Aspen HYSYS E_m model

The calculated temperature profiles with the HYSYS E_m model are shown in the figure 4-5. The measured temperatures for the cases Goal1 and 2B5 are included to show the ranges of the measured temperatures. The calculations show less differences than the measured temperatures. The base stage efficiency profile Zhu was developed for the case H14 and determines to a large degree the temperature profile.

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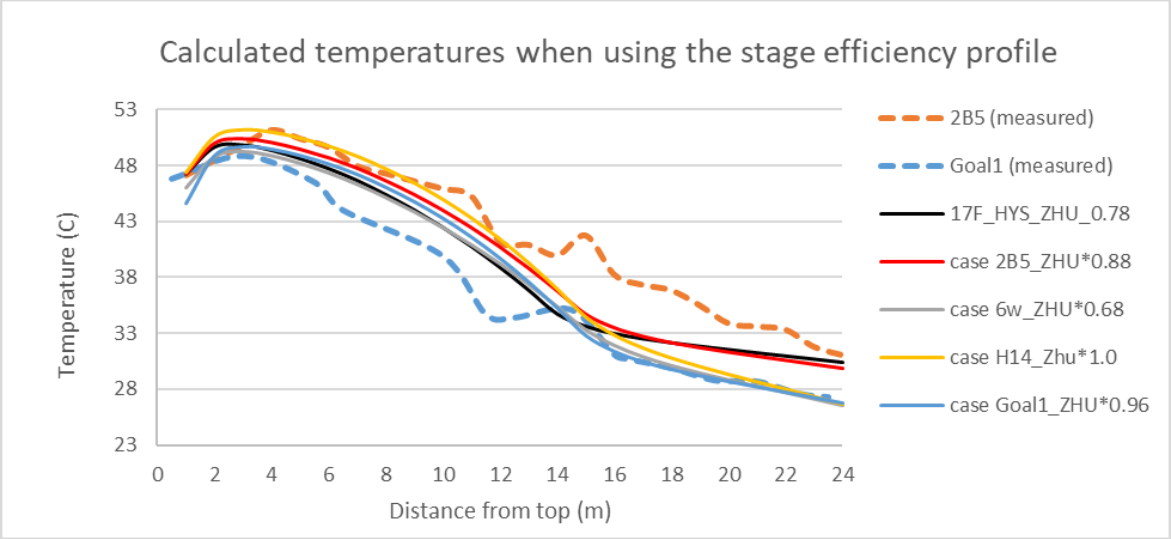

Figure 4-5: Calculated temperatures with the profiled stage efficiencies. Measured values included with dotted lines for comparison. (CO_2 removal equals test results for all calculations)

When using a constant efficiency value for all stages, the calculated temperature profiles are very different. The measured profile for the case 2B5, the highest measured temperatures, is included for comparison in the figure 4-6.

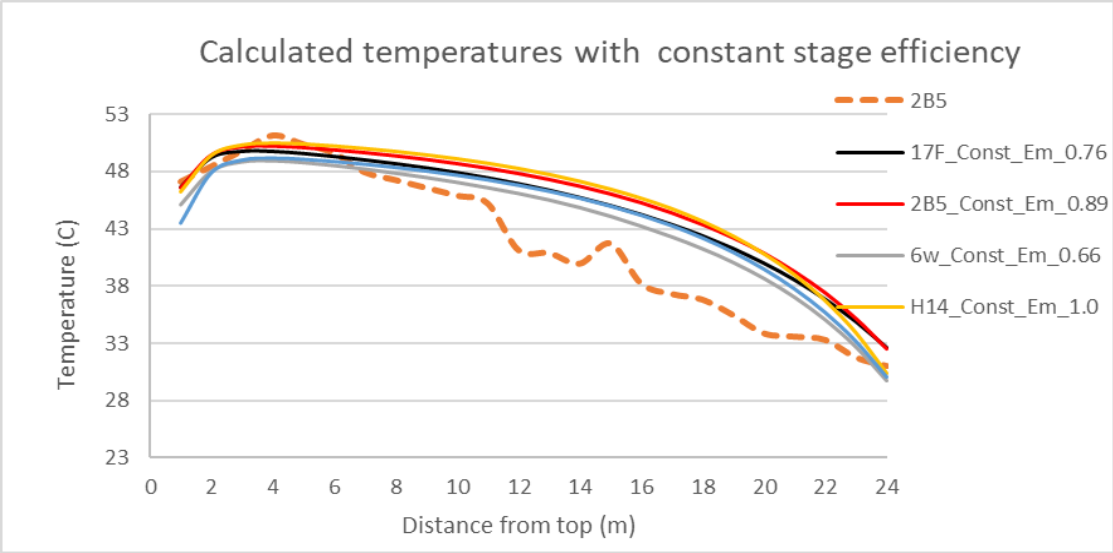

Figure 4-6: Calculated temperatures with constant stage efficiencies. Measured value included with dotted lines for comparison. (CO_2 removal equals test results for all calculations)

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4.3 Calculations with the Aspen Plus rate-based model

The rate-based model calculates the CO_2 removal based on the given input on lean amine and flue gas compositions and flowrates, and the specified dimensions and packing material for the absorber. The liquid holdup factor has been used for tuning to test performance data. The reason why the interfacial area factor is not used, is explained in chapter 4.3.3

The rate-based model calculates the Murphree stage efficiency that corresponds to the calculated stage efficiencies. The ratio of the mean efficiencies for two cases correspond to an E_m factor between those cases. In chapter 4.3.4 it is evaluated if these E_m factors from the rate-based model calculations can be used with Aspen HYSYS E_m model.

4.3.1 Rate-based model CO_2 removal calculations

The calculated removal efficiencies without model tuning, and the required tuning of the liquid hold-up factor to calculate CO_2 removal as measured, are listed in the table 4-5.

Table 4-5: Key input data from test cases and calculated CO_2 removal

Case	17F	Goal1	H14	2B5	6w
Key input:					
- Lean amin loading (mole CO_2/mole MEA)	0.20	0.20	0.23	0.23	0.25
- Lean amin / flue gas flow ratio	0.793	0.777	0.958	0.865	0.967
- MEA wt% (without CO_2)	31.0	32.3	30.0	31.6	30.4
CO2 removal (%)					
Test result	*83.5*	*90.1*	*90*	*87.3*	*79*
Rate-based (not tuned)	83.6	88.0	88.7	85.7	85.7
Holdup factor tuned model	1.0	2.2	1.5	1.6	0.1

Except for the case 6w, the calculated CO_2 removal with the rate-based model match quite well with the test results. For case 6w the reported CO_2 removal is 79% while the calculated value is 85.6%.

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4.3.2 Comparison with earlier work for the rate-based model

The rate-based model used in earlier work was provided by TCM and the input file was not possible to use.

The case H14 is used for comparison. The earlier work calculated the CO_2 removal to 88.8%. The model used in this work calculates 88.7% removal efficiency. The calculated temperatures are compared in figure 4-7.

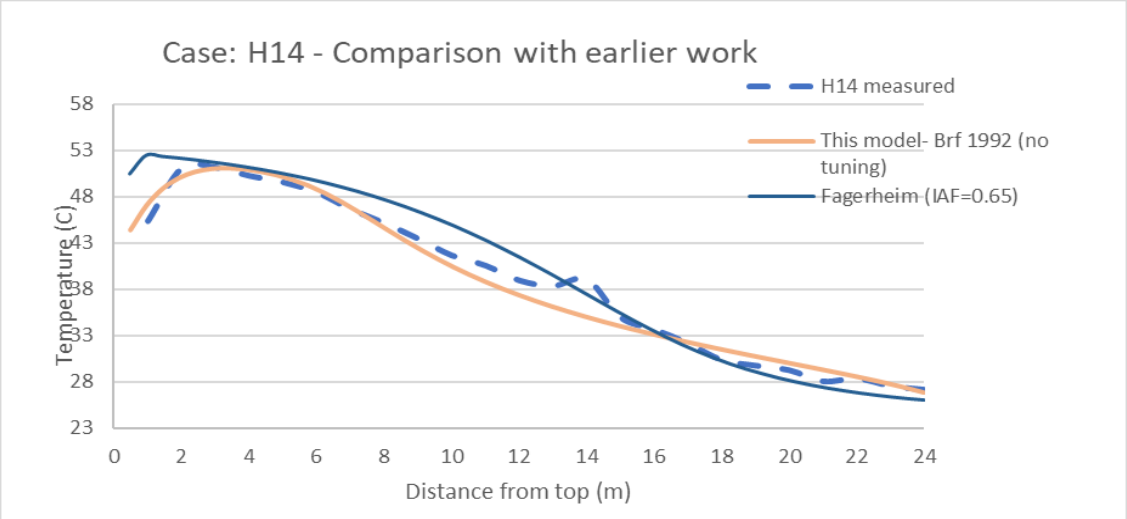

Figure 4-7: Comparison of case H14 temperature calculations with earlier work and with measured temperatures

Both models match the measured temperatures well. In the earlier work the interface area factor was used for tuning. The factor used for the earlier work curve in figure 4-7 was 0.65. The model used in this work is not tuned. When tuned with the liquid hold-up factor to match the CO_2 removal results, the calculated temperatures do not change.

4.3.3 Temperature calculations with the rate-based model

The temperature calculations are very much dependent on the chosen mass transfer correlation BRF-1992, together with fluid property package RK-ENRTL.

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The rate-based model does not assume equilibrium between bulk gas and liquid volumes and therefore calculates both liquid and gas temperatures. The observed radial horizontal spread in the temperature measurements at TCM is assumed mainly to be due to differences in gas and liquid temperatures. The figure 4-8 shows the individual measurements for case 2B5. The average of the values is used to present the measured temperatures, included as the grey line in the figure. Also included is the calculated gas and liquid temperatures.

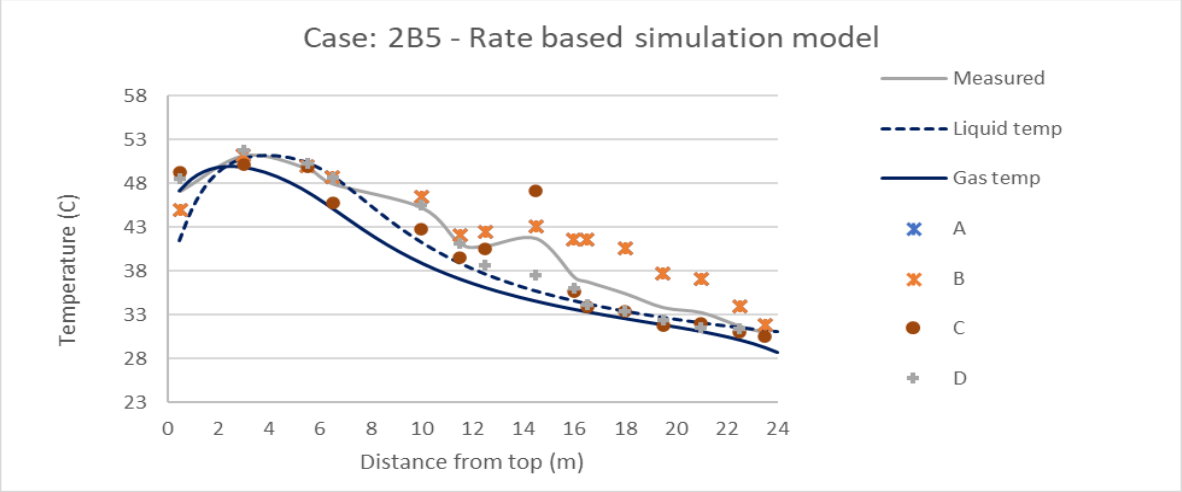

Figure 4-8: Measured and calculated temperatures for the case 2B5 with rate-based model

There is a considerable spread in the temperature measurements in the lower part of the column. The calculated liquid and gas temperatures does not show the same pattern as the measured temperatures.

It is possible to obtain higher differences in the lower part of the column by assuming an interface area factor less than 1. This is shown in the figure 4-9., where “iaf” in the legend is the interface area coefficient. However, this reduces the temperatures at the top of column, and reduces the CO_2 removal, which is not supported by the measurements.

The heat transfer between gas and liquid is uncertain, but the CO_2 removal calculations are not sensitive to changes in assumptions. It is possible to calculate larger differences in gas and liquid temperatures by reducing this heat transfer. But this gives largest differences at the top of column, and thus, does not agree with measurements.

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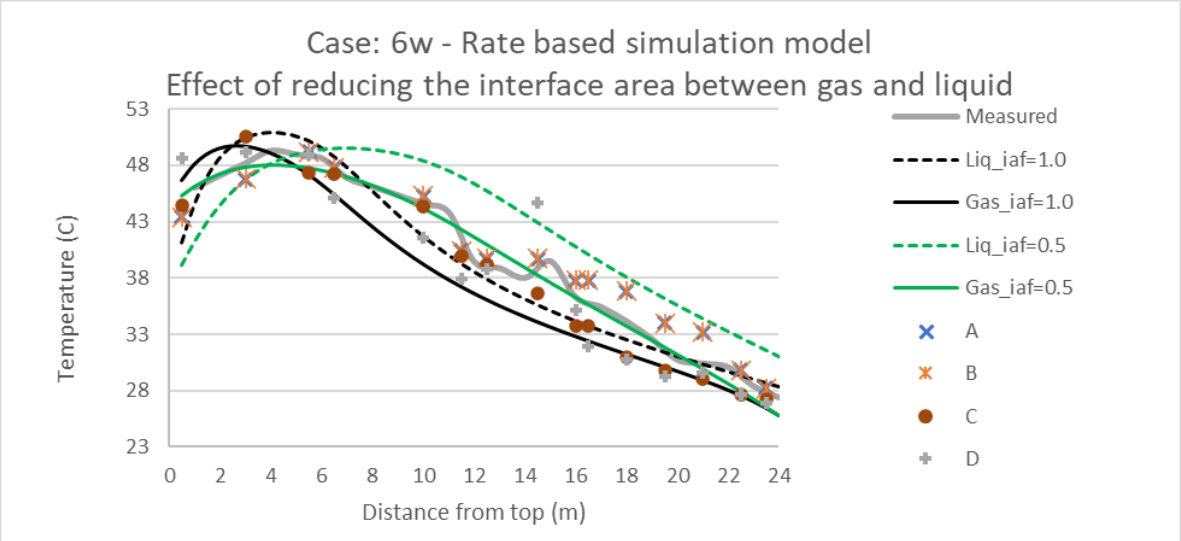

Figure 4-9: Measured and calculated temperatures for the case 6w with rate-based model

The calculated absorber temperature is assumed to be the average of the calculated gas and liquid temperatures. The calculated temperature profiles for the six cases are shown in the figure 4-10. The measured temperature profiles for the cases 2B5 and Goal1 are included to show the range of the measured temperatures.

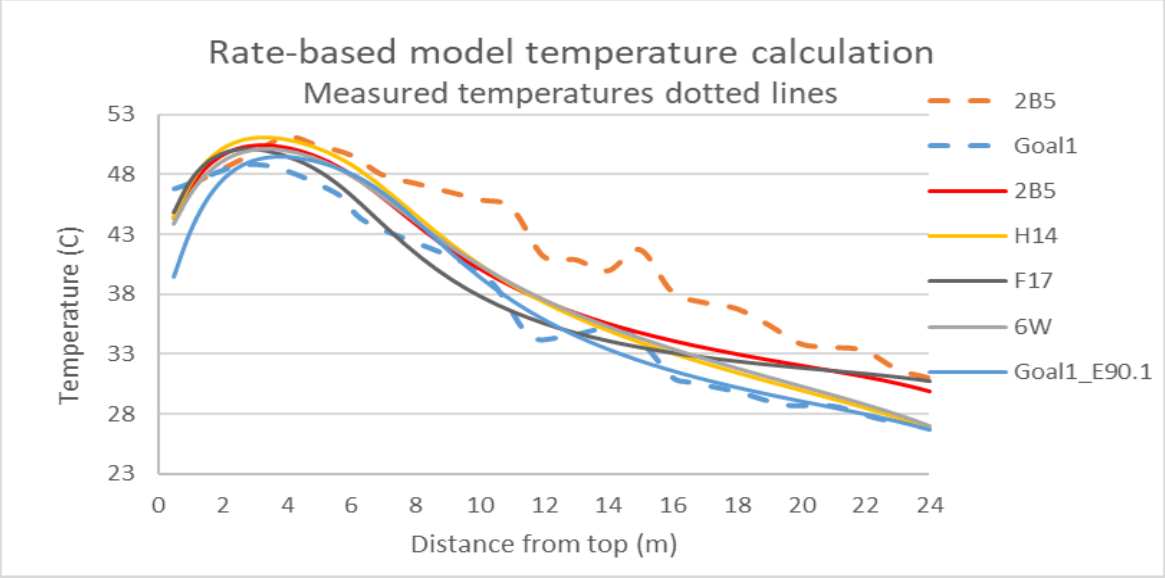

Figure 4-10: Calculated temperatures for the test cases with rate-based model. Measured temperatures with dotted lines for comparison. (CO_2 removal equals test results for all calculations)

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Comparison with the results from the Aspen HYSYS model in figure 4-4, and the complete set of test temperatures in figure 4-3, shows that it is possible to obtain a better average fit between calculations and measurements when using the Murphree efficiency factors with HYSYS. But the rate-based model calculations are also good.

4.3.4 Using the rate-based model to calculate E_m factors

The rate-based model calculates Murphree stage efficiencies. The ratio of calculated stage efficiencies between two cases can be compared with the E_m factor used in the Aspen HYSYS model.

The average Murphree stage efficiencies for the different cases are calculated. The results are shown in the table 4-3 including a comparison with the E_m factors estimated with the Aspen HYSYS model. The case H14 has been used as basis for calculations of ratios. This corresponds to the E_m equal 1.0 in table 4-4 for the E_m model.

The stage efficiency ratios calculated with the tuned the rate-based model, have been used to calculate new values with the Aspen HYSYS Em model, to compare the calculated CO_2 removals.
The calculated Murphree stage efficiencies are consistent when using the liquid hold-up factor.

Table 4-6: Comparison of Em factors in Aspen HYSYS and calculated changes in the stage efficiencies with the rate-based model, using case H14 as reference stage efficiencies

Table 4-6: Comparison of Em factors in Aspen HYSYS and calculated changes in the stage efficiencies with the rate-based model, using case H14 as reference stage efficiencies

Case	17F	Goal1	H14	2B5	6w
E_m factors					
HYSYS_Zhu from table 4-1	0.78	0.96	1.0	0.88	0.68
Calculated with tuned model	0.79	0.96	1.0	0.96	0.48

There is a good consistency between the rate-based model and the Aspen HYSYS Em model for three of the cases; H14, 17F and Goal1. However, for the case 6w, the deviation is large.

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4.4 Possible correlation to predict the Em-factor

This presented idea is purely empirical approach where easy estimation of the Em factor is the main idea. The intention has been to find a relatively simple approach to adjust the user defined stage efficiencies within a limited range of operational conditions. The ranges presented by the test cases in table 4-1 is assumed relevant.

It was imagined three sets of stage efficiencies called state A, B, C.

- State B can be calculated with the efficiency profile of A times an Em factor, - call it kab.
- State C can be calculated with the efficiency profile of B times an E_m factor, - call it kbc. Since state B be is estimated by state A multiplied with kab, state C can be estimated by the profile of A times the product of kab and kbc
- State C may also be calculated as state A times a constant kac. Thus kac = kab * kbc

It is assumed that in general a set of changes can be represented by multiplying a given efficiency profile with a corresponding set of factors. Stage efficiencies from a base case must be assumed known. The given stage efficiencies for the base case is multiplied with the set of factors to calculate a new state.

Flue gas flowrate and composition are assumed as known and constant values. The lean amine flowrate and load will typically vary with different process configurations. The amine concentration (wt%,not including CO_2) may also be subject to optimisation. It is assumed that the E_m factor should adjust for changes from a defined base case in:

- Lean amine load (mol CO_2/ mol MEA)
- Lean amine flowrate (kg/hr)
- Amine concentration (weight % not including CO_2)

A change in one of the above variables input assumptions will mean a change in the absorber CO_2 removal efficiency. The new absorber efficiency shall be calculated by assuming the base

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case efficiency profile multiplied by the factor to determine the user defined stage efficiencies.

The rate-based model was used to generate stage efficiency profiles. Only one of the three considered variables was changed at a time. The ratio between the generated stage efficiency profiles for the two conditions was calculated. It was assumed a linear relationship between the changes in the ratios and changes in the considered process variable. And it is assumed that relevant gradients are similar within the assumed operational ranges. These are approximations. One tuning factor for each variable is included which may also allow adjustments. The tuning factor is common to all predictions, to ensure consistency.

For each of the three assumed variables a simple equation 4-2 was assumed

$$k = c*(case\_input - base\_case\_value) \quad (4\text{-}2)$$

The "case_input" in the equation 4-2 is the input value of loading (mol CO_2/mol MEA), flowrate (1000 kg/hr) or concentration (wt%). The "base_case_value" is the relevant value from a reference case. If kl, kf and kc is the factors for lean loading, lean amine flowrate and MEA concentration respectively, the resulting E_m factor to include changes in all three variables can be calculated as the product of the three k-factors.

$$E_m = kl * kf * kc \quad (4\text{-}3)$$

The average stage efficiencies were calculated with simple calculations as described above. The case 17F was used as base case. Two new cases, called M1 and M2, were assumed after the tuning was performed. The calculated CO_2 removals for the cases M1 and M2 matched very well between the models. The results are given in the table 4-7.

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Table 4-7: Key input data, CO_2 removal and E_m factors calculated with simple correlation

Case	17F	H14	2B5	M1	M2
Key input:					
- Lean amin loading (mole CO_2/moleMEA)	0.20	0.23	0.23	0.215	0.215
Lean amin / flue gas flow ratio	0.793	0.958	0.865	0.877	0.835
- MEA wt% (without CO_2)	31.0	30.0	31.6	30.5	31.3
Calculated Em factors using the simple correlation	0.78	0.92	0.90	0.87	0.84
CO_2 removal (%)					
Test result	*83.5*	*90*	*87.3*		
Ratebased (not tuned)	83.6	88.7	85.7	87.4	86.5
HYSYS E_m model using the calcuted E_m factors	83.6	88.2	88.0	87.3	86.4

4.5 Comments to the calculations for the CHP flue gas cases

The deviations in the calculations of case 6w

The reported test data for the rich amine loading, 0.49 [(Sætre)] agrees with the calculated value with the untuned rate-based model. If the model is tuned to achieve 79% removal efficiency, the calculated rich amin loading is just below 0.48. Inconsistencies in the test measurements may explain the relatively large difference between reported and calculated CO_2 removal. But there are uncertainties in the measured values. (Test data for rich amin loading for other cases are given with only one digit, “0.5”)

Previous rate-based model assumptions

Previous student work used the ELECNRTL fluid property method and BRF-1985 correlations for mass transfer and interface area calculations. The previous model was developed by TCM and the input file was not possible to open. With the same assumptions the calculated CO_2 removal in this work deviated substantially from previous work. Some work was performed to identify that the RK-ENERTL fluid property correlation together with the BRF-1992 mass transfer, interface area and hold-up correlations, gave a good match with the measured results and previous calculations. The used correlations are among those available by default for the absorber packing material type.

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Previous student work used the interfacial area factor (IAF) for tuning. Model tuning to fully match the measured CO_2 removal was not possible for all the cases. Also, the tuning with IAF changed the calculated temperatures. There was generally not a good match with both temperatures and removal efficiency at the same time. When using the liquid hold-up factor (LHUF) for tuning, it has been possible to match the CO_2 removal efficiencies for all cases. And the temperature calculations are quite god with and without this tuning. Also, if IAF is changed, the calculated Murphree stage efficiencies cannot be compared between cases. However, it has not been evaluated if the results on CO_2 removal and temperature when using LHUF for tuning, could depend on other choices as the combination of the RK-ENERTL fluid property and the BRF-1992 mass transfer correlation.

Measured temperature spread in lower part of absorber

The reason for the radial spread in measured temperatures are assumed to be differences in gas and liquid temperatures. Another explanation may possibly be that the gas is not fully mixed in the structured packing and thus not a bulk gas temperature.

Temperature calculations with the rate-based model

Calculations with other correlations for mass transfer than the BRF-1992 can deviate substantially. The figure 4-11 below shows examples for case H14 when using the BRF-1985 correlations. The calculated temperatures are very dependent on the value of the interface area factor. The changes are not the same when using BRF-1992 correlations.

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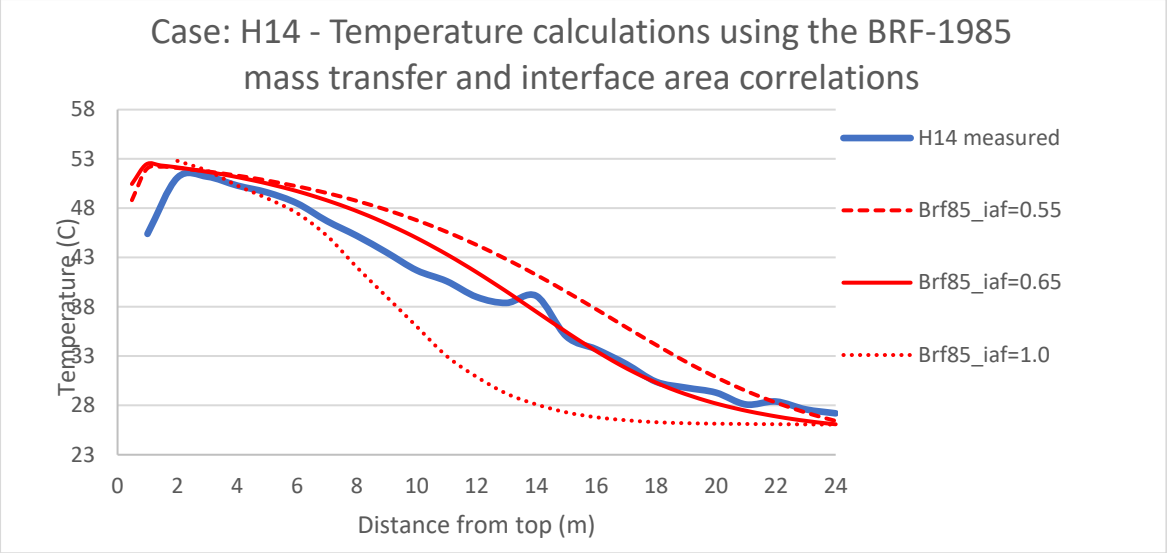

Figure 4-11: Measured and calculated temperatures for the case H14 and sensitivity to correlations and interface area factor (Fagerheim 2019)

Using a factor value of 1.0 with BRF-1985 will generally mean that the calculated temperatures are much too low for a large part of the column height than measured. And using a factor value below 1 is not always in line with measured CO_2 removal. It could be expected that the calculated temperatures in the upper part of the column should have differed more between the different interface area factor values, when the differences are that large in the middle.

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5 Results – RCC flue gas cases

Flue gas from coal power plants typically contain 12 – 15 mol% CO_2, compared to approximately 4 mol% from natural gas combined cycles power plants. The higher CO_2 concentration represents a higher driving force for separation and therefore tests and model calculations will differ. Flue gas from coal power often contain impurities which must be removed before CO_2 removal. This is performed and evaluated at TCM but is not discussed in this work.

Six test cases in a Specific Reboiler Duty (SRD) optimisation campaign performed by TCM in the period 2017-2018 have been used as a basis for this exercise. The comparison between test cases and models is based on test data that has been published (Sha, et al. 2018). The MEA wt% was only available as a range, and not case specific. It was therefore required to make some important assumptions linked to the calculations, as explained in chapter 5.1.2.

The same rate-based model as in chapter 4 is used and tuned with the liquid hold-up factor. To evaluate the suggested tuning to the SRD test cases, published test data for four other tests performed at TCM within the MEA Campaign 4 (Fosbøl 2019], were used. For one of these cases, the temperature profile in the absorber is published, which allowed for comparison with the models.

Comparison has also been made against four test cases that were performed at the pilot plant in Esbjerg in 2014. With an absorber diameter of 1.1 meters and a height of 17 meters, it is possible to consider the TCM plant as an upscaling of Esbjerg. It was therefore interesting to see how well calculations with the suggested rate-based model matched with published test results from the Esbjerg pilot plant test cases. Only calculations with the rate-based model have been done for the Esbjerg test cases.

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5.1 TCM SRD test cases

5.1.1 SRD test cases main input data

The flue gas composition assumed is given in table 5-1

Table 5-1: Flue gas composition RCC cases

Component	Mol%
N_2	70.1
O_2	12.2
CO_2	13.5
H_2O	4.2
	100.0
MW	30.36
Density (kg/Sm3)	1.28

The key input data from the six test cases in the SRD optimisation campaign used for the rate-based model tuning, and for Aspen HYSYS E_m model evaluation, are given in table 5-2. The lean amine flowrate and loading values differs significantly between cases. The measured CO_2 removal values do not vary that much. Higher loading is compensated by higher flowrates. The lean amine and flue gas inlet temperatures is 55 and 29 ^oC respectively.

Table 5-2: Key input data and test results for the TCM SRD test cases

Case	6c	6a	8a	5c	3	4
Key input:						
- Lean amin loading (mole CO_2/moleMEA)	0.16	0.19	0.199	0.204	0.251	0.273
Lean amine flowrate (kg/hr)	99670	114873	120360	116455	136867	160821
Flue gas flowrate (Smr/hr)	33908	33900	33934	33918	33699	33874
Flue gas flowrate used (for simplicity) (kg/hr)	43500	43500	43500	43500	43250	43500
Mass ratio lean amine / flue gas	2.29	2.64	2.77	2.68	3.16	3.70
Flue gas CO_2 content (mole %)	13.5	13.5	13.5	13.5	13.5	13.5
Measured CO_2 removal efficiency (%)	*88.3*	*87.3*	*87.4*	*87.3*	*88.1*	*85.9*

The rate-based model was used to estimate specific MEA concentrations. These values were used also as input for the Aspen HYSYS E_m model.

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The presentation of the results starts with the rate-based model in chapter 5.1.1. The temperature calculations for both the rate-based and the Aspen HYSYS E_m model is presented in chapter 5.1.2, including comparisons with test results and of the two models. Chapter 5.1.3 includes Aspen HYSYS model E_m factor calculations to obtain the same CO_2 removal efficiencies as measured.

5.1.2 SRD cases: CO_2 removal calculations with the rate-based model

Model tuning and case specific MEA wt% estimation

The first set of calculations was performed assuming an MEA concentration of 30 wt % (not including CO_2) for all the cases. Table 5-3 shows the results.

Table 5-3: CO_2 removal and model tuning with MEA 30 wt%

Case	6c	6a	8a	5c	3	4
CO_2 removal (%)						
Test result	*88.3*	*87.3*	*87.4*	*87.3*	*88.1*	*85.9*
Rate-based (not tuned)	87.9	91.5	92.5	88.9	86.7	90.2
Hold-up factors to calculate test results	1.1	0.4	0.3	0.7	1.3	0.4

The given MEA wt% range has been used to reduce the deviations between calculations and measurements. It has been assumed that case 8a represents the lower limit of the given MEA wt% range with 28 wt% (including CO_2). Case 3 is assumed as the upper limit with 30.2 wt% (including CO_2). The cases 8a and 3 are recalculated and the results are in table 5-4.

Table 5-4: Assumed input and resulting CO_2 removal for the cases 8a and 3

Case	8a	3
Assumed MEA concentration:		
- including CO_2 (wt%)	28.0	30.2
- not including CO_2 (wt%)	29.2	31.9
CO_2 removal (%):		
Test result	*87.4*	*88.1*
Rate-based (not tuned)	89.9	88.9
Holdup factors to calculate test results	0.6	0.84

For a generic model for RCC flue gas it is assumed a hold-up factor of 0.72. This is the middle value of the tuned values for the cases 8a and 3, as shown the table 5-4. The model with this

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hold-up factor is used to calculate the CO_2 removal for all cases. Each case assumes the MEA concentrations, within the given range, that gives the lowest deviation between calculated CO_2 removal and test results.

CO_2 removal calculated for the SRD test cases

The calculated removal and assumed MEA concentrations are given in table 5-5. The key input data is repeated for convenience.

Table 5-5: Key input data and measured and calculated CO_2 removal for the SRD cases

Case	6c	6a	8a	5c	3	4
Key input:						
- Lean amin loading	0.16	0.19	0.199	0.204	0.251	0.273
Flow ratio: Lean amin / flue gas	2.29	2.64	2.77	2.68	3.16	3.70
MEA wt% (without CO_2)	31.1	29.2	29.2	30.0	31.8	29.6
CO_2 removal (%)						
Test result	*88.3*	*87.3*	*87.4*	*87.3*	*88.1*	*85.9*
Liquid hold-up factor 0.72	88.3	*87.3*	*88.3*	87.3	87.5	*86.3*
Holdup factor, case specific			0.6		0.84	0.65

With the assumptions made, the calculated CO_2 removal efficiencies are in good agreement with the test results. Some further tuning on the liquid holdup factor is required for the cases 8a, 3 and 4 to match the test results accurately, as shown in the table 5-5.

5.1.3 SRD cases: Temperature calculations

The absorber temperature calculations are shown and discussed for both the Aspen HYSYS and the Aspen Plus models. A figure with measured temperatures for one case is published (Shah et al. 2018). This is assumed to be for Case 4 as this case matches the measured removal efficiency informed in the figure text in the reference. Comparison is in addition made between the models.

SRD Case 4 temperatures

The figure 5-1 shows measured and calculated temperatures for case 4.

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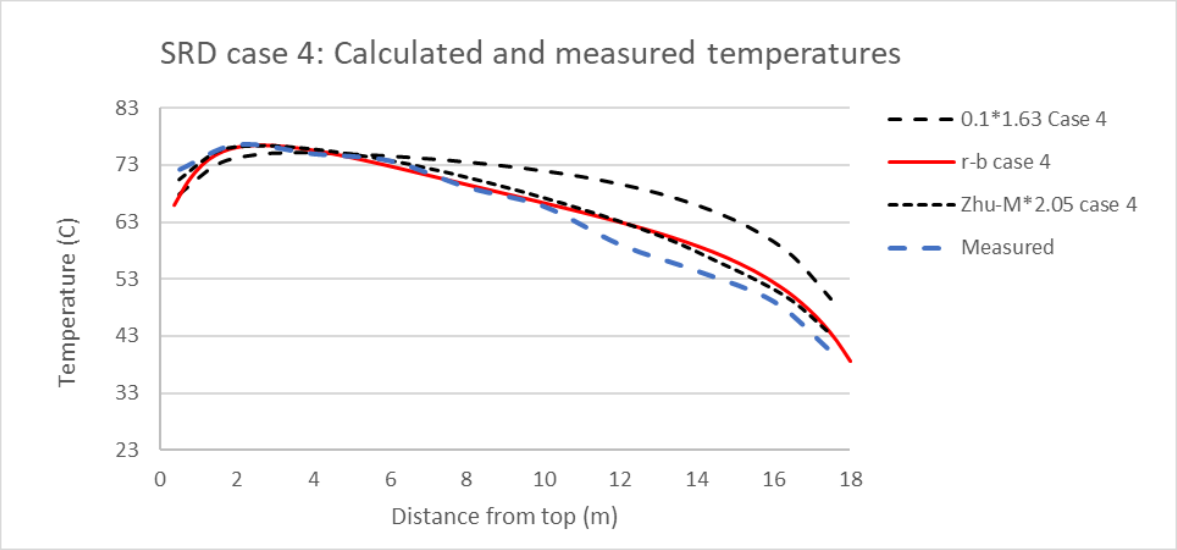

Figure 5_1: Calculated and measured temperatures for SRD case 4. (CO_2 removal equals test results for all calculations)

The rate-based model and the Aspen HYSYS E_m model using the Zhu_M profile calculate almost equal temperatures. The match with the test results is good, with some deviation on the lower part of the packed column. As expected, the calculated temperatures deviate when using a constant stage efficiency. The calculated E_m factor to obtain test result CO_2 removal differ significantly between the two profiles.

SRD temperature calculations with the rate-based model

The figure 5-2 below shows the calculated temperatures with the rate-based model for the six SRD cases. The figure includes the cases with specific tuning to match measured CO_2 removal. The differences in the calculated temperatures using the generic holdup factor of 0.72, was very small, and therefore not shown.

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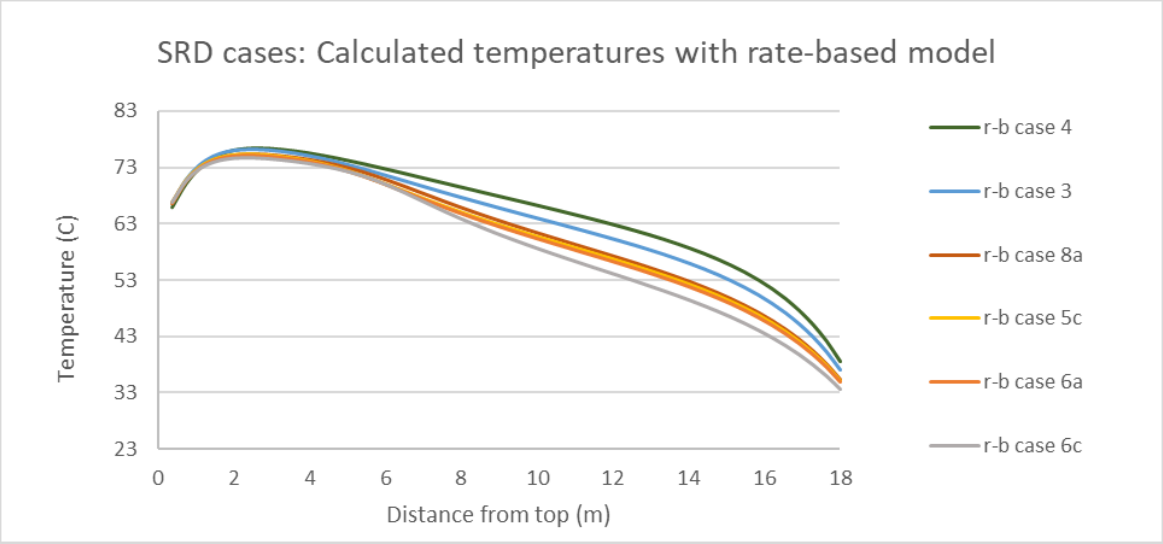

Figure 5-2: Calculated temperatures for SRD cases with the rate-based model. (CO_2 removal equals test results for all calculations)

SRD temperature calculations with the Aspen HYSYS Em model

The calculated temperatures with the Aspen HYSYS E_m model are shown in the figure 5-3. For comparison, the highest (case 4) and lowest (case 6c) temperature profiles from the rate-based model calculations are included.

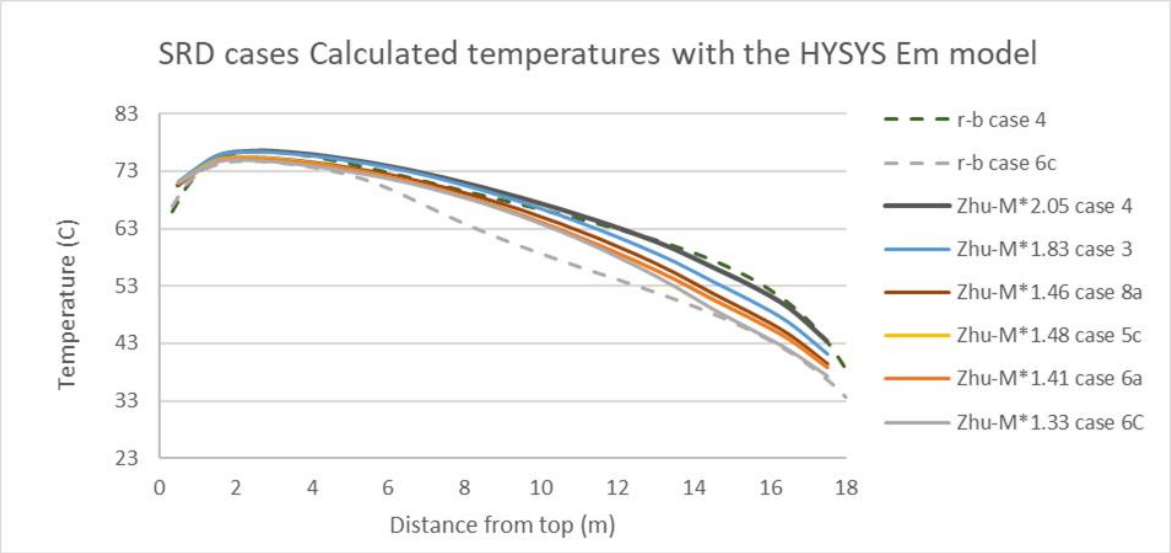

Figure 5-3: Calculated temperatures for the SRD test cases with the Aspen HYSYS Em model using the Zhu-M profile as a basis. The rate-based model calculations for cases 4 and 6c included for comparison. (CO_2 removal equals test results for all calculations)

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The rate-based model has a wider spread in the temperature calculations between the cases. One may observe that the order of temperature profiles from highest to lowest is the same for both models. It is the same order as for the lean amine loading and flowrate values. More CO_2 requires more MEA and thus more chemical reactions. The predicted E_m factor for the cases also follows the same order; highest E_m factor for case 4 with 2.05 and lowest for the case 6c with 1.33.

5.1.4 SRD cases: Estimation of E_m factor with the Aspen HYSYS model

The base stage efficiencies assumed, the Zhu_M profile and constant value 0.1, have been multiplied with a factor, the E_m factor, so that the calculated CO_2 removal efficiencies equal the test results. Table 5-6 repeats key input data the SRD cases in chapter 5.1, together with the tuned E_m factors for these cases.

Table 5-6: Key input data for SRD test cases, and the calculated Em factors

Case	6c	6a	8a	5c	3	4
Key input:						
- Lean amin loading (mole CO_2/mole MEA)	0.16	0.19	0.199	0.204	0.251	0.273
Mass flow ratio: Lean amin / flue gas	2.29	2.64	2.77	2.68	3.16	3.70
MEA wt% (without CO_2)	31.1	29.2	29.2	30.0	31.8	29.6
CO_2 removal (%)						
Test result	*88.3*	*87.3*	*87.4*	*87.3*	*88.1*	*85.9*
Calculated E_m factors:						
Zhu-M	1.33	1.41	1.46	1.48	1.83	2.05
Const 0.1	1.31	1.32	1.34	1.36	1.60	1.63

There are significant differences between the E_m factors estimated for Zhu_M and constant 0.1. Thus, the temperature profile is important for the CO_2 removal calculations for the RCC flue gas. Also, there are significant changes in the values for the cases 3 and 4, compared to the other cases.

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5.2 TCM Campaign 4 test cases

Campaign 4 included sixteen cases (Fosbøl et al. 2019). Four of them have been used to see how calculations with the proposed tuned rate-based model and the Aspen HYSYS E_m model compare with the test results and the observations for the SRD cases. The four cases represent a large range in lean amine flow and loading. They also included the highest and lowest measured CO_2 removal of the sixteen cases in the campaign.

The four cases selected from the TCM Campaign 4 are shown in the table 5-7. Measured temperatures are published for case 1A-1 and used for comparison with calculated temperatures.

Table 5-7: Key input data and test results from the TCM Campaign 4 test cases

Case	1A-1	1C	1D	2B
Key input:				
Lean amin loading (mol CO_2 / mol MEA)	0.215	0.29	0.318	0.266
Mas flow lean amin (kg/hr)	120100	200500	200600	165600
Mass flow flue gas (kg/hr)	43500	43500	43500	43500
Flue gas CO_2 content (mole %)	13.5	13.5	13.5	13.5
Measured CO_2 removal efficiency (%)	*90.1*	*89.7*	*78.7*	*89.4*

The MEA concentration is described as 30 wt% MEA. Case specific MEA values are not given, nor is a range. The same MEA range as for the six SRD test cases have been assumed and the MEA concentration is estimated the same way as in table 5-5 for the SRD cases.

5.2.1 Campaign 4 cases: CO_2 removal calculations with the rate-based model

The rate-based model used is the same as the in chapter 5.1 for the SRD cases. The result obtained are shown in the table 5-8. The lean amine flow and loading values for the cases 1C and 1D are well outside the ranges of the six SRD test cases in table 5-5. The deviation between calculations and test results for these cases are larger for these cases.

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Table 5-8: Key input data from the Campaign 4 test cases and calculated CO_2 removal

Case	1A-1	1C	1D	2B
Key input:				
Lean amin loading (mol CO_2 / mol MEA)	0.215	0.29	0.318	0.266
Mas flow ratio: Lean amin / flue gas	2.76	4.61	4.61	3.81
MEA wt% (without CO_2)	31.6	29.6	29.7	29.6
CO_2 removal (%)				
Test result	*90.1*	*89.7*	*78.7*	*89.4*
Rate-based with liquid holdup factor 0.72	89.4	*92.2*	*82.6*	89.3
Holdup factor case specific tuning	0.85	0.38	0.2	
Rich amine loading				
Measured (mol CO_2 / mol MEA)	0.483	0.507	0.507	0.513
Calculated (mol CO_2 / mol MEA)	0.513	0.493	0.501	0.512

The model does not predict the case 1D very well. Comparing the cases 1C and 1D, the measured consequence of an increased lean amine loading from 0.29 to 0.318 was a substantial reduction in CO_2 removal, which was only partly calculated by the model if not specifically tuned for the case.

The rich amine loading has been published and values are compared in the table. The values for case 1A-1 may indicate a higher MEA concentration than assumed for the calculations. If so, the higher limit for the MEA wt% range was larger than assumed.

5.2.2 Campaign 4 cases: Temperature calculations

The absorber temperature calculations are presented for both the Aspen HYSYS and the Aspen Plus models. The calculated temperatures are compared with measured for the case 1A-1.

Campaign 4 case 1A-1 temperatures

The calculated temperatures with the rate-based model agrees a bit better than the Aspen HYSYS model with the Zhu_M profile. As expected, the constant profile differs in temperatures. It also differs in the mean stage efficiency value. The stage efficiency to obtain the test result in CO_2 removal was 0.158 with a constant value stage efficiency. The corresponding mean stage efficiency with the Zhu_M profile was 0.172. A new profile was

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made to show that it possible to adjust the temperatures to better fit measured temperatures and maintaining the CO_2 removal efficiency. The new profile is called "Adjusted" in the figure 5.4.

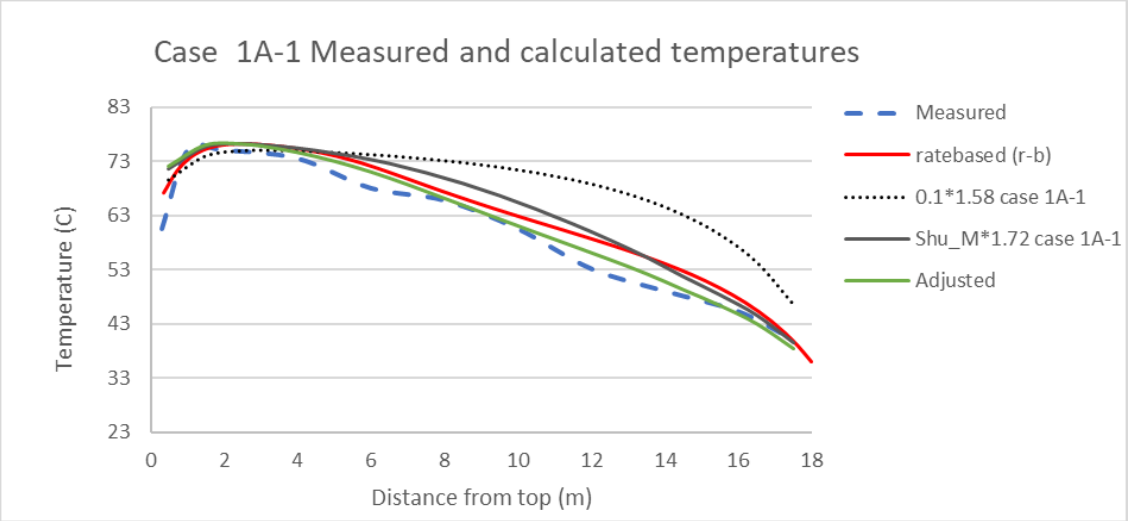

Figure 5-4: Calculated and measured temperatures for 1A-1 test case. (CO_2 removal equals test results for all calculations)

The stage efficiency profiles for Zhu-M*1.72 and for the Adjusted are listed in the table 5-9. There are substantial differences in the profiling. Still, the average stage values are quite close, with 0.168 compared to 0.172 for the Zhu_M profile.

*Table 5-9: Stage efficiencies according to Zhu-M*1.72 and Adjusted*

Stage	Zhu_M*1.72	Adjusted	Stage	Zhu_M*1.72	Adjusted
1	0.310	0.414	10	0.180	0.133
2	0.296	0.375	11	0.165	0.112
3	0.281	0.338	12	0.150	0.097
4	0.267	0.303	13	0.136	0.083
5	0.252	0.270	14	0.121	0.070
6	0.243	0.244	15	0.013	0.007
7	0.238	0.223	16	0.013	0.007
8	0.209	0.182	17	0.013	0.006
9	0.194	0.157	18	0.013	0.006
			Mean	0.172	0.168

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Campaign 4 temperature calculations with the rate-based model

The figure 5-5 below shows the calculated temperatures with the rate-based model for the four selected cases. The heavy tuning of the case 1D with a holdup factor of 0.2 did not matter for the temperature calculations.

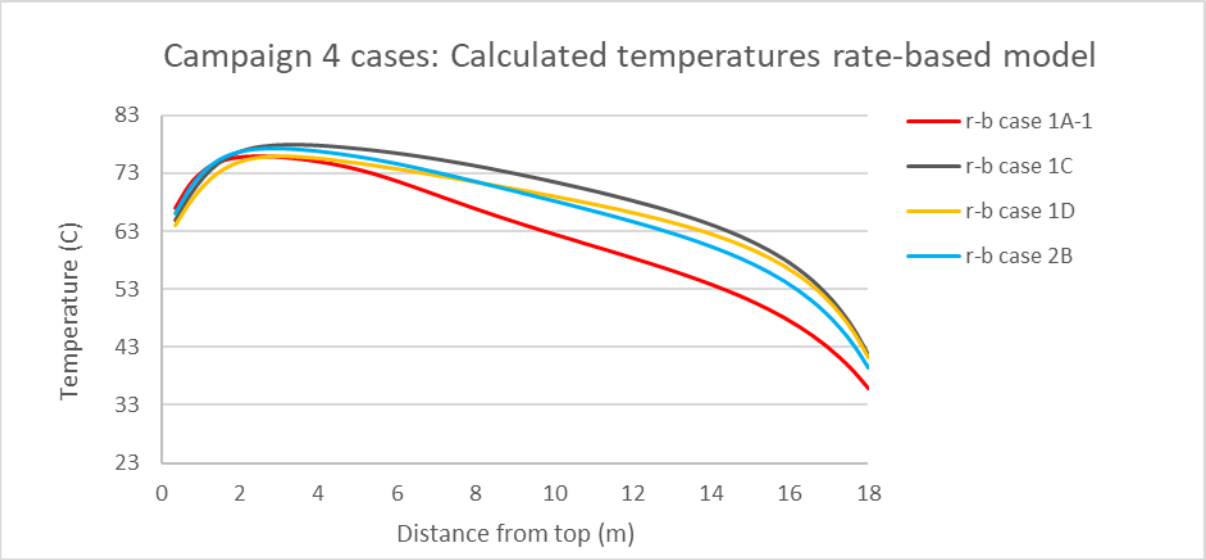

Figure 5-5: Calculated temperatures for SRD cases with the rate-based model. (CO_2 removal equals test results for all calculations)

SRD temperature calculations with the Aspen HYSYS Em model

For comparison, the highest (case 1C) and lowest (case 1A-1) temperature profiles from the rate-based model calculations are included with dotted lines in the figure 5-6, together with the results from the Aspen HYSYS E_m model. The comparison shows that the two models agree very well for all four cases.

There was some deviation from the measured values for case 1A-1, as shown in the figure 5-4. But the Zhu_M profile fitted quite well with the case 4 measurements from the SRD cases, as shown in figure 5-1. The Zhu profile is therefore useful for the RCC flue gas, as it was for the CHP flue gas cases in chapter 4.

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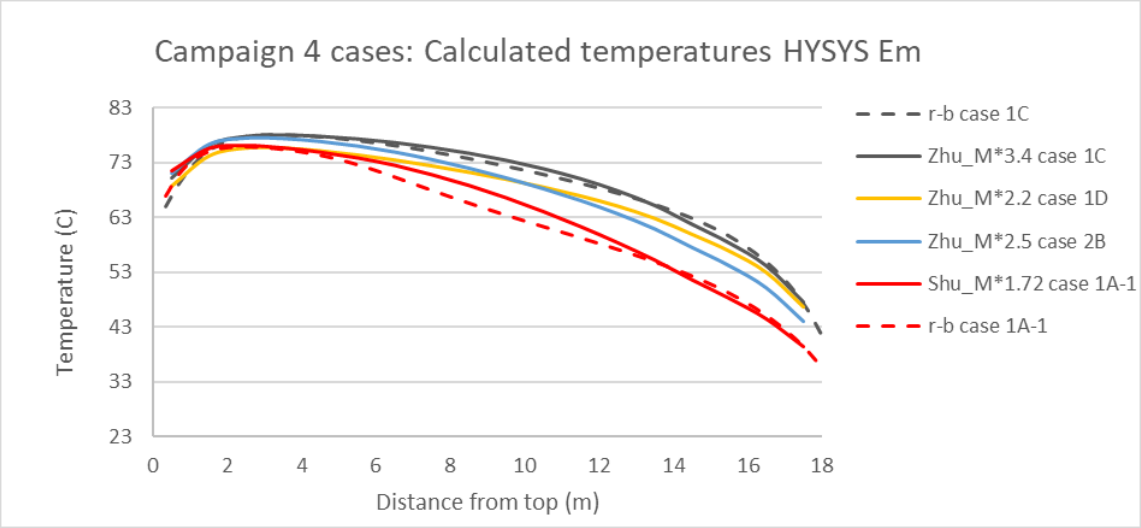

Figure 5-6: Calculated temperatures for the selected Campaign 4 test cases with the Aspen HYSYS Em model using the Zhu-M profile as a basis. The rate-based model calculations for cases 1C and 1A-1 are included for comparison. (CO_2 removal equals test results for all calculations)

5.2.3 Campaign 4 cases: Calculation of Em factor with the Aspen HYSYS model

The tuned Em factor to achieve the measured CO_2 removal efficiencies are shown in the table 5-10. The differences between the constant value profile and the Zhu_M profile are significant.

It can be observed that higher lean amine load cases generate higher E_m factors when high removal efficiencies are obtained in the result. The stage efficiencies had to be increased very much to match test results for the case 1C. In this case a removal efficiency of 89.7% was measured with a relatively high lean amine loading, 0.29, and a very high lean amine flowrate. When the lean amine loading in the case 1D is higher, 0.318, while the flowrate is maintained, the measured CO_2 removal efficiency drops significantly to 78.7%. Very different E_m factors had to be used for the two cases to calculate CO_2 removal efficiencies as measured.

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Table 5-10: Key input data for the selected Campaign 4 cases and calculated Em factors

Case	1A-1	1C	1D	2B
Key input:				
- Lean amin loading (mole CO_2/mole MEA)	0.215	0.29	0.318	0.266
Mass flow ratio: Lean amin / flue gas	2.76	4.61	4.61	3.81
MEA wt% (without CO_2)	31.6	29.6	29.8	29.6
CO_2 removal (%)				
Test result	*90.1*	*89.7*	*78.7*	*89.4*
Calculated E_m **factors:**				
Zhu-M	1.72	3.4	2.2	2.5
Const 0.1	1.58	2.47	1.15	2.0

5.3 Esbjerg pilot plant test cases

Results from several absorber and desorber performance test campaigns have been performed since year 2000 on several pilot plants and results have been made available. Important research programs before TCM (2012), and later, have been performed on pilot plants in Texas (USA), Regina (Canada) and Esbjerg (Denmark) (Wang et al 2011). The CASTOR and CESAR test programs in Esbjerg also had specific goal on reducing cost of CO_2 removal.

Published results from test cases from the Esbjerg pilot plant (Razi et al. 2013 a, b) has been used to see how well the proposed rate-based model compare with the reported CO_2 results. Calculations have been performed with the rate-based model only. The rate-based model is changed to represent the dimensions and packing material. The diameter is 1.1 meter and packed column height 17 meter. The packing material is Sulzer Mellapak 2X. Otherwise, the model used is the same as for the TCM cases.

The flue gas CO_2 concentration was 12 mol% and absorber inlet temperature between 48 and 50 ^oC. The lean amine inlet temperature was 40 ^oC. The MEA wt% was given as 30. Other key input is given in the table 5-11 together with results. The name of the cases has been changed to distinguish from the name of the TCM cases.

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Table 5-11: Key input data from Esbjerg test cases and CO_2 removal results

Case	E-1	E-2	E-3	E-4
Key input:				
Lean amin loading (mol CO_2 / mol MEA)	0.29	0.258	0.222	0.181
Lean amine flowrate (kg/hr))	23808	20832	17856	14880
Flu gas flowrate (kg/hr)	6304	6333	6364	6364
Mass flow ratio lean amine /flue gas	3.78	3.30	2.83	2.36
CO_2 removal (%)				
Test result	*88*	*90*	*88*	*87*
Rate-based (LHUF= 0.72)	86.7	*88.7*	*88.8*	86.7

The calculations of CO_2 removal seem to agree quite well with the reported results. There is an uncertainty with the assumed MEA wt% of 30. It may have been some variations between the cases. The use of liquid holdup factor (LHUF) of 0.72 is in accordance with suggested model for the TCM RCC fuel gas cases.

The figure 7 shows the calculated temperatures for the four cases compared with reported measured temperatures. The calculated temperatures agree very well with measurements.

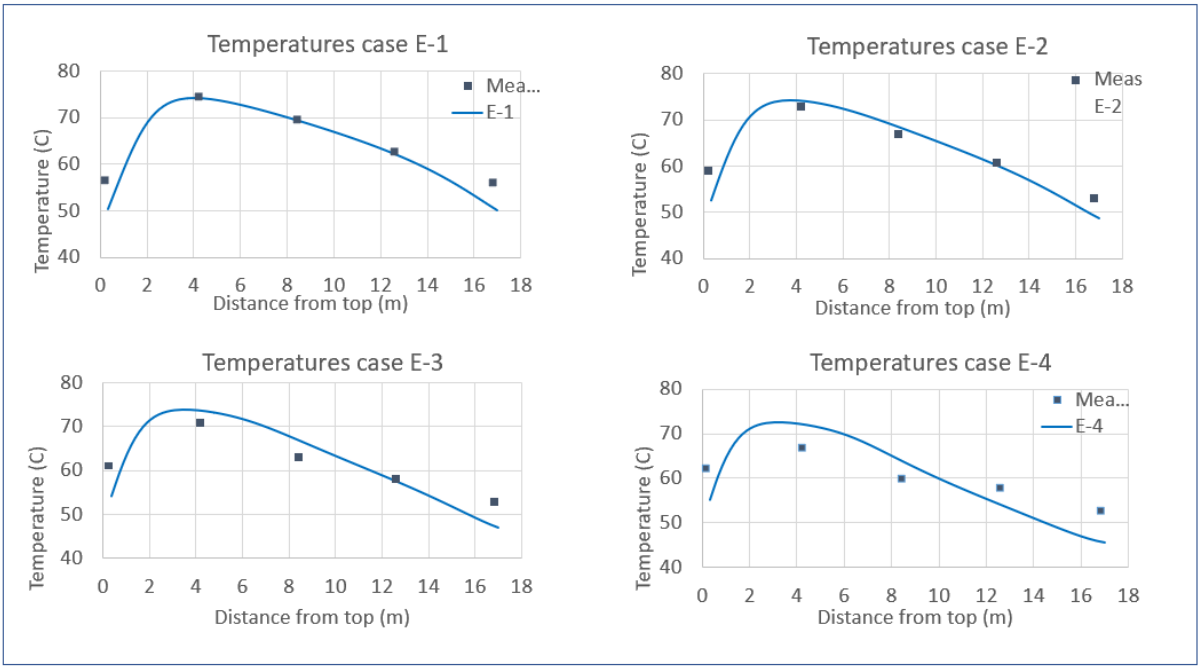

Figure 5-7: Calculated temperatures compared with measurements for the Esbjerg cases. (Liquid holdup factor 0.72 for all calculations)

The assumed gas composition is shown in table 5-12.

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Table 5-12: Gas composition assumed for Esbjerg cases

Component	Mol%
N_2	68.5
O_2	15.3
CO_2	12
H_2O	4.2
SUM	100.0
MW	30.11
Density (kg/Nm3)	1.34

5.4 Possible correlation to predict the absorber removal efficiency

The possible easy way to update Aspen HYSYS stage efficiencies with changes in input as presented in the chapter 4.3 will not work in this case for the RCC flue gas calculations. The model predictions are not consistent in the stage efficiencies. Instead, a similar approach is used to estimate the absorber efficiency when input values for lean amine loading, flowrate and/or MEA wt% are changing.

For convenience, the assumed simple correlations are repeated:

$$k = c*(case\_input - base\_case\_value) \quad (4\text{-}2).$$

$$E_m = kl*kf*kc \quad (4\text{-}3)$$

If there is a change in only one variable from a reference case, for instance lean amine flowrate, the new efficiency can be calculated by multiplying the reference case efficiency by a factor k. Similarly for lean amin loading and MEA wt%. If there is a change in all the three variables, the assumption is that it is possible to calculate the change in the removal efficiency as the product of the three factors for the individual changes. The factors kl, kf, and kc are the k factors calculated for the three variables when individual changes. The E_m factor in equation 4-3 is then not the Murphree stage efficiency factor but an overall absorber efficiency factor.

To estimate average slopes for the individual variable changes, some cases were calculated with the rate-based model, as shown in the table 5-13.

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Table 5-13: Absorber efficiency data used to estimate factor values for the simple correlation

Case	Base	1	2	3	4	5	6	7	8
Lean amine loading	0.225	0.2	0.2	0.2	0.2	0.25	0.25	0.25	0.25
Lean amine flowrate	112500	100000	100000	125000	125000	100000	100000	125000	125000
MEA wt%	31	30	32	30	32	30	32	30	32
Calculated efficiency	0.802	0.783	0.810	0.922	0.954	0.645	0.673	0.784	0.819
Re-calculated with simple correlation		0.778	0.809	0.920	0.958	0.662	0.689	0.784	0.816

From the cases 1-8, four different efficiency slopes can be calculated when only one of the variables are changed. The average of the four was used as the c-factor in the equation 4-3. The cases 1 – 8 were recalculated with the simple correlation. However, the mean slope for the lean amine flowrate was reduced with 15% (tuning factor 0.85) since that matched the results better when the efficiencies where recalculated. As shown in last rows, the recalculated values are very close to the calculated efficiencies. Since the calculated efficiencies with the rate-based model were used to generate the correlation, it should of course match well.

Without further tuning the simple correlation was used to recalculate the TCM SRD cases. The estimates are shown in the table 5-14.

Table 5-14: Recalculation of the TCM SRD cases using simple correlation

Case	Base	6c	6a	8a	5c	3	4
Lean amine loading	0.225	0.16	0.19	0.199	0.204	0.251	0.273
Lean amine flowrate	112500	99670	114873	120360	116455	136867	160821
MEA wt%	31	31.1	29.2	29.2	30	31.8	29.6
Test result		0.883	0.873	0.874	0.873	0.881	0.859
Recalculated with simple correlation		0.887	0.873	0.882	0.861	0.869	0.874

The calculated values with the simple correlation agree well for the SRD cases. Similarly, the selected four cases from the TCM campaign 4 were recalculated. These cases included

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significantly different input assumptions. The results in the second bottom row in the table 5-15, show large errors for the cases 1C and 1D.

The main change between the cases 1C and 1D is the lean amine loading. The test results indicate a much steeper slope for the lean amine loading than applied in the simple correlation. The last row in the table 5-15 is the calculated values if the lean amine loading factor is multiplied by 1.25. The results are then much better. But that change would have given poorer results for the SRD cases in the table 5-14.

Table 5-15: Recalculation of the TCM Campaign 4 cases using simple correlation

Case	Base	1A-1	1C	1D	2B
Lean amine loading	0.225	0.215	0.29	0.318	0.266
Lean amine flowrate	112500	140000	200500	200600	165600
MEA wt%	31	30	29.6	29.7	29.6
Test result		0.901	0.897	0.787	0.894
Recalculated with simple correlation		0.886	0.980	0.871	0.916
Recalculated with tuning factor 1.25 on lean amine loading		0.885	0.915	0.779	0.882

5.5 Comments to the MEA wt% assumptions

To be able to utilize the TCM test data it was necessary to make assumptions on the MEA wt% for the individual cases. The assumptions made are described together with results in the chapter 5.1.1. The upper and lower limit values in the given range was assigned to the two cases 8a and 3. The holdup factor was tuned for these two cases to match the CO_2 removal test results. The other cases were recalculated using the average of tuning factor of 8a and 3, which was 0.72. In these calculations it was assumed an MEA wt% within the range that gave the lowest deviation from the measured CO_2 removals. The assumptions made give about as low as possible deviations between measured and calculated CO_2 removals using a rate-based model with liquid holdup factor 0.72. The actual MEA concentrations will differ from those assumed.

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6 Sensitivity analysis

Some sensitivity calculations were performed to see if they could help to better understand the results presented in the chapters 4 and 5. The main attention is on the following two observations from chapter 4 and 5:

- For some test cases there are relatively large differences between calculated and measured results
- For the CHP flue gas cases there were a consistency between the Murphree CO_2 stage efficiencies used in Aspen HYSYS and those calculated by the rate-based model, with respect to changes from one case to another. This was not so for the RCC flue gas cases in chapter 4.

Calculations to show model behaviour when only one input varies at a time are used to comment on the two observations. These calculations do not consider the TCM stripper capacity.

6.1.1 HYSYS model using model default stage efficiencies

Another Aspen HYSYS model was found useful. The stage efficiencies are not user defined. Instead, the number of stages has been tuned to match calculated and measured CO_2 removal, thus utilising the model default values for stage efficiencies. The model is not generic. To match test results exactly, the number of stages will change. It is included with 88 stages model, which matched the CO2 removal efficiency for the 17F case.

6.1.2 The TCM CHP flue gas

When lean amine loading is changed, and everything else is assumed constant, the CO_2 removal efficiency will change. In the figure 6-1 below, the lean amin flowrate, and the flue gas composition and flowrate, are all kept constant. Two cases for MEA concentrations are included, 30 wt% and 33 wt%, where the 30 wt% line is dotted. The Aspen HYSYS E_m model results are shown with green lines. The E_m profile is the Zhu*0.78, which also corresponds to the 17F case.

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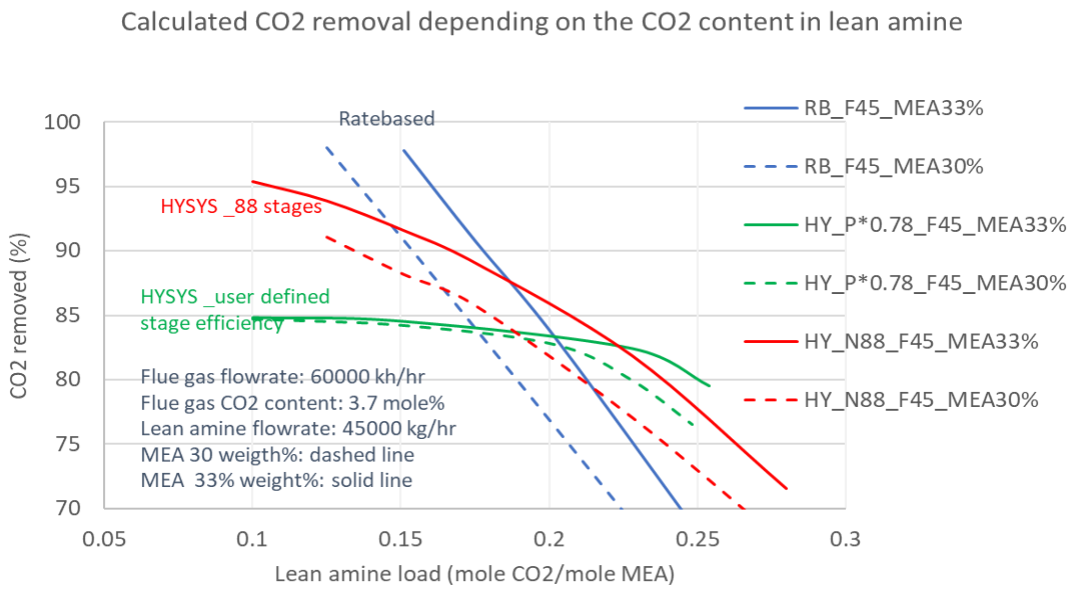

Figure 6-1: Sensitivity to lean amine load for lean amine flowrate of 45000 kg/hr

The 88 stages Aspen HYSYS model calculates a slope that differs from the rate-based model. The number of stages to match the test results will vary. Some difference is therefore as expected. The slope towards the 100% efficiency limit is very different from the rate-based line.

In the figure 6-2 similar results are generated with a higher lean amine flowrate. For both the rate-based and the 88 stages Aspen HYSYS model, the slope of the curves becomes steeper. But the Aspen HYSYS E_m model differ very much. It is almost horizontal, between 84 and 85% efficiency, for a large range of conditions. A different stage efficiency profile will assumingly give a similar curve on another CO_2 removal efficiency level. The calculated absorber efficiency is almost entirely given by the user defined stage efficiencies.

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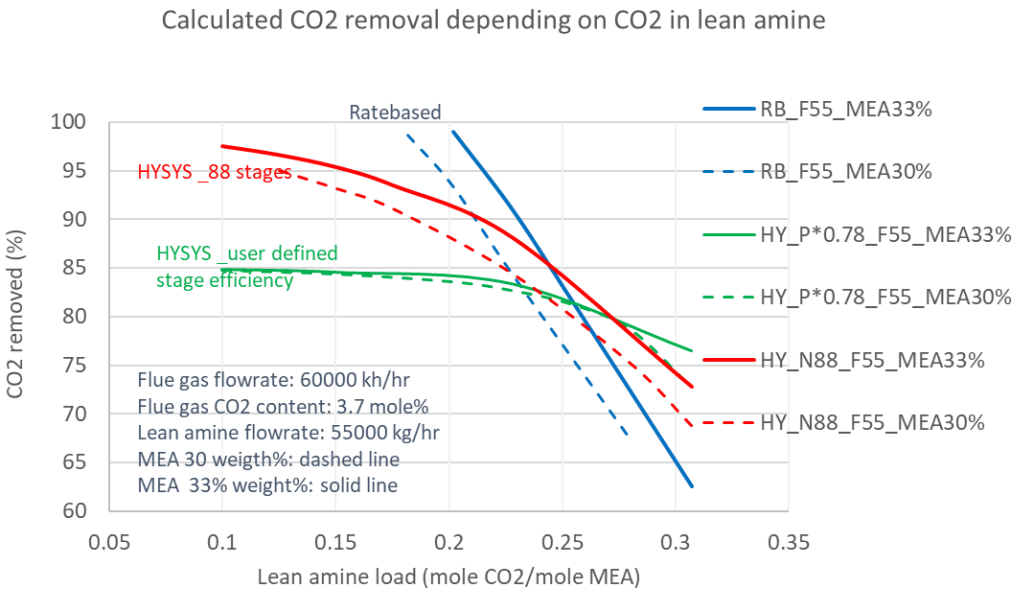

Figure 6-2: Sensitivity to lean amine load for lean amine flowrate of 55000 kg/hr

6.1.3 The TCM RCC flue gas cases

The figure 6-3 shows similar curves for the RCC flue gas. One main difference from the CHP flue gas is the slope of the Aspen HYSYS E_m model. For the CHP flue gas case the calculated efficiency was almost entirely defined by the user specified stage efficiency for a significant range of lean loading values. In the case of the RCC flue gas, the calculated efficiencies depend on the input values for lean amine loading, flowrate (or flow ratio to the flue gas) and MEA wt%, in addition to the user defined number of stages and efficiencies.

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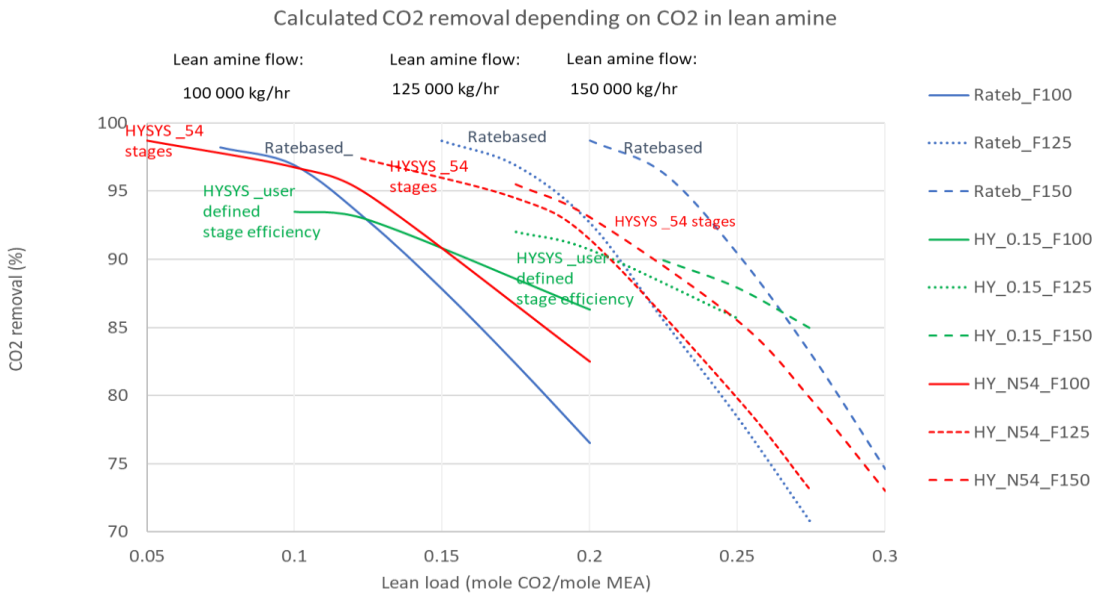

Figure 6-3: Sensitivity to lean amine load for RCC flue gas

The Aspen HYSYS model using model default efficiency values was developed with 54 stages, which matched the 6c test case. This test case has lean amine flowrate close to 100' kg/hr which explain that the curve is closest to the rate-based model for that lean amine flowrate in figure 6-3. If the number of stages was tuned to a case with higher flowrates, the curve would have been lifted and closer to the rate-based for the higher lean amine flowrates. For both models increased lean amine flowrates result in steeper curves. But the Aspen HYSYS model seem to start to bend towards the 100% efficiency line at a lower efficiency level. The deviation in the slopes between the two models may result in very different results. If case comparison with flowrates of about 125' kg/r and loading range 0.2 – 0.25, the models could wrongly be concluded to agree well.

Comments to the simple correlations for absorber efficiency

The ratio calculated with the rate-based model between two cases was not the same as the E_m factor required to update the Aspen HYSYS E_m model for the RCC flue gas cases. However, when changing the approach to estimate the absorber efficiency and not the stage efficiency in the Aspen HYSYS model, the reference case is a constant absorber efficiency value. Thus, the absorption capacity slopes calculated by the rate- based model could be used for the simple estimation of absorber efficiency. The E_m factor can be tuned based on the absorber efficiency.

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7 Discussion

The work is based on previously reported results from master's studies at USN. An important observation from previous work is that the CO_2 removal for one case can be calculated in Aspen HYSYS by multiplying the stage efficiencies used in another case, by a factor. The factor was named Murphree efficiency factor, E_m. Estimation of the E_m factor was central in this work. For a performed test case, the factor can be estimated by tuning of the model to get the measured removal efficiency. The challenge is how to estimate if *you* do not know the absorber efficiency.

7.1 Aspen HYSYS equilibrium model

The gas properties package used in Aspen HYSYS is not the same as in previous student work. This was due to new version of Aspen HYSYS (HYSYS v11). Results were compared. Slightly higher CO_2 removal efficiency was calculated when the same input was used.

There were clear differences between the calculations performed for the CHP flue gas and the RCC flue gas. For the CHP flue gas cases the calculated CO_2 removal was mainly dependent on the average user defined stage efficiencies. It did not matter much if a constant value for all stages, or a profile with large differences between stages, was used. If the average stage efficiency value was the same, the CO_2 removal calculated was the same. Changing inputs on lean amine loading, flowrate, or MEA wt%, did not change the calculated CO_2 removal much if the mean user defined stage efficiency was not changed. Case ratios of stage efficiencies calculated with the rate-based model was approximately equal to the ratios of the tuned stage efficiencies for the Aspen HYSYS model for the same cases. However, for one of the five test cases, case 6 w, the deviation was substantial between the two.

For the RCC flue gas cases, the calculated CO_2 removal may vary significantly with changing input in lean amine loading, flowrate, and MEA wt%, when the stage efficiencies are kept constant. But multiplying the stage efficiencies with an E_m factor is still required to match the test results. The estimated E_m factor can differ much between using profiled stage

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efficiencies and constant stage efficiencies in HYSYS. The ratio of stage efficiencies calculated for two cases with the rate-based model differ from those ratios estimated with the Aspen HYSYS models for the same cases. The reasons for the differences from the CHP flue gas cases is assumed linked to the CO_2 content of the flue gas with the respective changes in fluid flowrates and compositions.

Sensitivity calculations were performed which confirmed the differences observed between the CHP and the RCC flue gas cases.

The calculated absorber temperature profile depends on the user defined stage efficiency profile. The value of the Em factor is of secondary importance for the temperature calculations. If a constant stage efficiency value is used, the calculated temperatures will clearly deviate from the measured. When the profiled stage efficiencies are used, the calculated temperatures agree quite well with the measured temperatures. For the RCC flue gas cases, comparisons with temperature measurements are performed for two published cases only.

It was developed a stage efficiency profile to specifically match the Campaign 4 case 1A-1 measured temperature profile. However, it is not assumed likely that this adjusted profile in general will match the measurements better than the profile used for all cases. It would of course be an advantage for the evaluation if measured temperatures for more tests with the RCC flue gas, are made available.

The Esbjerg pilot plant tests was not simulated with the Aspen HYSYS E_m model. The TCM cases showed that the model could be adjusted for all cases. It was assumed not likely that the Esbjerg cases should provide new knowledge in the use of the Aspen HYSYS E_m model. But there could be of interest to compare the temperature calculations with the measurements. It is therefore included in recommendation for further work.

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7.2 Aspen Plus rate-based model

The rate-based model that was used in previous work was not possible to use. The version of Aspen HYSYS used could not read the TCM developed input file. As a part of familiarisation with the software, some effort was made to determine use of the RK-ENERTL fluid property package together with the BRF-1992 correlations for mass transfer.

The CO_2 removal calculations for the CHP flue gas are close to what was calculated in previous work. They matched test results quite well for four of the five cases. No generic tuning is suggested. For the RCC flue gas cases, assumptions had to be made with respect to MEA wt%. With these assumptions, it was observed that the model calculated too high CO_2 removal efficiencies, in the order of 2% in average. The model was therefore tuned with a liquid holdup factor of 0.72, as a general approach for the RCC flue gas cases. Most of the cases was then quite well calculated.

The model calculates the temperatures quite well, for some cases very well, and none poorly. The temperature calculations are not sensitive to the model tuning on the CO_2 removal with the liquid holdup factor (LHUF). In the previous work the interface area factor (IAF) had to be specified to a value lower than one to calculate temperatures that agreed with measurements (without any sound explanation). One may say that the IAF in the model used in earlier work gave a tool for temperature tuning. But this model calculates the temperatures just as good, and better, and thus is much better on predictive temperature calculations.

It is possible to use the LHUF to match all test cases on CO2 removal efficiencies. That was not possible for all cases with the IAF. And when tuning with the IAF to better match CO2 removal, some cases deviated very much on the measured temperatures in the earlier work.

Four cases from the Esbjerg pilot plant were also calculated. The CO_2 content was like the RCC flu gas. Both the CO_2 removal and the temperature agreed very well with the test results.

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The calculated CO_2 removal do not agree well for three cases. With respect to the case 6w within the CHP flue gas cases, this was also an observation in previous students work. Comparison of calculated rich amine loading with the rich amine loading value reported by TCM, may suggest that there are some uncertainties with the measurements. Model error may also be the reason. Within the CHP flue gas cases, this was the test with the highest lean amine loading and flowrate.

Two RCC test cases deviated more than others. They both had high amine flowrates compared to other tests, which was the reason why these cases were selected. They differed in the lean amine loading, and the measured CO_2 removal efficiencies were 89.7% and 78.7%. The model calculated 92.2% and 82.6%, which could be argued as reasonably well estimated given the conditions. But it also shows that accuracy of calculations will vary. It can be important to be aware of which ranges of conditions good accuracy can be expected.

Sensitivity calculations were made to see how changes in lean amine loading influenced the absorber removal efficiency. It is commented as a risk that the calculations may be too optimistic for conditions with very high removal efficiencies. This is based on comparison with a Aspen HYSYS model using model default efficiencies. There are not any test results for comparison.

The number of stages used in the rate-based model were 50. The results did not change for the CHP flue gas cases when the number of stages was increased to 96. When the number was reduced to 20, the calculated CO2 removal was reduced. Reduction was also observed when using RCC flue gas type. If the number of stages had been reduced in the generic model suggested for the RCC flue gas, the proposed liquid holdup factor could have been closer to 1.0. It has not been considered whether reducing the number of sections could have been a better approach than (only) tuning with the liquid holdup factor.

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7.3 Model comparison

Test data for model validation is required to ensure the accuracy of the calculations with a rate-based model. With the Em model, the user needs to know the absorber efficiency, which can be based on test cases. The case considered cannot deviate too much from test cases. Comparisons with more tests are necessary to define validity of the rate-based model. Calculations with the Em model depend on user having such a good insight into the process that he knows approximately what the efficiency should be. Alternatively, and as suggested, is that some simple correlations can possibly be used to estimate the removal efficiency. The Em model is easy to use, and the user can control the results.

The rate-based model has been used by researchers to develop correlations for mass transfer that agrees with observations. It is possible to analyse type of sensitivities that is not possible with the Em model. While the Em model can more easily be used in a work process to look at economic sensitivities to some relatively well defined alternatives with respect to technical assumptions.

7.4 Simple correlation for use with Aspen HYSYS Em model

If the rate-based model calculates accurately, the overall absorber efficiency calculated with the rate-based model can be used for tuning the Em factor to an Aspen HYSYS Em model. However, if an optimisation study requires a lot of calculations, it will be time consuming.

A simple correlation has been suggested to estimate an absorber efficiency multiplication factor that multiplied with the efficiency of reference case can calculate the stage efficiency. It is assumed that the factor can be calculated as the product of several factors. Each of these factors represents individual changes in lean amin loading, flowrate and MEA wt%. A simple exercise performed was positive. The set of factors and the reference case were developed by rate-based model calculations. But one set of factors will not be valid for a wide range of conditions. Model development will be required. The set of factors and reference case efficiency must be assigned case specifically, assumingly by interpolating between values generated for relatively equal conditions. Model development work would

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be required. One advantage with this absorber efficiency approach is that it could be possible to use results from tests, and not only the rely on rate-based model results, as the basis for the factor estimations.

Initially the attempt was to use this simple correlation approach to generate E_m factors for use with Aspen HYSYS E_m model. Applicability is likely limited and therefore not recommended for further work.

7.5 Recommendations further work

It is somewhat cumbersome to estimate the absorber efficiency with the rate-based model and then tune the Aspen HYSYS model. It is not identified another general way of finding the Em factor than by tuning. It is therefore suggested to evaluate the possibility of including the Aspen HYSYS model in an extended software package. This package must include a model, or correlation, that generates the absorber efficiency and some routine that tunes the Aspen HYSYS model. The E_m factor approach could possibly be used in an automatic tuning.

More work can be done in comparing tests and calculations, to suggest how models can be tuned, and to determine how the validity of a given version can be described within a given range of operating conditions. This is considered particularly important for further development of a rate-based model. But comparison with measured temperatures for RCC flue gas type should also be interesting for studies with the Aspen HYSYS E_m model.

It is suggested to evaluate the number of stages assumed in the rate-based model, and if the recommended number could depend on the CO_2 content in flue gas. Reduced number of stages for the RCC flue gas would mean reduced tuning with liquid holdup factor.

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8 Conclusion

Many new CO_2 removal plants are likely to be installed. Successful design and operations can be supported by methods and models. A good overview of process alternatives and options are important.

The work is based on previous student work to improve calculations models. During the work process it was considered of special interest to look further into the potential use of the Murphree efficiency factor E_m with the Aspen HYSYS model.

It is difficult to determine the E_m factor without knowing the efficiency of the absorber for given conditions. A simple correlation has been suggested and assumed possible to include in model development. If successfully developed the benefits may be:

- Efficient simulation work when performing energy and cost optimization studies
- Possibility to include measured values as cases used to generate the slope factors and not only rely on calculations with the rate-based model.

If successful, the model could then be a mean to systemize the knowledge of the absorber operations. But a user demand analyses should be performed to understand the potential and the required model user interface.

The rate-based model was tuned with the liquid holdup factor (LHUF). For the RCC flue gas cases it is suggested to use a LHUF of 0.72 as it would otherwise generally calculate too high CO_2 removal efficiencies. For the CHP flue gas cases no general tuning was recommended. This use of the LHUF may be linked to the model choices made for fluid property, mass transfer and interfacial area calculations. Earlier student work used the interfacial area coefficient (IAF) for case specific tuning. The use of IAF was not successful along with the model choices in this work.

The rate-based model is an important tool to estimate the absorber efficiency. The model used calculated most of the cases quite well and some very well. The deviations are higher

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for the cases with high lean amine flowrates than for the other cases. The number of tests that has been analysed (16) may not reveal all model deficiencies. The risk that the model also may calculate too high CO_2 removal when the efficiencies are high (above 90%), is commented. It is however possible to make versions of the model that predicts well within a given range of operating conditions.

The Aspen HYSYS E_m model is easy to use. With correct user input, it calculates accurately for a wide range of operating conditions. This user-control is assumed to be interesting to exploit. The use of E_m factor is an elegant way to update calculations.

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Appendix A: Task description

University of South-Eastern Norway

Faculty of Technology, Natural Sciences and Maritime Sciences, Campus Porsgrunn

FMH606 Master's Thesis

Title: Process simulation of CO_2 absorption data fitted to performance efficiency at TCM Mongstad

USN supervisor: Lars Erik Øi, Co-supervisors: Sumudu Karunarathne (USN), Ismail Shah (TCM)

External partner: CO_2 Technology Centre Mongstad (TCM)

Task background:
Technology Centre Mongstad (TCM) is the world's largest facility for testing and improving CO_2 capture, and started in 2006 when the Norwegian government and Statoil (now Equinor) made an agreement to establish the world's largest full scale CO_2 capture and storage project. To be able to predict process behaviour it is necessary to have good and robust simulation models.

There have been performed several projects at Telemark University College/ University of South-Eastern Norway on process simulation of amine based CO_2 capture processes. Most of the simulations have been performed with the program Aspen HYSYS, but the process has also been simulated using Aspen Plus. In several Master Thesis projects from 2014 to 2020, both programs have been used to simulate the monoethanol amine (MEA) based CO_2 capture process at TCM. These projects have mainly been limited to the absorption column using 24 meter of packing. There are available data for other conditions and also performance data for the stripping column.

Task description:
The aim of the project is to develop simulation models for amine based CO_2 capture.

1. A literature search on process simulation of stage efficiency in CO_2 capture by absorption and desorption.
2. Perform Aspen HYSYS and/or Aspen Plus simulations of the MEA based CO_2 capture process at TCM
3. Compare process simulations with performance data and design data
4. Develop the simulation models further and make suggestions for improvements

Student category: EET or PT

The task is suitable for online students (not present at the campus): Yes (but it must be possible to run the Aspen HYSYS program)

Practical arrangements:
The work will be carried out mainly in Porsgrunn or from home. A visit to TCM Mongstad is a possibility. The aim is to base the work on open available data, so that the thesis can be open. In case confidential information from TCM Mongstad is utilized, this information must however be treated confidentially.

Supervision:
As a general rule, the student is entitled to 15-20 hours of supervision. This includes necessary time for the supervisor to prepare for supervision meetings (reading material to be discussed, etc).

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Appendix B: Input data

Content:

B1: Input data for the CHP cases

H14 input data for process simulations --90% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	54900	Flow [kmol/h]	1986
Temperature [°C]	36.5	Temperature [°C]	25
MEA [mol%]	10.94	CO2 [mol%]	3.7
H2O [mol%]	86.54	H2O [mol%]	2.95
CO2 [mol%]	2.52	O2 [mol%]	13.6
Pressure [bara]	1.0313	N2 [mol%]	79.75
Loading	0.23	Pressure [bara]	1.063
MEA wt%	30		

Goal1 input data for process simulations -90.1% removal

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	44391	Flow [kmol/h]	1981
Temperature [°C]	28.6	Temperature [°C]	25
MEA [mol%]	12.04	CO2 [mol%]	3.62
H2O [mol%]	85.55	H2O [mol%]	3.1
CO2 [mol%]	2.41	O2 [mol%]	14.3
Pressure [bara]	1.0313	N2 [mol%]	79
Loading	0.2	Pressure [bara]	1.063
MEA wt%	32.3		

6w input data for process simulations -79% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	54915	Flow [kmol/h]	1970
Temperature [°C]	36.9	Temperature [°C]	25
MEA [mol%]	11.07	CO2 [mol%]	3.57
H2O [mol%]	86.16	H2O [mol%]	3
CO2 [mol%]	2.77	O2 [mol%]	13.6
Pressure [bara]	1.0313	N2 [mol%]	79.83
Loading	0.25	Pressure [bara]	1.063
MEA wt%	30.4		

F17 input data for process simulations -83.5% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	57434	Flow [kmol/h]	2512
Temperature [°C]	37	Temperature [°C]	29.8
MEA [mol%]	11.44	CO2 [mol%]	3.7
H2O [mol%]	86.27	H2O [mol%]	3.7
CO2 [mol%]	2.29	O2 [mol%]	14.6
Pressure [bara]	1.0313	N2 [mol%]	78
Loading	0.2	Pressure [bara]	1.01
MEA wt%	31		

2B5 input data for process simulations -87.3% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	49485	Flow [kmol/h]	1986
Temperature [°C]	36.8	Temperature [°C]	28.2
MEA [mol%]	11.67	CO2 [mol%]	3.57
H2O [mol%]	85.65	H2O [mol%]	3.7
CO2 [mol%]	2.68	O2 [mol%]	14.6
Pressure [bara]	1.0313	N2 [mol%]	78.13
Loading	0.2	Pressure [bara]	1.063
MEA wt%	31.6		

`

B2: Input data for the SRD cases

6c input data for process simulations --88.3% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	99670	Flow rate [kg/h]	43500
Temp. [°C]	55	Temp. [°C]	29
MEA [mol%]	11.50	CO2 [mol%]	13.5
H2O [mol%]	86.66	H2O [mol%]	4.2
CO2 [mol%]	1.84	O2 [mol%]	12.2
Pressure [bara]	1.0313	N2 [mol%]	70.1
Loading	0.16	Press. [bara]	1.063
MEA wt%	31.1		

5c input data for process simulations --87.3% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	116455	Flow rate [kg/h]	43500
Temp. [°C]	55	Temp. [°C]	29
MEA [mol%]	11.00	CO2 [mol%]	13.5
H2O [mol%]	86.76	H2O [mol%]	4.2
CO2 [mol%]	2.24	O2 [mol%]	12.2
Pressure [bara]	1.0313	N2 [mol%]	70.1
Loading	0.204	Press. [bara]	1.063
MEA wt%	30		

6a input data for process simulations --87.3% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	114873	Flow rate [kg/h]	43500
Temp. [°C]	55	Temp. [°C]	29
MEA [mol%]	10.60	CO2 [mol%]	13.5
H2O [mol%]	87.39	H2O [mol%]	4.2
CO2 [mol%]	2.01	O2 [mol%]	12.2
Pressure [bara]	1.0313	N2 [mol%]	70.1
Loading	0.19	Press. [bara]	1.063
MEA wt%	29.2		

3 input data for process simulations --88.1% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	136867	Flow rate [kg/h]	43250
Temp. [°C]	55	Temp. [°C]	29
MEA [mol%]	11.75	CO2 [mol%]	13.5
H2O [mol%]	85.30	H2O [mol%]	4.2
CO2 [mol%]	2.95	O2 [mol%]	12.2
Pressure [bara]	1.0313	N2 [mol%]	70.1
Loading	0.251	Press. [bara]	1.063
MEA wt%	31.8		

8a input data for process simulations --87.4% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	120360	Flow rate [kg/h]	43500
Temp. [°C]	55	Temp. [°C]	29
MEA [mol%]	10.60	CO2 [mol%]	13.5
H2O [mol%]	87.29	H2O [mol%]	4.2
CO2 [mol%]	2.11	O2 [mol%]	12.2
Pressure [bara]	1.0313	N2 [mol%]	70.1
Loading	0.199	Press. [bara]	1.063
MEA wt%	29.2		

6c input data for process simulations--85.9% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	160821	Flow rate [kg/h]	43500
Temp. [°C]	55	Temp. [°C]	29
MEA [mol%]	10.70	CO2 [mol%]	13.5
H2O [mol%]	86.38	H2O [mol%]	4.2
CO2 [mol%]	2.92	O2 [mol%]	12.2
Pressure [bara]	1.0313	N2 [mol%]	70.1
Loading	0.273	Press. [bara]	1.063
MEA wt%	29.6		

`

B1: Input data for the Campaign 4 cases

1A-1 input data for process simulations --90.1% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	120100	Flow rate [kg/h]	43500
Temp. [°C]	55	Temp. [°C]	29
MEA [mol%]	11.70	CO2 [mol%]	13.5
H2O [mol%]	85.79	H2O [mol%]	4.2
CO2 [mol%]	2.51	O2 [mol%]	12.2
Pressure [bara]	1.0313	N2 [mol%]	70.1
Loading	0.215	Press. [bara]	1.063
MEA wt%	31.6		

1D input data for process simulations --78.7% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	200600	Flow rate [kg/h]	43500
Temp. [°C]	55	Temp. [°C]	29
MEA [mol%]	10.70	CO2 [mol%]	13.5
H2O [mol%]	85.90	H2O [mol%]	4.2
CO2 [mol%]	3.40	O2 [mol%]	12.2
Pressure [bara]	1.0313	N2 [mol%]	70.1
Loading	0.318	Press. [bara]	1.063
MEA wt%	29.7		

1C input data for process simulations --89.7% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	200500	Flow rate [kg/h]	43500
Temp. [°C]	55	Temp. [°C]	29
MEA [mol%]	10.70	CO2 [mol%]	13.5
H2O [mol%]	86.20	H2O [mol%]	4.2
CO2 [mol%]	3.10	O2 [mol%]	12.2
Pressure [bara]	1.0313	N2 [mol%]	70.1
Loading	0.19	Press. [bara]	1.063
MEA wt%	29.6		

2B input data for process simulations --89.4% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	165600	Flow rate [kg/h]	43500
Temp. [°C]	55	Temp. [°C]	29
MEA [mol%]	10.70	CO2 [mol%]	13.5
H2O [mol%]	86.45	H2O [mol%]	4.2
CO2 [mol%]	2.85	O2 [mol%]	12.2
Pressure [bara]	1.0313	N2 [mol%]	70.1
Loading	0.266	Press. [bara]	1.063
MEA wt%	29.6		

`

B1: Input data for the Esbjerg cases

E-1 input data for process simulations --88% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	23808	Flow rate [kg/h]	6303
Temp. [°C]	40	Temp. [°C]	50
MEA [mol%]	10.90	CO2 [mol%]	12
H2O [mol%]	85.94	H2O [mol%]	4.2
CO2 [mol%]	3.16	O2 [mol%]	15.3
Pressure [bara]	1.0313	N2 [mol%]	68.5
Loading	0.29	Press. [bara]	1.063
MEA wt%	31.6		

E-3 input data for process simulations --88% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	17856	Flow rate [kg/h]	6364
Temp. [°C]	40	Temp. [°C]	48
MEA [mol%]	10.90	CO2 [mol%]	12
H2O [mol%]	86.68	H2O [mol%]	4.2
CO2 [mol%]	2.42	O2 [mol%]	15.3
Pressure [bara]	1.0313	N2 [mol%]	68.5
Loading	0.222	Press. [bara]	1.063
MEA wt%	29.7		

E-2 input data for process simulations --90% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	20832	Flow rate [kg/h]	6333
Temp. [°C]	40	Temp. [°C]	49
MEA [mol%]	10.90	CO2 [mol%]	12
H2O [mol%]	86.29	H2O [mol%]	4.2
CO2 [mol%]	2.81	O2 [mol%]	15.3
Pressure [bara]	1.0313	N2 [mol%]	68.5
Loading	0.258	Press. [bara]	1.063
MEA wt%	29.6		

E-4 input data for process simulations --87% removal.

Amine inlet		Flue gas inlet	
Flow rate [kg/h]	14880	Flow rate [kg/h]	6364
Temp. [°C]	40	Temp. [°C]	48
MEA [mol%]	11.00	CO2 [mol%]	12
H2O [mol%]	87.00	H2O [mol%]	4.2
CO2 [mol%]	2.00	O2 [mol%]	15.3
Pressure [bara]	1.0313	N2 [mol%]	68.5
Loading	0.181	Press. [bara]	1.063
MEA wt%	29.6		

`

Appendix C: Temperatures for the CHP cases

Content:

C1: Measured temperatures (average)

Stage / distance from top (m)	Measured temperature profiles					
	Data from Fagerheim (Fagerheim 2019)				Based on TCM data (Sætre 2016)	
	17F	2B5	6w	H14	Distance from top (m)	Goal1
1	47.4	47.1	46.05	45.4	0.5	46.8
2	51.7	48.44	47.15	51.1	3	48.9
3	51.6	49.79	48.25	51.2	5.5	46.5
4	50.5	51.14	49.35	50.3	6.5	44.0
5	49.9	50.36	49.01	49.6	10	39.9
6	48.9	49.59	48.68	48.5	11.5	34.7
7	47.2	47.92	46.9	46.7	12.5	34.4
8	46	47.24	46.14	45.2	14.5	35.1
9	44.4	46.56	45.38	43.5	16	31.1
10	43.1	45.88	44.61	41.7	16.5	30.7
11	42.2	45.2	43.85	40.6	18	29.9
12	40.9	41.13	39.45	39	19.5	28.8
13	40.6	40.86	38.88	38.4	21	28.7
14	41.6	39.94	38	39.1	22.5	27.6
15	37.4	41.7	39.5	35	23.5	27.3
16	37.1	38.2	36.27	33.7		
17	35.9	37.28	35.4	32.2		
18	34.3	36.79	34.13	30.4		
19	34.1	35.43	32.55	29.8		
20	33.8	33.84	30.7	29.3		
21	32.9	33.56	30.38	28.1		
22	33.2	33.27	30.05	28.4		
23	32.5	31.73	28.35	27.6		
24	32.4	30.99	27.33	27.2		

`

C2: Calculated Aspen HYSYS Zhu profile

Stage	Calculated temperatures with Zhu profile				
	17F	Goal1	H14	2B5	6w
1	47.3	44.6	47.4	47.3	46.0
2	49.7	48.9	50.5	50.0	48.8
3	49.9	49.6	51.2	50.4	49.2
4	49.4	49.4	50.9	50.1	48.8
5	48.7	48.9	50.4	49.5	48.1
6	47.8	48.1	49.7	48.7	47.3
7	46.7	47.2	48.8	47.8	46.3
8	45.4	46.0	47.7	46.6	45.1
9	44.0	44.7	46.4	45.4	43.8
10	42.5	43.2	44.9	44.0	42.4
11	40.8	41.6	43.3	42.4	40.9
12	39.0	39.7	41.4	40.7	39.2
13	36.9	37.5	39.3	38.8	37.3
14	34.8	35.2	37.0	36.8	35.3
15	33.7	32.8	34.5	34.7	33.3
16	33.0	31.3	32.8	33.5	31.9
17	32.6	30.4	31.7	32.7	30.9
18	32.2	29.7	30.8	32.2	30.1
19	31.9	29.2	30.0	31.7	29.4
20	31.6	28.7	29.3	31.3	28.8
21	31.3	28.2	28.7	30.9	28.2
22	31.0	27.7	28.0	30.6	27.7
23	30.7	27.2	27.4	30.2	27.1
24	30.4	26.7	26.7	29.9	26.5
Em- value	0.78	0.96	1	0.88	0.68
CO2 -rem (%)	83.5	90.1	90	87.3	79
Calc r.am.load	0.478	0.489	0.489	0.484	0.477
Calc r.am.load = calculated rich amine loading					

`

C3: Calculated Aspen HYSYS 0.1 profile

Stage	Calculated temperatures with Zhu profile				
	17F	Goal1	H14	2B5	6w
1	46.7	43.5	46.2	46.6	45.1
2	49.3	48.0	49.4	49.5	48.1
3	49.8	49.1	50.3	50.2	48.9
4	49.8	49.2	50.5	50.2	49.0
5	49.6	49.1	50.4	50.1	48.8
6	49.4	48.9	50.2	49.9	48.6
7	49.1	48.7	50.0	49.7	48.2
8	48.7	48.4	49.7	49.4	47.9
9	48.4	48.1	49.4	49.1	47.5
10	48.0	47.7	49.1	48.7	47.1
11	47.5	47.3	48.7	48.3	46.6
12	47.0	46.9	48.2	47.8	46.1
13	46.4	46.3	47.7	47.3	45.5
14	45.8	45.7	47.1	46.7	44.9
15	45.1	45.0	46.4	46.1	44.1
16	44.3	44.2	45.6	45.3	43.3
17	43.4	43.3	44.7	44.4	42.3
18	42.4	42.2	43.6	43.4	41.3
19	41.3	41.0	42.3	42.2	40.1
20	40.0	39.5	40.8	40.9	38.7
21	38.6	37.8	39.0	39.3	37.0
22	36.9	35.7	36.7	37.4	35.1
23	34.9	33.2	33.9	35.2	32.7
24	32.7	30.0	30.4	32.6	29.7
Em- value	0.76	0.96	1	0.89	0.66
CO2 -rem (%)	83.5	90.1	90	87.3	79
Calc r.am.load	0.478	0.488	0.488	0.484	0.477

Calc r.am.load = calculated rich amine loading

`

C4: Aspen Plus rate-based temperature

Stage	Case														
	17F			Goal1			H14			2B5			6w		
	Gas	Liq	Aver	Gas	Liq	Aver	Gas	Liq	Aver	Gas	Liq	Aver	Gas	Liq	Aver
1	47.3	42.3	44.8	44.4	35.8	40.1	47.5	41.6	44.6	47.5	42.1	44.8	47.3	42.3	44.8
2	48.7	46.0	47.3	46.7	41.2	44.0	49.1	45.5	47.3	48.9	45.8	47.4	48.7	46.0	47.3
3	49.4	48.3	48.8	48.1	45.1	46.6	50.1	48.1	49.1	49.8	48.3	49.0	49.4	48.3	48.8
4	49.7	49.7	49.7	48.9	47.6	48.2	50.7	49.8	50.3	50.1	49.9	50.0	49.7	49.7	49.7
5	49.7	50.4	50.1	49.3	49.1	49.2	50.9	50.9	50.9	50.2	50.8	50.5	49.7	50.4	50.1
6	49.5	50.8	50.1	49.3	50.0	49.7	50.9	51.6	51.2	50.0	51.3	50.6	49.5	50.8	50.1
7	49.1	50.9	50.0	49.1	50.5	49.8	50.7	51.9	51.3	49.6	51.5	50.5	49.1	50.9	50.0
8	48.5	50.8	49.7	48.7	50.7	49.7	50.3	52.0	51.2	49.1	51.4	50.2	48.5	50.8	49.7
9	47.8	50.6	49.2	48.1	50.7	49.4	49.8	51.9	50.9	48.3	51.2	49.8	47.8	50.6	49.2
10	47.0	50.2	48.6	47.3	50.5	48.9	49.2	51.7	50.4	47.5	50.7	49.1	47.0	50.2	48.6
11	46.0	49.6	47.8	46.4	50.1	48.2	48.4	51.3	49.8	46.5	50.0	48.2	46.0	49.6	47.8
12	45.0	48.7	46.8	45.3	49.4	47.3	47.5	50.7	49.1	45.5	49.0	47.2	45.0	48.7	46.8
13	43.9	47.5	45.7	44.2	48.3	46.2	46.5	49.8	48.2	44.5	47.9	46.2	43.9	47.5	45.7
14	42.7	46.3	44.5	43.0	47.0	45.0	45.5	48.8	47.1	43.4	46.7	45.0	42.7	46.3	44.5
15	41.7	45.0	43.3	41.8	45.6	43.7	44.4	47.7	46.0	42.5	45.5	44.0	41.7	45.0	43.3
16	40.6	43.7	42.2	40.7	44.2	42.4	43.4	46.5	44.9	41.5	44.3	42.9	40.6	43.7	42.2
17	39.7	42.5	41.1	39.6	42.9	41.3	42.4	45.4	43.9	40.7	43.2	42.0	39.7	42.5	41.1
18	38.9	41.3	40.1	38.7	41.7	40.2	41.5	44.2	42.8	39.9	42.2	41.1	38.9	41.3	40.1
19	38.1	40.3	39.2	37.8	40.5	39.2	40.6	43.2	41.9	39.2	41.3	40.3	38.1	40.3	39.2
20	37.5	39.4	38.4	37.0	39.5	38.2	39.8	42.2	41.0	38.6	40.5	39.5	37.5	39.4	38.4
21	36.8	38.6	37.7	36.3	38.5	37.4	39.0	41.3	40.1	38.0	39.8	38.9	36.8	38.6	37.7
22	36.3	37.9	37.1	35.6	37.7	36.7	38.3	40.4	39.4	37.5	39.1	38.3	36.3	37.9	37.1
23	35.8	37.2	36.5	35.0	36.9	36.0	37.7	39.6	38.6	37.0	38.5	37.7	35.8	37.2	36.5
24	35.4	36.7	36.0	34.5	36.2	35.3	37.1	38.9	38.0	36.5	37.9	37.2	35.4	36.7	36.0
25	35.0	36.1	35.6	34.0	35.6	34.8	36.5	38.2	37.3	36.1	37.4	36.7	35.0	36.1	35.6
26	34.6	35.7	35.1	33.5	35.0	34.2	35.9	37.6	36.7	35.7	36.9	36.3	34.6	35.7	35.1
27	34.3	35.2	34.8	33.1	34.4	33.8	35.4	37.0	36.2	35.3	36.5	35.9	34.3	35.2	34.8
28	34.0	34.9	34.4	32.7	33.9	33.3	34.9	36.4	35.7	35.0	36.0	35.5	34.0	34.9	34.4
29	33.7	34.5	34.1	32.3	33.5	32.9	34.5	35.9	35.2	34.7	35.7	35.2	33.7	34.5	34.1
30	33.5	34.2	33.9	31.9	33.1	32.5	34.0	35.4	34.7	34.4	35.3	34.9	33.5	34.2	33.9
31	33.3	33.9	33.6	31.6	32.7	32.1	33.6	34.9	34.2	34.1	35.0	34.6	33.3	33.9	33.6
32	33.1	33.7	33.4	31.3	32.3	31.8	33.2	34.4	33.8	33.9	34.7	34.3	33.1	33.7	33.4
33	32.9	33.4	33.2	31.0	31.9	31.5	32.8	34.0	33.4	33.6	34.4	34.0	32.9	33.4	33.2
34	32.7	33.2	33.0	30.7	31.6	31.2	32.4	33.6	33.0	33.4	34.1	33.7	32.7	33.2	33.0
35	32.5	33.0	32.8	30.4	31.3	30.9	32.0	33.2	32.6	33.1	33.9	33.5	32.5	33.0	32.8
36	32.4	32.8	32.6	30.1	31.0	30.6	31.6	32.8	32.2	32.9	33.6	33.3	32.4	32.8	32.6
37	32.2	32.7	32.5	29.9	30.7	30.3	31.3	32.4	31.8	32.7	33.4	33.0	32.2	32.7	32.5
38	32.1	32.5	32.3	29.6	30.5	30.1	30.9	32.0	31.5	32.5	33.2	32.8	32.1	32.5	32.3
39	32.0	32.4	32.2	29.4	30.2	29.8	30.6	31.7	31.1	32.3	32.9	32.6	32.0	32.4	32.2
40	31.8	32.2	32.0	29.1	30.0	29.6	30.2	31.3	30.8	32.1	32.7	32.4	31.8	32.2	32.0
41	31.7	32.1	31.9	28.9	29.7	29.3	29.8	31.0	30.4	31.8	32.6	32.2	31.7	32.1	31.9
42	31.6	32.0	31.8	28.6	29.5	29.1	29.5	30.6	30.1	31.6	32.4	32.0	31.6	32.0	31.8
43	31.5	31.9	31.7	28.4	29.3	28.8	29.1	30.3	29.7	31.4	32.2	31.8	31.5	31.9	31.7
44	31.3	31.8	31.6	28.1	29.1	28.6	28.7	30.0	29.3	31.2	32.0	31.6	31.3	31.8	31.6
45	31.2	31.7	31.4	27.8	28.9	28.3	28.3	29.6	29.0	30.9	31.9	31.4	31.2	31.7	31.4
46	31.1	31.6	31.3	27.5	28.7	28.1	27.9	29.3	28.6	30.6	31.7	31.1	31.1	31.6	31.3
47	30.9	31.5	31.2	27.1	28.5	27.8	27.4	29.0	28.2	30.2	31.5	30.9	30.9	31.5	31.2
48	30.7	31.4	31.1	26.7	28.3	27.5	26.9	28.7	27.8	29.8	31.4	30.6	30.7	31.4	31.1
49	30.4	31.4	30.9	26.2	28.2	27.2	26.4	28.3	27.4	29.4	31.2	30.3	30.4	31.4	30.9
50	30.2	31.3	30.7	25.6	28.0	26.8	25.7	28.0	26.9	28.8	31.1	29.9	30.2	31.3	30.7
CO2 rem			83.6			90.1			90.0			87.1			79.5
R. am load			0.485			0.495			0.494			0.460			0.473
LHUF			1			2.2			1.5			1.6			0.1

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Appendix D: Temperatures for the SRD cases

Content:

D1: Measured temperatures (average)

D2: Calculated Aspen HYSYS Zhu profile

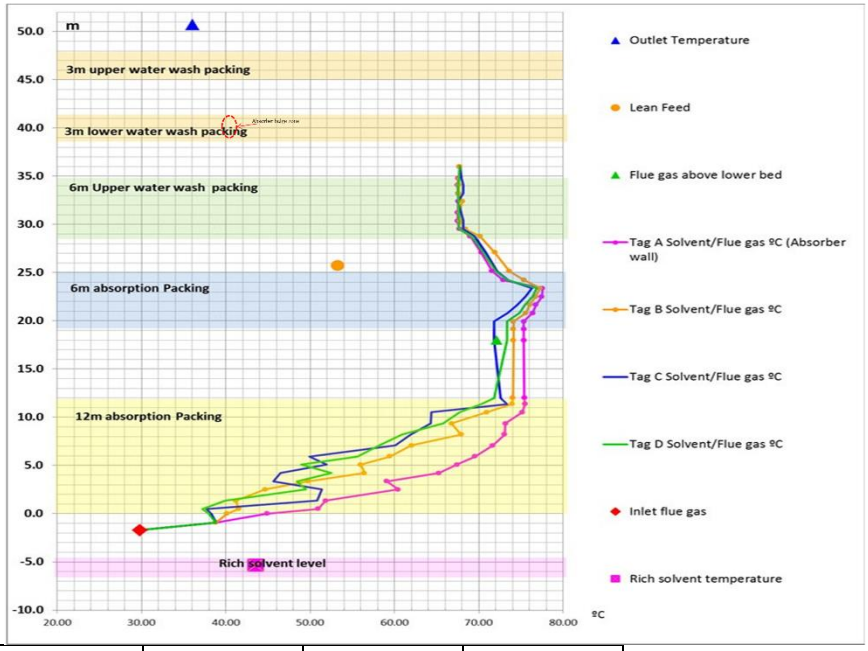
D3: Calculated Aspen HYSYS 0.1 profile

D4: Aspen Plus rate-based

D1: Measured temperatures (average)

One measured profile available, assumed case 4 based on given removal efficiency.

The figure (Shah 2018) was enlarged, and data read, average calculated, as seen in table below



Dist. from top (m)	Average temp (°C)	a	b	c	d
0.5	72.25	71.5	73.5	72	72
2	76.625	77	77	76	76.5
4	75	76	75	74	75
6	73.75	75.5	74	72	73.5
8	69.125	75.5	70	64	67
10	65.75	73	68	62	60
12	59	70	60	50	56
14	54.375	65	54	46.5	52
16	49	57	43	52	44
17.5	40.125	45	40	38	37.5

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°C

D2: Calculated Aspen HYSYS Zhu profile

Stage	Calculated temperatures with Zhu profile					
	6c	6a	8a	5c	3	4
1	71.1	70.9	70.9	71.0	71.2	70.5
2	74.5	74.8	74.9	74.8	75.7	75.5
3	74.8	75.2	75.5	75.3	76.4	76.5
4	74.3	74.7	75.0	74.7	76.0	76.2
5	73.4	73.8	74.2	73.8	75.3	75.5
6	72.3	72.7	73.1	72.7	74.3	74.5
7	70.9	71.3	71.8	71.2	73.0	73.2
8	69.2	69.6	70.2	69.4	71.4	71.7
9	67.3	67.6	68.3	67.4	69.6	70.1
10	65.1	65.4	66.3	65.2	67.6	68.3
11	62.5	62.9	63.9	62.7	65.3	66.4
12	59.6	60.2	61.3	60.1	62.8	64.3
13	56.4	57.3	58.5	57.2	60.1	62.0
14	52.9	54.2	55.3	54.2	57.2	59.4
15	49.0	50.7	51.7	50.7	53.7	56.2
16	45.5	47.4	48.4	47.4	50.4	53.0
17	41.8	43.7	44.6	43.8	46.5	49.2
18	37.3	38.8	39.5	38.9	41.1	43.3
Em- value	1.33	1.41	1.46	1.48	1.83	2.05
CO2 -rem (%)	88.3	87.3	87.4	87.3	88.1	85.9
Calc r.am.load	0.510	0.509	0.506	0.512	0.504	0.499

Calc r.am.load = calculated rich amine loading

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D3: Calculated Aspen HYSYS 0.1 profile

Stage	Calculated temperatures with 0.1 profile					
	6c	6a	8a	5c	3	4
1	69.4	68.9	68.8	69.1	69.0	67.9
2	73.1	73.1	73.1	73.3	73.8	73.2
3	73.8	74.0	74.2	74.2	75.0	74.9
4	73.7	74.0	74.2	74.2	75.2	75.2
5	73.4	73.7	73.9	73.9	75.0	75.1
6	73.0	73.2	73.5	73.5	74.7	74.8
7	72.4	72.7	73.0	72.9	74.2	74.4
8	71.8	72.1	72.4	72.3	73.7	73.9
9	71.0	71.3	71.6	71.5	73.0	73.3
10	70.1	70.3	70.7	70.6	72.2	72.5
11	68.9	69.2	69.6	69.4	71.2	71.5
12	67.5	67.8	68.3	68.1	70.0	70.4
13	65.8	66.2	66.6	66.3	68.4	68.9
14	63.6	64.1	64.6	64.2	66.4	67.1
15	60.9	61.4	62.0	61.4	63.9	64.8
16	57.2	58.0	58.6	57.8	60.5	61.6
17	52.1	53.1	53.8	52.9	55.7	57.1
18	44.5	45.6	46.3	45.5	48.0	49.5
Em- value	1.31	1.32	1.34	1.36	1.6	1.63
CO2 -rem (%)	88.3	87.3	87.4	87.3	88.1	85.9
Calc r.am.load	0.511	0.510	0.506	0.512	0.504	0.499

Calc r.am.load = calculated rich amine loading

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D4: Aspen Plus rate-based temperature

Stage	Case																	
	6c			6a			8a			5c			3			4		
	Gas	Liq	Aver	Gas	Liq	Aver	Gas	Liq	Aver	Gas	Liq	Aver	Gas	Liq	Aver	Gas	Liq	Aver
1	70.8	63.0	66.9	70.6	62.7	66.6	70.6	62.6	66.6	70.7	62.8	66.7	70.9	62.6	66.8	70.0	61.8	65.9
2	72.8	68.5	70.6	72.8	68.2	70.5	72.9	68.1	70.5	72.9	68.3	70.6	73.4	68.4	70.9	72.7	67.3	70.0
3	73.9	71.8	72.8	74.0	71.6	72.8	74.2	71.6	72.9	74.1	71.8	73.0	74.9	72.2	73.6	74.5	71.2	72.8
4	74.4	73.6	74.0	74.6	73.7	74.1	74.8	73.7	74.3	74.8	73.8	74.3	75.7	74.5	75.1	75.5	73.8	74.6
5	74.6	74.6	74.6	74.8	74.8	74.8	75.1	74.9	75.0	75.0	74.9	75.0	76.1	75.8	75.9	76.0	75.3	75.7
6	74.5	75.1	74.8	74.8	75.3	75.1	75.1	75.5	75.3	75.0	75.5	75.2	76.1	76.4	76.3	76.2	76.2	76.2
7	74.4	75.2	74.8	74.6	75.5	75.1	75.0	75.7	75.4	74.8	75.7	75.2	76.0	76.7	76.3	76.1	76.6	76.4
8	74.1	75.2	74.7	74.3	75.5	74.9	74.8	75.8	75.3	74.5	75.7	75.1	75.7	76.7	76.2	75.9	76.7	76.3
9	73.8	75.1	74.4	74.0	75.4	74.7	74.5	75.7	75.1	74.1	75.6	74.9	75.3	76.6	76.0	75.6	76.6	76.1
10	73.3	75.0	74.2	73.5	75.2	74.4	74.1	75.5	74.8	73.6	75.4	74.5	74.9	76.4	75.6	75.3	76.4	75.9
11	72.9	74.8	73.8	73.0	75.0	74.0	73.6	75.3	74.4	73.1	75.1	74.1	74.4	76.0	75.2	74.9	76.1	75.5
12	72.3	74.5	73.4	72.3	74.6	73.5	73.0	75.0	74.0	72.4	74.7	73.6	73.8	75.6	74.7	74.4	75.8	75.1
13	71.6	74.2	72.9	71.6	74.1	72.9	72.4	74.6	73.5	71.7	74.2	73.0	73.2	75.1	74.1	73.9	75.3	74.6
14	70.9	73.8	72.3	70.8	73.6	72.2	71.7	74.1	72.9	70.9	73.6	72.2	72.5	74.5	73.5	73.4	74.9	74.1
15	70.0	73.2	71.6	70.0	72.8	71.4	70.9	73.5	72.2	70.1	72.8	71.4	71.9	73.9	72.9	72.8	74.4	73.6
16	69.0	72.5	70.7	69.1	72.0	70.5	70.1	72.8	71.4	69.2	72.0	70.6	71.2	73.2	72.2	72.3	73.8	73.0
17	68.0	71.5	69.8	68.1	71.1	69.6	69.2	72.0	70.6	68.3	71.1	69.7	70.5	72.5	71.5	71.7	73.3	72.5
18	66.9	70.5	68.7	67.2	70.1	68.6	68.3	71.1	69.7	67.3	70.1	68.7	69.8	71.8	70.8	71.1	72.7	71.9
19	65.8	69.3	67.5	66.3	69.1	67.7	67.4	70.1	68.8	66.5	69.2	67.8	69.1	71.1	70.1	70.5	72.1	71.3
20	64.7	68.1	66.4	65.4	68.1	66.7	66.5	69.2	67.9	65.6	68.2	66.9	68.4	70.3	69.4	69.9	71.5	70.7
21	63.6	66.9	65.3	64.5	67.1	65.8	65.6	68.2	66.9	64.7	67.3	66.0	67.7	69.6	68.7	69.4	70.9	70.2
22	62.6	65.8	64.2	63.6	66.2	64.9	64.8	67.3	66.1	63.9	66.4	65.2	67.0	68.9	68.0	68.8	70.4	69.6
23	61.6	64.7	63.2	62.8	65.3	64.1	64.0	66.4	65.2	63.1	65.5	64.3	66.3	68.2	67.3	68.2	69.8	69.0
24	60.7	63.6	62.2	62.0	64.4	63.2	63.2	65.6	64.4	62.3	64.7	63.5	65.7	67.6	66.6	67.6	69.2	68.4
25	59.8	62.6	61.2	61.2	63.6	62.4	62.4	64.7	63.5	61.6	63.9	62.7	65.0	66.9	66.0	67.1	68.6	67.8
26	58.9	61.7	60.3	60.5	62.8	61.6	61.6	63.9	62.8	60.8	63.1	62.0	64.4	66.2	65.3	66.5	68.1	67.3
27	58.0	60.7	59.4	59.7	62.0	60.9	60.8	63.1	62.0	60.1	62.3	61.2	63.7	65.6	64.7	65.9	67.5	66.7
28	57.2	59.9	58.5	59.0	61.3	60.1	60.1	62.3	61.2	59.4	61.6	60.5	63.1	65.0	64.0	65.3	66.9	66.1
29	56.4	59.0	57.7	58.3	60.5	59.4	59.4	61.6	60.5	58.7	60.9	59.8	62.4	64.3	63.4	64.7	66.3	65.5
30	55.6	58.2	56.9	57.5	59.8	58.7	58.6	60.9	59.7	57.9	60.2	59.0	61.8	63.7	62.7	64.1	65.8	64.9
31	54.8	57.4	56.1	56.8	59.1	57.9	57.9	60.1	59.0	57.2	59.5	58.3	61.1	63.1	62.1	63.5	65.2	64.3
32	54.0	56.6	55.3	56.0	58.4	57.2	57.1	59.4	58.3	56.5	58.8	57.6	60.4	62.4	61.4	62.8	64.6	63.7
33	53.2	55.8	54.5	55.3	57.7	56.5	56.4	58.7	57.5	55.7	58.1	56.9	59.7	61.8	60.7	62.1	64.0	63.1
34	52.3	55.0	53.7	54.5	57.0	55.7	55.6	58.0	56.8	54.9	57.4	56.2	58.9	61.1	60.0	61.4	63.4	62.4
35	51.5	54.3	52.9	53.7	56.2	55.0	54.8	57.3	56.0	54.1	56.7	55.4	58.2	60.4	59.3	60.7	62.8	61.7
36	50.6	53.5	52.1	52.9	55.5	54.2	53.9	56.5	55.2	53.3	55.9	54.6	57.4	59.8	58.6	59.9	62.1	61.0
37	49.7	52.7	51.2	52.0	54.8	53.4	53.0	55.8	54.4	52.4	55.2	53.8	56.5	59.1	57.8	59.1	61.4	60.3
38	48.8	51.9	50.4	51.1	54.0	52.5	52.1	55.0	53.6	51.5	54.5	53.0	55.6	58.3	57.0	58.2	60.7	59.5
39	47.8	51.1	49.5	50.1	53.3	51.7	51.1	54.2	52.7	50.5	53.7	52.1	54.6	57.6	56.1	57.3	60.0	58.6
40	46.8	50.3	48.5	49.0	52.5	50.7	50.0	53.4	51.7	49.5	52.9	51.2	53.5	56.8	55.2	56.2	59.2	57.7
41	45.7	49.5	47.6	47.9	51.6	49.8	48.9	52.6	50.7	48.3	52.0	50.2	52.4	55.9	54.1	55.0	58.4	56.7
42	44.5	48.6	46.5	46.6	50.7	48.7	47.6	51.7	49.7	47.1	51.2	49.1	51.0	55.0	53.0	53.7	57.5	55.6
43	43.1	47.6	45.4	45.3	49.8	47.5	46.2	50.8	48.5	45.7	50.2	48.0	49.6	54.1	51.8	52.2	56.6	54.4
44	41.7	46.7	44.2	43.8	48.8	46.3	44.7	49.7	47.2	44.2	49.3	46.7	47.9	53.1	50.5	50.5	55.6	53.0
45	40.1	45.6	42.9	42.1	47.8	44.9	42.9	48.7	45.8	42.5	48.2	45.3	46.0	52.0	49.0	48.6	54.4	51.5
46	38.3	44.5	41.4	40.1	46.6	43.4	40.9	47.5	44.2	40.5	47.0	43.8	43.8	50.7	47.3	46.2	53.2	49.7
47	36.3	43.4	39.8	37.9	45.4	41.6	38.6	46.2	42.4	38.3	45.8	42.0	41.3	49.4	45.3	43.5	51.8	47.6
48	34.0	42.1	38.0	35.4	44.0	39.7	36.0	44.8	40.4	35.7	44.4	40.0	38.2	47.9	43.0	40.1	50.2	45.2
49	31.4	40.7	36.0	32.4	42.5	37.4	32.9	43.2	38.1	32.6	42.9	37.7	34.6	46.1	40.4	36.1	48.4	42.2
50	28.4	39.1	33.7	28.9	40.7	34.8	29.2	41.4	35.3	29.1	41.1	35.1	30.2	44.1	37.2	31.1	46.2	38.6
CO2 rem			88.3			87.3			87.4			87.3			88.1			85.9
R. am load			0.517			0.518			0.513			0.520			0.512			0.506
LHUF			0.72			0.72			0.6			0.72			0.84			0.65

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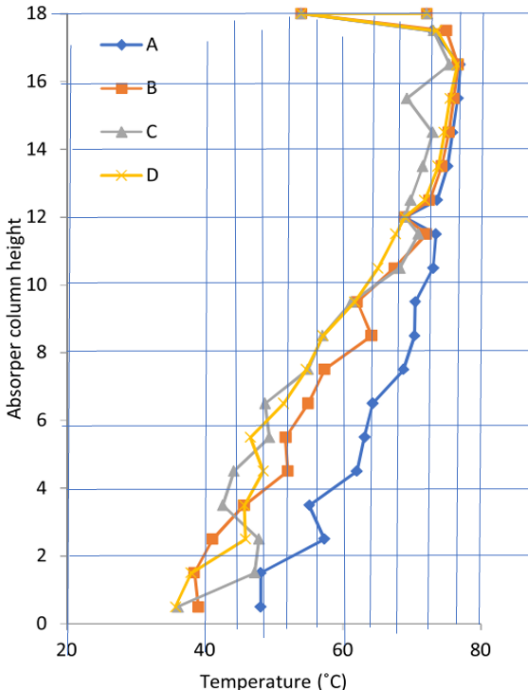
Appendix E: Temperatures for the Campaign-4 cases

Content:



E1: Measured temperatures (average)

One case published (Fosbøl 2020):

Dist. from top (m)	A	B	C	D	Average temp (°C)
0.3		68		53	60.5
1	75	75	75	75	75
2	76	76	72	76	75
4	74	74	72	74	73.5
6	68	68	68	68	68
8	71.5	64	64	63.5	65.75
10	69	61	56	56	60.5
12	63.5	53	48	48	53.125
14	58	48	43	47	49
16	52	40	47	42	45.25
17.5	48	40	36	36	40

`

E2: Calculated Aspen HYSYS Zhu profile

Stage	Calculated temperatures with Zhu profile			
	1A-1	1C	1D	2B
1	71.5	70.3	68.8	71.0
2	75.6	76.3	74.3	76.3
3	76.1	77.9	75.8	77.4
4	75.7	78.2	75.8	77.3
5	74.9	77.9	75.3	76.8
6	73.9	77.5	74.5	76.0
7	72.5	76.8	73.6	74.9
8	70.8	75.9	72.5	73.5
9	68.8	74.8	71.3	72.0
10	66.6	73.5	70.1	70.2
11	64.1	72.0	68.6	68.2
12	61.3	70.1	67.0	66.1
13	58.4	67.9	65.1	63.7
14	55.2	65.2	62.9	60.9
15	51.6	61.8	60.0	57.6
16	48.3	58.4	56.9	54.3
17	44.5	54.2	53.0	50.3
18	39.4	47.5	46.7	44.2
Em- value	1.73	3.4	2.2	2.5
CO2 -rem (%)	90.1	89.7	79	89.4
Calc r.am.load	0.510	0.479	0.485	0.485
Calc r.am.load = calculated rich amine loading				

`

E3: Calculated Aspen HYSYS 0.1 profile

Stage	Calculated temperatures with 0.1 profile			
	1A-1	1C	1D	2B
1	69.5	66.2	65.9	68.0
2	73.9	72.5	71.8	73.5
3	74.9	75.1	74.2	75.4
4	74.9	76.0	75.0	75.8
5	74.7	76.3	75.1	75.8
6	74.4	76.3	75.0	75.7
7	73.9	76.2	74.6	75.4
8	73.4	76.0	74.2	75.0
9	72.7	75.7	73.7	74.4
10	71.9	75.3	73.0	73.8
11	70.8	74.7	72.2	73.0
12	69.5	73.9	71.2	72.0
13	67.9	72.9	69.9	70.6
14	65.8	71.6	68.3	68.9
15	63.1	69.7	66.2	66.7
16	59.5	66.9	63.4	63.6
17	54.4	62.6	59.3	58.9
18	46.6	54.7	51.9	51.1
Em- value	1.58	2.47	1.15	2
CO2 -rem (%)	90.1	89.7	78	89.7
Calc r.am.load	0.510	0.480	0.483	0.495
Calc r.am.load = calculated rich amine loading				

`

E4: Aspen Plus rate-based

Stage	Case											
	1A-1			1C			1D			2B		
	Gas	Liq	Aver	Gas	Liq	Aver	Gas	Liq	Aver	Gas	Liq	Aver
1	71.1	62.9	67.0	69.1	60.7	64.9	67.9	60.3	64.1	70.3	61.8	66.0
2	73.4	68.6	71.0	72.3	66.0	69.1	70.8	65.1	67.9	73.1	67.4	70.3
3	74.8	72.2	73.5	74.6	70.2	72.4	72.9	69.0	70.9	75.0	71.5	73.2
4	75.5	74.3	74.9	76.2	73.4	74.8	74.4	71.9	73.1	76.1	74.2	75.1
5	75.7	75.5	75.6	77.2	75.5	76.3	75.2	73.8	74.5	76.8	75.8	76.3
6	75.8	76.1	75.9	77.8	76.8	77.3	75.7	75.1	75.4	77.0	76.8	76.9
7	75.7	76.3	76.0	78.1	77.7	77.9	75.9	75.8	75.8	77.1	77.2	77.2
8	75.4	76.4	75.9	78.2	78.1	78.2	75.9	76.1	76.0	77.0	77.5	77.2
9	75.1	76.3	75.7	78.2	78.4	78.3	75.8	76.3	76.0	76.9	77.5	77.2
10	74.8	76.1	75.5	78.2	78.4	78.3	75.6	76.2	75.9	76.6	77.4	77.0
11	74.3	75.9	75.1	78.0	78.4	78.2	75.3	76.1	75.7	76.3	77.3	76.8
12	73.8	75.6	74.7	77.9	78.4	78.1	75.0	75.8	75.4	76.0	77.0	76.5
13	73.2	75.2	74.2	77.7	78.2	78.0	74.7	75.6	75.1	75.6	76.7	76.2
14	72.5	74.8	73.6	77.5	78.1	77.8	74.4	75.3	74.8	75.2	76.4	75.8
15	71.7	74.2	73.0	77.2	77.9	77.6	74.0	74.9	74.5	74.7	76.0	75.4
16	70.9	73.5	72.2	76.9	77.7	77.3	73.6	74.6	74.1	74.2	75.6	74.9
17	70.1	72.7	71.4	76.6	77.5	77.0	73.2	74.2	73.7	73.7	75.2	74.4
18	69.2	71.9	70.6	76.3	77.2	76.7	72.8	73.8	73.3	73.2	74.7	73.9
19	68.4	71.0	69.7	75.9	76.9	76.4	72.4	73.4	72.9	72.6	74.1	73.4
20	67.5	70.1	68.8	75.5	76.6	76.1	72.0	73.0	72.5	72.0	73.6	72.8
21	66.7	69.2	67.9	75.1	76.2	75.7	71.6	72.6	72.1	71.4	73.0	72.2
22	65.9	68.3	67.1	74.7	75.8	75.3	71.1	72.2	71.7	70.9	72.5	71.7
23	65.0	67.4	66.2	74.2	75.4	74.8	70.7	71.8	71.2	70.3	71.9	71.1
24	64.3	66.6	65.4	73.7	75.0	74.4	70.3	71.4	70.8	69.7	71.3	70.5
25	63.5	65.8	64.6	73.2	74.5	73.9	69.8	70.9	70.4	69.1	70.7	69.9
26	62.7	65.0	63.9	72.7	74.1	73.4	69.3	70.5	69.9	68.4	70.1	69.3
27	62.0	64.2	63.1	72.2	73.5	72.8	68.9	70.0	69.5	67.8	69.5	68.7
28	61.2	63.5	62.3	71.6	73.0	72.3	68.4	69.6	69.0	67.2	68.9	68.0
29	60.5	62.7	61.6	71.0	72.5	71.7	67.9	69.1	68.5	66.6	68.3	67.4
30	59.7	62.0	60.9	70.4	71.9	71.2	67.4	68.7	68.0	65.9	67.7	66.8
31	59.0	61.2	60.1	69.8	71.3	70.5	66.8	68.2	67.5	65.3	67.1	66.2
32	58.2	60.5	59.4	69.1	70.8	69.9	66.3	67.7	67.0	64.6	66.4	65.5
33	57.4	59.8	58.6	68.4	70.1	69.3	65.7	67.2	66.4	63.9	65.8	64.8
34	56.6	59.1	57.9	67.7	69.5	68.6	65.1	66.6	65.9	63.1	65.1	64.1
35	55.8	58.4	57.1	66.9	68.9	67.9	64.4	66.1	65.3	62.4	64.5	63.4
36	55.0	57.6	56.3	66.1	68.2	67.2	63.7	65.5	64.6	61.6	63.8	62.7
37	54.1	56.9	55.5	65.3	67.5	66.4	63.0	64.9	64.0	60.7	63.1	61.9
38	53.1	56.1	54.6	64.4	66.7	65.6	62.2	64.3	63.2	59.8	62.4	61.1
39	52.1	55.3	53.7	63.4	66.0	64.7	61.3	63.6	62.5	58.8	61.6	60.2
40	51.0	54.5	52.7	62.3	65.1	63.7	60.3	62.9	61.6	57.7	60.8	59.3
41	49.8	53.6	51.7	61.1	64.3	62.7	59.2	62.1	60.7	56.5	59.9	58.2
42	48.5	52.7	50.6	59.7	63.3	61.5	57.9	61.3	59.6	55.1	59.0	57.1
43	47.1	51.7	49.4	58.1	62.3	60.2	56.5	60.4	58.4	53.6	58.0	55.8
44	45.5	50.7	48.1	56.3	61.2	58.7	54.8	59.4	57.1	51.8	57.0	54.4
45	43.7	49.6	46.6	54.1	60.0	57.0	52.7	58.2	55.5	49.8	55.8	52.8
46	41.6	48.4	45.0	51.5	58.6	55.1	50.3	57.0	53.6	47.4	54.5	50.9
47	39.3	47.1	43.2	48.3	57.0	52.7	47.3	55.5	51.4	44.5	53.0	48.8
48	36.5	45.6	41.1	44.4	55.2	49.8	43.5	53.9	48.7	41.0	51.4	46.2
49	33.3	44.0	38.6	39.4	53.1	46.3	38.8	51.9	45.3	36.8	49.5	43.1
50	29.4	42.2	35.8	33.1	50.6	41.9	32.7	49.5	41.1	31.5	47.2	39.3
CO2 rem			90.0			89.8			78.7			89.3
R. am load			0.513			0.493			0.503			0.500
LHUF			0.85			0.38			0.2			1

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Appendix F: Temperatures for the Esbjerg cases

Content:

E1: Measured temperatures

E2: Aspen Plus rate-based

E1: Measured temperatures

Temperature figures (Neda 2013a) was enlarged, and measurements were read

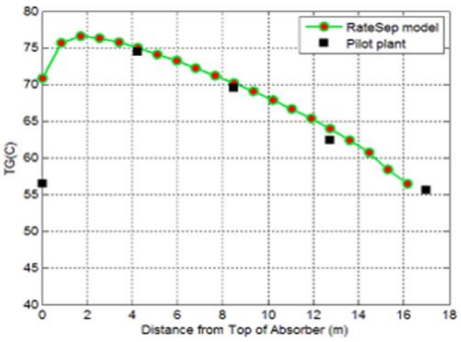


fig. 1. Test 1A-1- Absorber Gas Temperature Profiles

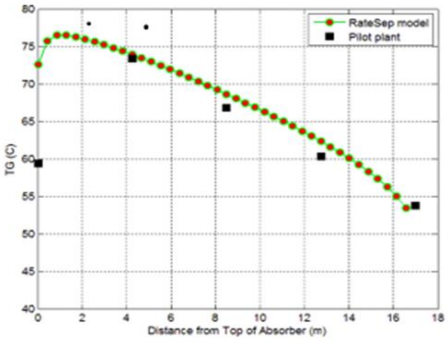
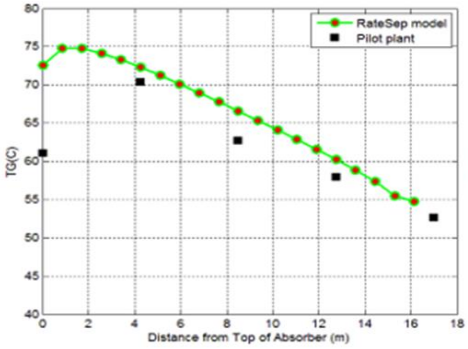
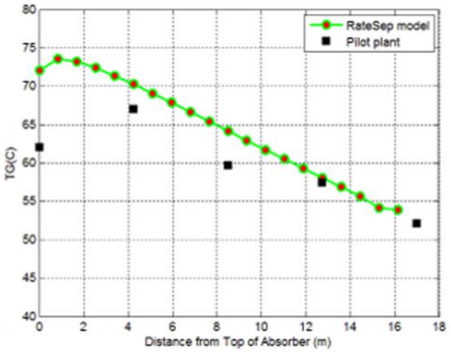


fig. 2. Test 1A-2- Absorber Gas Temperature Profiles





Dist from topm, m	E-1	E-2	E-3	E-4
0.2	56.3	59	61	62
4.2	74.3	73	70.8	67
8.4	69.5	67	63	59.8
12.6	62.5	60.7	58	57.8
16.8	55.8	53	53	52.5

Temperatures in C

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E2: Aspen Plus rate-based

Stage	Case											
	E-1			E-2			E-3			E-4		
	Gas	Liq	Aver	Gas	Liq	Aver	Gas	Liq	Aver	Gas	Liq	Aver
1	56.6	44.3	50.4	59.5	45.6	52.6	61.5	46.8	54.2	62.7	47.8	55.2
2	60.5	49.0	54.8	63.5	51.4	57.5	65.3	53.5	59.4	66.1	54.9	60.5
3	64.0	54.0	59.0	66.8	57.1	62.0	68.3	59.4	63.8	68.6	60.9	64.7
4	67.0	58.8	62.9	69.4	62.2	65.8	70.4	64.3	67.4	70.3	65.3	67.8
5	69.4	63.1	66.3	71.3	66.3	68.8	71.9	68.0	69.9	71.4	68.5	69.9
6	71.2	66.8	69.0	72.6	69.4	71.0	72.8	70.5	71.6	72.0	70.5	71.3
7	72.5	69.5	71.0	73.5	71.5	72.5	73.3	72.2	72.7	72.3	71.8	72.1
8	73.3	71.5	72.4	73.9	73.0	73.5	73.6	73.2	73.4	72.4	72.6	72.5
9	73.7	72.9	73.3	74.1	73.9	74.0	73.6	73.8	73.7	72.3	73.0	72.6
10	73.9	73.7	73.8	74.2	74.4	74.3	73.5	74.1	73.8	72.1	73.1	72.6
11	73.9	74.2	74.1	74.1	74.7	74.4	73.4	74.3	73.8	71.9	73.2	72.5
12	73.8	74.4	74.1	73.9	74.8	74.3	73.1	74.3	73.7	71.5	73.1	72.3
13	73.6	74.5	74.0	73.6	74.7	74.2	72.8	74.2	73.5	71.1	73.0	72.0
14	73.3	74.4	73.9	73.2	74.6	73.9	72.4	74.0	73.2	70.7	72.8	71.7
15	73.0	74.2	73.6	72.9	74.3	73.6	72.0	73.8	72.9	70.2	72.5	71.3
16	72.6	73.9	73.3	72.4	74.1	73.2	71.5	73.5	72.5	69.6	72.2	70.9
17	72.3	73.6	72.9	72.0	73.7	72.8	70.9	73.1	72.0	68.9	71.8	70.3
18	71.8	73.3	72.5	71.4	73.3	72.4	70.3	72.7	71.5	68.2	71.3	69.7
19	71.4	72.9	72.1	70.9	72.8	71.9	69.7	72.2	70.9	67.4	70.7	69.0
20	70.9	72.5	71.7	70.3	72.4	71.3	69.0	71.6	70.3	66.5	70.0	68.2
21	70.4	72.0	71.2	69.7	71.8	70.8	68.3	71.0	69.6	65.7	69.1	67.4
22	70.0	71.6	70.8	69.1	71.3	70.2	67.6	70.3	68.9	64.8	68.3	66.5
23	69.5	71.1	70.3	68.5	70.7	69.6	66.8	69.6	68.2	63.9	67.3	65.6
24	68.9	70.6	69.8	67.9	70.1	69.0	66.1	68.8	67.4	63.0	66.4	64.7
25	68.4	70.1	69.3	67.3	69.5	68.4	65.3	68.0	66.7	62.1	65.5	63.8
26	67.9	69.6	68.8	66.6	68.8	67.7	64.5	67.3	65.9	61.3	64.5	62.9
27	67.3	69.1	68.2	66.0	68.2	67.1	63.8	66.5	65.1	60.4	63.6	62.0
28	66.8	68.6	67.7	65.3	67.6	66.4	63.0	65.7	64.4	59.6	62.7	61.2
29	66.2	68.1	67.1	64.6	66.9	65.8	62.3	65.0	63.6	58.8	61.9	60.3
30	65.6	67.5	66.6	64.0	66.3	65.1	61.5	64.2	62.9	58.0	61.0	59.5
31	65.0	67.0	66.0	63.3	65.6	64.5	60.8	63.5	62.1	57.3	60.2	58.7
32	64.4	66.4	65.4	62.6	65.0	63.8	60.0	62.7	61.4	56.5	59.4	58.0
33	63.8	65.9	64.8	61.9	64.3	63.1	59.3	62.0	60.6	55.7	58.6	57.2
34	63.2	65.3	64.2	61.2	63.6	62.4	58.5	61.2	59.9	55.0	57.8	56.4
35	62.5	64.7	63.6	60.5	63.0	61.7	57.8	60.5	59.1	54.3	57.1	55.7
36	61.8	64.1	62.9	59.7	62.3	61.0	57.0	59.8	58.4	53.5	56.3	54.9
37	61.1	63.4	62.2	59.0	61.6	60.3	56.2	59.0	57.6	52.8	55.6	54.2
38	60.3	62.8	61.5	58.2	60.9	59.5	55.4	58.3	56.8	52.1	54.8	53.5
39	59.5	62.1	60.8	57.4	60.1	58.7	54.6	57.5	56.1	51.4	54.1	52.7
40	58.7	61.4	60.0	56.5	59.4	57.9	53.8	56.7	55.3	50.7	53.3	52.0
41	57.8	60.6	59.2	55.7	58.6	57.1	53.0	55.9	54.5	50.0	52.5	51.3
42	56.9	59.8	58.4	54.8	57.7	56.3	52.2	55.1	53.6	49.3	51.7	50.5
43	56.0	59.0	57.5	53.9	56.9	55.4	51.4	54.2	52.8	48.7	50.9	49.8
44	55.0	58.0	56.5	53.0	55.9	54.5	50.6	53.3	51.9	48.1	50.1	49.1
45	54.0	57.1	55.5	52.1	55.0	53.5	49.8	52.4	51.1	47.5	49.2	48.4
46	53.0	56.0	54.5	51.2	53.9	52.5	49.1	51.3	50.2	47.1	48.3	47.7
47	52.1	54.8	53.5	50.4	52.8	51.6	48.4	50.3	49.4	46.8	47.4	47.1
48	51.2	53.5	52.4	49.6	51.5	50.6	47.9	49.1	48.5	46.6	46.4	46.5
49	50.5	52.0	51.3	49.1	50.1	49.6	47.6	47.9	47.7	46.7	45.3	46.0
50	50.0	50.4	50.2	48.8	48.6	48.7	47.6	46.5	47.0	47.1	44.2	45.7
CO2 rem			86.7			88.7			88.8			86.7
R. am load			0.494			0.496			0.499			0.499
LHUF			0.72			0.72			0.72			0.72

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APPENDIX G: Simple correlations for E_m factor used on CHP gas chap 4

The ratios of Em values calculated by Aspen Plus where only one variable was varied at a time, were used. The table shows the values and ratios. The case 17F was used as reference for the ratios. (The case was modified for flowrates to be equal to the other flowrates, by correspondingly reducing the lean amine flowrate)

Only the 5 first stages are shown for illustration:

	LA: 55000kg/hr, MEA 30%			LA: 55000kg/hr, l.a. load 0.228			Load:0.23, wt%: 30		
	Leanload	Leanload		MEA wt%	MEA wt%		l.a flow	l.a flow	
	0.182	0.281		33	30		55000 kg/hr	45000 kg/hr	
	Em	Em	Ratio Em	Em	Em	Ratio Em	Em	Em	Ratio Em
1	0.102	0.114	1.116	0.113	0.108	1.205	0.108	0.104	1.197
2	0.112	0.123	1.100	0.124	0.119	1.206	0.119	0.114	1.199
3	0.119	0.129	1.082	0.132	0.126	1.203	0.126	0.121	1.201
4	0.124	0.130	1.050	0.137	0.131	1.198	0.131	0.125	1.207
5	0.127	0.126	0.993	0.140	0.135	1.195	0.135	0.126	1.229

The c- factors were calculated:

C factors		
Loading	MEA wt%	Lean amine flow (1000 kg/hr)
-4.0384	0.1183	0.0544

And then the Em factor for the cases (ref table 4.7)

	Ref 17F_M				
	17F_M	M1	H14	2B5	M2
Key input:					
- Lean amin loading (moleCO2/moleMEA)	0.20	0.215	0.23	0.23	0.215
- Lean amin flowrate (kg/hr)	45400	50150	54900	49485	47442.5
- MEA wt% (without CO2)	31.0	30.5	30	31.6	31.3
- CO2 in fluegas (mole%)	3.7	3.62	3.7	3.57	3.57
- Flue gas flowrate (kg/hr)	57220	57157	57300	57193	56788
Em fact	**0.78**	**0.87**	**0.92**	**0.90**	**0.84**

`

APPENDIX H: Simple correlations for absorber efficiency used in chap 5

Reference is made to table 5-13:

Case	Base	1	2	3	4	5	6	7	8
Lean amine loading	0.225	0.2	0.2	0.2	0.2	0.25	0.25	0.25	0.25
Lean amine flowrate	112500	100000	100000	125000	125000	100000	100000	125000	125000
MEA wt%	31	30	32	30	32	30	32	30	32
Calculated efficiency	0.802	0.783	0.810	0.922	0.954	0.645	0.673	0.784	0.819

The mean slopes when only one variable value differed were calculated:

Loading	MEA wt%	Lean amine Flow (1000 kg/hr)
-3.2	0.02	0.006715

The factor above for lean amine flow includes a tuning of 0.85. (the other are 1.0)

The SRD cases was calculated with this factor with “Base” above as reference values:

	6c	6a	8a	5c	3	4
Factor	1.106	1.089	1.099	1.074	1.084	1.090
Factor* ref efficiency	0.887	0.873	0.882	0.861	0.869	0.874
Test result	0.883	0.873	0.874	0.873	0.881	0.859

The reference efficiency (“Base”) is 0.802. There are substantial differences in input values.