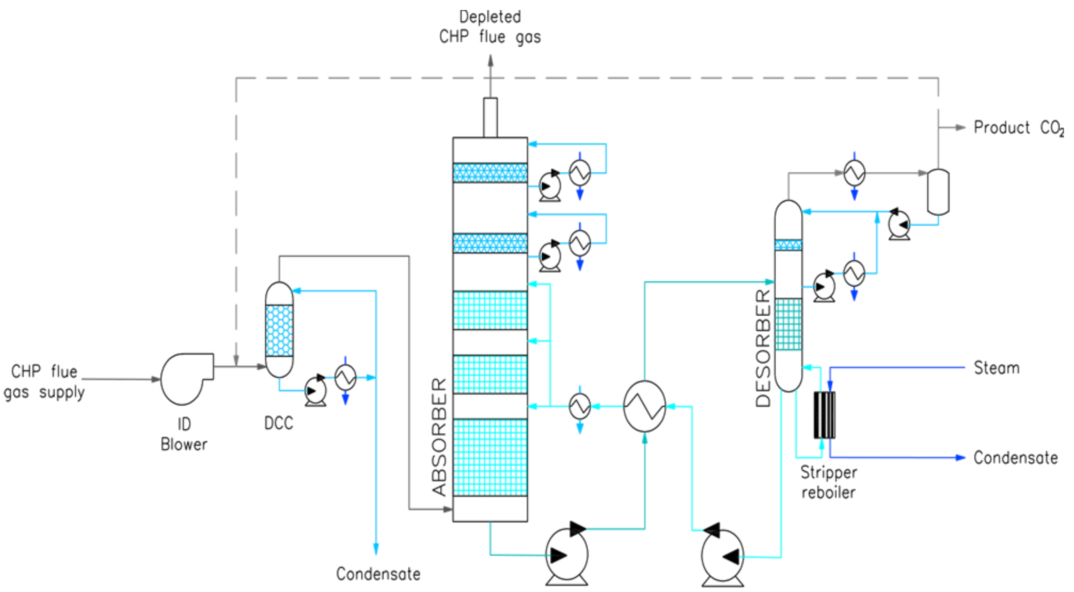
University of
South-Eastern Norway

www.usn.no

FMH606 Master's Thesis 2019

Energy and Environmental Technology

Process simulation of CO_2 absorption at TCM Mongstad



Sofie Fagerheim

Faculty of Technology, Natural sciences and Maritime Sciences
Campus Porsgrunn

University of
South-Eastern Norway

www.usn.no

Course: FMH606 Master's Thesis, 2019

Title: Process simulation of CO_2 absorption at TCM Mongstad

Number of pages: 140

Keywords: Absorption, Aspen Plus, Aspen HYSYS, CO_2 capture, MEA, simulation, TCM

Student:	Sofie Fagerheim
Supervisor:	Lars Erik Øi
External partner:	CO_2 Technology Centre Mongstad (TCM)
Availability:	Open

Summary:

Developing robust and predictable process simulation tools for CO_2 capture is important for improving carbon capture technology and reduce man made CO_2 emissions.

In this thesis, five different scenarios of experimental data from the amine based CO_2 capture process at TCM have been simulated in rate-based model in Aspen Plus and equilibrium-based model in Aspen HYSYS and Aspen Plus. The simulations have been compared based on the prediction reliability for removal grade, temperature profile and rich loading.

In previous work, these five scenarios have been simulated and compared in Aspen HYSYS and Aspen Plus. Some of the results from earlier work are verified in this thesis.

The main purpose have been to fit the simulated results with performance data from TCM, and evaluate whether fitted parameters for one scenario gives reasonable predictions at other conditions. Two new E_M-profiles were estimated, and scaled to fit all five scenarios by developing an E_M-factor. From this work the new model with fitted parameters gave a reliable prediction of removal grade and temperature profile for all scenarios, and predicted more reliable results than rate-based model with estimated IAF.

The scenarios were also simulated with default E_M-profile in Aspen HYSYS, where the removal grade was fitted to performance data by adjusting number of stages. The scenarios were also simulated with three different amine packages in Aspen HYSYS, Kent-Eisenberg, Li-Mather and Acid Gas - Liquid Treating.

Preface

This report was written during the spring 2019 as my master thesis, and is 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.

The project focus is on performing process simulations of test data from the 2013 and 2015 campaign at TCM in Aspen HYSYS and Aspen Plus, and compare process simulations with performance data and earlier simulations of the same test data. The main purpose is to fit the removal grade, temperature profile and rich loading with performance data from TCM. Another purpose is to evaluate whether fitted parameters for one scenario gives reasonable predictions at other conditions.

I want to express my gratitude towards my supervisor, Professor Lars Erik Øi, for his supervision, guidance and great support during this thesis. Especially I appreciate that he made it possible for me to carry out all the work from Bodø, so that I was able to continue my job at Multiconsult and be with my family during the duration of this project.

I would also like to thank my family for their help and support during this work. Especially, I want to show gratitude to my boyfriend, Stefan, for his patience and help taking care of our son, Philip Edward, who turned two years during this project. I would like to thank him for giving me the time I needed to complete. Hopefully we will get more time together in the years to come.

The data-tools used during this project was:

Aspen HYSYS V10, Aspen Plus V10, MS Word 2013, MS Excel 2013 and AutoCAD Plant 3D 2018.

Bodø, 05.05.19

Sofie Fagerheim

Sofie Fagerheim

Contents

Nomenclature

A-G	Acid Gas - Liquid Treating (Amine package in Aspen HYSYS)
CCS	Carbon capture and storage
CHP	Combined Heat and Power plant
DCC	Direct-Contact Cooler
DEA	Diethanolamine
E_M	Murphree Efficency
e-NRTL	Electrolyte non-random two-liquid (Amine package in Aspen Plus)
IAF	Interfacial area factor
ID blower	Inducted Draft blower
IPCC	Intergovernmental Panel on Climate Change
K-E	Kent-Eisenberg (Amine package in Aspen HYSYS)
L-M	Li-Mather (Amine package in Aspen HYSYS)
MDEA	Methyl diethanolamine
MEA	Monoethanol amine
NOAA	National Oceanic and Atmosperic Administration
RFCC	Refinery Residue Fluid Catalytic Cracker
TCM	Technology Centre Mongstad
USN	University of South-Eastern Norway, *Earlier known as Telemark University College and University College of Southeast Norway*
Lean loading	The CO_2 low amine entering the absorber
Removal grade	Percent of CO_2 captured
Rich loading	The CO_2 rich amine exiting the absorber

1 Introduction

1.1 Background

TCM (Technology Centre Mongstad) is the world's largest facility for testing and improving CO_2 capture, and was 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 behavior, plan campaigns and verify results it is necessary to have good and robust simulation models.

There have been performed several projects at the University of Southeastern Norway, on process simulation of amine based CO_2 capture processes using Aspen HYSYS and Aspen Plus. Over the last decade, the MEA based CO_2 capture process at TCM have annually been simulated in master theses.

The focus of this report is on performing a literature review on process simulation of amine based CO_2 capture by absorption. Perform Aspen HYSYS and Aspen Plus simulations of the MEA based CO_2 capture process at TCM, and compare process simulations with performance data, and do a verification of some of the earlier work on this subject, performed in earlier master theses at USN.

1.2 Outline of the thesis

In chapter 2, the carbon related climate change, and the carbon capture and storage technology is briefly described. The Process description of the CO_2 capture process at TCM is presented with a P&ID, followed by the chemistry of MEA and CO_2 absorption. A short presentation of the earlier work on the subject is reviewed. The chapter finishes with a problem description.

In chapter 3, the simulation methodology is presented, introducing different simulation tools, Murphree efficiency, and necessary calculations. A new method of estimating Murphree efficiency and fitting Murphree efficiencies with removal grade by introducing an E_M-factor is developed The five scenarios used in this thesis is introduced, with performance data and input data to simulation. The chapter finishes with specification of simulation tools.

In chapter 4, the earlier theses of Zhu, Sætre and Røsvik is verified in Aspen HYSYS and Aspen Plus for all five scenarios. The simulations with the new estimated Murphree efficiency profiles in Aspen HYSYS, and simulations with the new estimated Murphree efficiency profiles and estimated interfacial area factor in Aspen Plus is presented. Followed by a comparison of the results from Aspen HYSYS and Aspen Plus. In the end the scenarios have been simulated with default Murphree efficiencies estimated by Aspen HYSYS, and with three different amine packages (Kent-Eisenberg, Li-Mather and Acid Gas).

In chapter 5, a method of estimating E_M-factor based on performance data is suggested.

In chapter 6, the results from the verification, and different simulations is evaluated. A comparison between results from earlier work and results from this work is discussed and some further work is suggested.

Chapter 7 is the conclusion of the thesis.

2 Background and problem description

This chapter gives a brief introduction to carbon related climate change, CO_2 capture technologies, description of the process at TCM, summary of earlier work on the subject, and in the end a problem description.

2.1 Climate change related to CO2 emission

When greenhouse gases are released to the atmosphere, they strengthen the greenhouse effect and trap heat, causing the planet surface to warm. CO_2 is the primary greenhouse gas emitted through human activities, mainly from burning fossil fuel. [1]

The graph in figure 2.1 shows atmospheric CO_2 levels measured in ppm at Mauna Loa Observatory in Hawaii, for a little more than a decade. The circle at the end of the graph shows the latest measurement from march 2019, where the level had passed 410 ppm. [2]

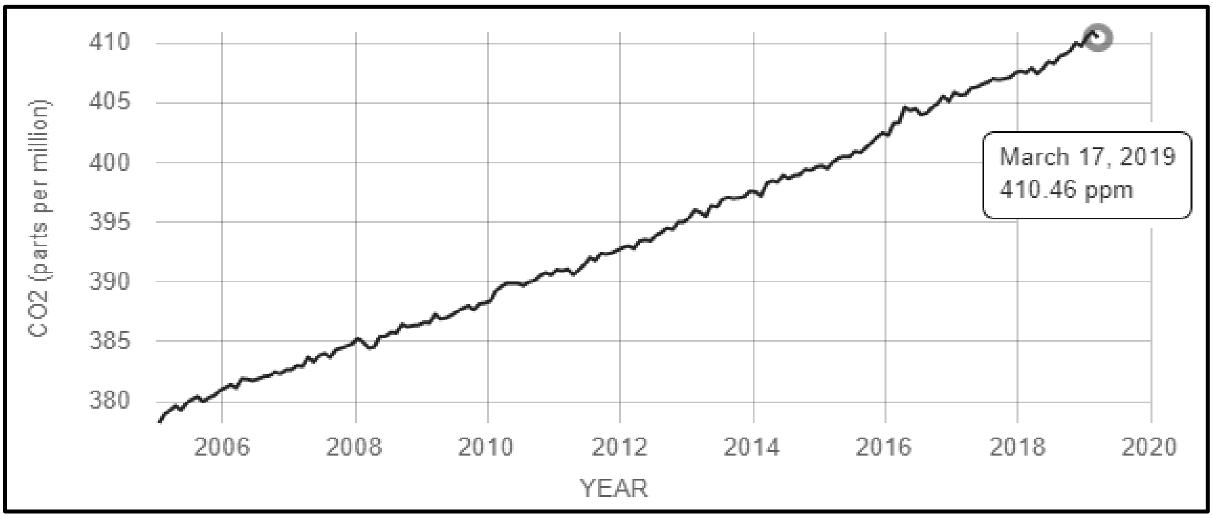


Figure 2.1: Atmospheric CO_2 levels measured at Mauna Loa Observatory, Hawaii. [2]

From the graph, it is clear that the CO_2 level in the atmosphere is increasing and will probably continue to increase in the years to come, if not some drastic changes are made. There have been implemented several protocols to reduce the global climate changes, the latest one in Paris 2015, where the main mitigation was focused on reducing emissions.

As mentioned, the largest source of CO_2 emissions from human activities comes from burning fossil fuels for electricity, heat and transportation. It is therefore implemented measures for these sources to emission. One measure is to develop technology to capture CO_2 and store it for sufficient time.

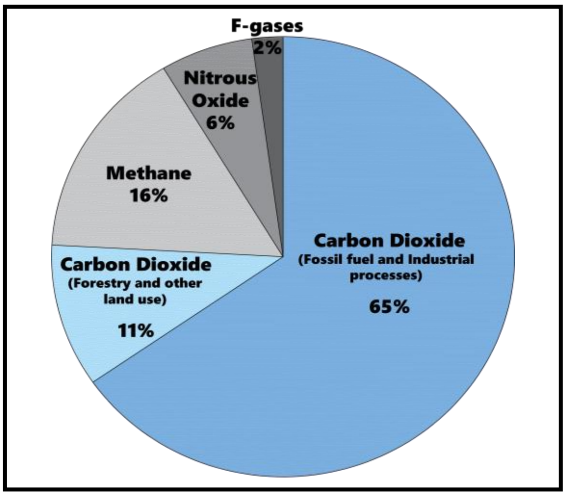


Figure 2.2: Global greenhouse gas emissions by gas, based on emissions from 2010. [1]

2.2 Carbon capture technologies

According to IPCC (Intergovernmental Panel on Climate Change) One considerable way to reduce climate change is CCS (Carbon Capture and Storage) [3].

There are mainly four ways to capture CO_2 from a combustion process [4, 5].

2.2.1 Pre-combustion CO_2 capture process

A pre-combustion system involves converting solid, liquid or gaseous fuel into syngas (a mixture of H_2 and CO_2) without combustion. This way the CO_2 can be removed from the mixture before the H_2 is used for combustion. Syngas can be produced in several ways e.g. gasification or pyrolysis.

2.2.2 Post-combustion CO_2 capture process

By post-combustion capture, CO_2 can be captured from the exhaust of a combustion process by absorbing it in a solvent. The absorbed CO_2 is liberated from the solvent and compressed for transportation and storage. Post-combustion technology is currently the most mature process for CO_2 capture.

2.2.3 Oxy-fuel combustion CO_2 capture process

In the process of oxy-fuel combustion, O_2, instead of air, is used for combustion. This oxygen-rich, nitrogen-free atmosphere results in final flue-gases consisting mainly of CO_2 and H_2O.

2.2.4 Chemical looping CO_2 capture process

The chemical looping process is similar to the oxy-fuel combustion, but a metal oxide is used as an oxygen carrier for the combustion, instead of pure oxygen. During the process, metal oxide is reduced to metal while the fuel is oxidized to CO_2 and water.

2.3 Carbon transport and storage

After capturing the CO_2, it needs to be transported by pipeline, ships, trucks or rail for storage at a suitable storage facility where it can remain for a long period of time. The transportation of CO_2 is very similar to transportation of natural gas, so the existing technology of transportation is considered safe [6].

Suited storage sites needs to obtain the pressure and temperature required for the CO_2 to remain in the liquid or supercritical phase. Such sites are typically located several kilometers under the earth's surface. Suitable storage sites include former oil and gas fields, deep saline formations or depleting oil fields where the injected CO_2 may increase the amount of oil recovered [4].

2.4 Process description at TCM

The TCM pilot-scale amine plant was designed and constructed by Aker Solutions and Kværner. The amine plant was designed to be flexible, to allow testing of different configurations, and has respective capacities of about 80 and 750 tons CO_2/day for CHP (Combined Heat and Power plant) and RFCC (refinery residue fluid catalytic cracker) flue gas operations. This paper is focused on the process with CO_2 capture of CHP flue gas [7]. Figure 2.3 shows a simplified process flow diagram, the numbers in the process description refers to this figure, the figure is inspired by Figure 1 in Thimsen et al., (2014) [8].

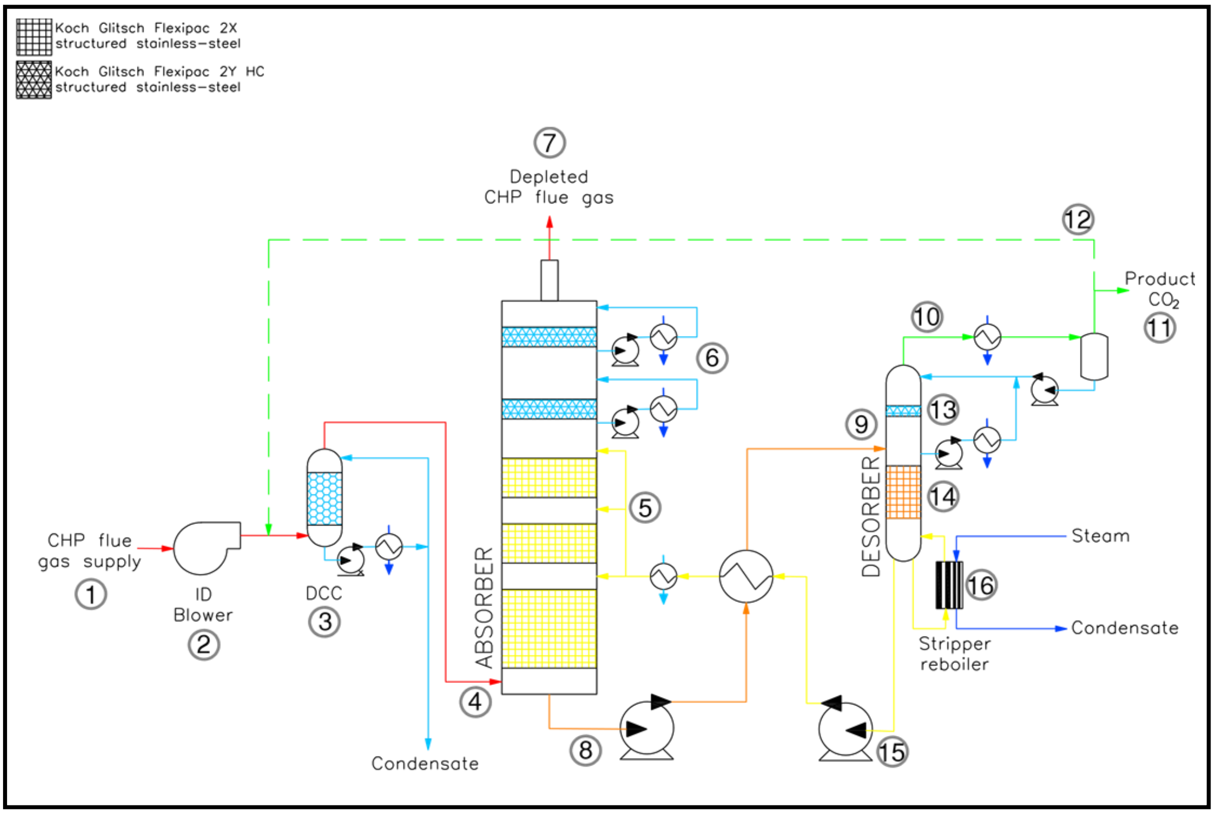


Figure 2.3: Simplified process flow diagram of the amine based CO_2 capture process plant at TCM

2.4.1 Flue gas treatment

1. The flue gas containing CO_2 comes from the CHP at Mongstad refinery, located close to TCM.
2. An ID (induced draft) blower sucks the flue gas out of the CHP chimney, and transports it to TCM through insulated pipes, to avoid temperature drops, which will lead to water condensation inside the pipelines. The ID blower prevents pressure drops and blows the flue gas through the plant with a blower output capacity of up to about 270 mbar and 70,000 Sm^3/h
3. A DCC (direct-contact cooler) system is placed after the ID blower, to quench and lower the temperature of the flue gas with a counter-current flow of water in order to improve the efficiency of the absorption process and provide pre-scrubbing on the flue gas.

2.4.2 CO_2 capture

4. The cooled flue gas enters an absorber, to remove CO_2 from the flue gas using an amine solvent called MEA (monoethanolamine). The absorber has a rectangular polypropylene-lined concrete column with a cross section measuring 3.55x2m and a total height of 62 m.
5. The amine solution contacts the flue gas in the lower region of the column, which consist of three sections of structured stainless-steel packing of 12 m, 6 m and 6 m of height.
6. In the upper region of the column, water-wash systems are located to scrub and clean the flue gas, particularly of any solvent carry over. The water-wash system consists of two sections of structured stainless-steel packing, both have a height of 3 m. The water-wash system is also used to maintain the water balance of the solvent by using heat exchangers to adjust the temperature of the circulating water.
7. The CO_2 depleted flue gas exits the absorber column through a stack located at the top of the absorber.
8. The rich amine exits at the bottom of the absorber, and is from there pumped to the top of the absorption packing in the stripper. During this transportation, the rich amine recovers heat from the lean amine exiting the stripper, through a cross-flow heat exchanger.

2.4.3 Amine regeneration

9. The stripper column recover the captured CO_2 and return lean solvent to the absorber. At TCM there is two independent stripper columns, the column used for CHP flue gas is cylindrical and has a diameter of 1.3 m and a height of 30 m. The other stripper column is larger and is utilized when treating flue gases of higher CO_2 content.
10. The stripper column has an overhead condenser system where CO_2 and water leaving the stripper is cooled down to separate the water, which is led back to the stripper, by a reflux drum, condenser and pumps.
11. The cooled and dried CO_2 is released in to the atmosphere at a safe vent location.
12. A portion of the product CO_2 can also be recycled back to the inlet of the DCC to increase the concentration of CO_2 in the inlet flue gas stream.
13. The upper region of the stripper column consist of a rectifying water-wash section of structured stainless-steel packing, with a height of 1.6 m.
14. The lower region of the stripper consist of structured stainless steel packing with a height of 8m.
15. The lean amine exits at the bottom of the desorber, and is pumped through a cross-flow heat exchanger where it releases energy to the rich amine entering the desorber. The stripped lean amine is cooled down in another heat exchanger before it enters the absorber above each of the three absorber packings.
16. A stream of lean amine is re-heated by steam in a stripper reboiler and put back to the stripper to keep the stripper at desired temperature.

2.5 Chemistry of the process

In this subchapter the advantages and disadvantages of using MEA for CO_2 capture is weighted and the chemical reactions of the CO_2 absorption is described briefly.

The CO_2 is absorbed in a 30/70 wt% mixture of MEA solvent and water. It is absorbed by direct contact with the solvent-mixture in a 24 meter high packing section, of structured stainless-steel.

2.5.1 Generally about MEA

MEA (monoethanolamine) is the amine used as solvent for the CO_2 absorbation in this paper. MEA has the formula $H_2NC_2H_4OH$, and is a primary alkanolamine that often is used for CO_2 removal. Other amines that rapidly is used for CO_2 removal is the secondary alkanolamine, DEA (diethanolamine) and the tertiary amine, MDEA (methyl diethanolamine).

When used as solvents, the amines are typically 20-40 wt% solutions in water. MEA in water solution reacts fast with dissolved CO_2 to form carbamate, and has a high CO_2 capacity. Reaction 2.1 shows how MEA reacts as a weak base in water. [9]

$$MEA + H_2O \leftrightarrow HMEA^+ + OH^- \qquad \text{R(2.1)}$$

2.5.2 Advantages and disadvantages of using MEA for CO_2 capture

The advantages of using MEA in CO_2 capture is its low molecular weight, which gives the MEA high capacity even at low concentrations. Another advantage is the high alkalinity of primary amines. MEA is also considered as a relatively cheap chemical compared with other amines available for CO_2 capture. The toxicity is relatively low and the environmental impact is less questionable than for other amines, because MEA occurs naturally in living organisms.

The disadvantages of using MEA is the high-energy consumption needed for desorption, which is a side effect of the high absorption efficiency. Another problem with MEA in contact with exhaust gas is its tendency to degrade in high temperature and react with oxygen and other components like sulphur oxides and nitrogen oxides [10, 9]. Another important issue is the CO_2 emitted during the production of MEA. When MEA is produced, CO_2 is emitted during the Haber-Bosch process. The regeneration of solvent after the absorption is also an indirect source of CO_2 emission, related to the use of fuels in i.e., combustion for energy supply. The evaluation of the overall balance of CO_2 emitted and captured is essential to determine the efficiency of the process [11].

2.5.3 Reactions of CO_2 absorption into MEA

The following reactions describes how CO_2 can be absorbed into the mixture of MEA solution Reaction 2.2 describes how CO_2 in a gas can be absorbed in an aqueous liquid. [9]

$$CO_2(g) \leftrightarrow CO_2(aq) \tag*{R(2.2)}$$

Since all the reactions in this system occurs in the aqueous phase, the “aq” notation is skipped. Reaction 2.3 describes how in the aqueous phase CO_2 reacts with hydroxide to bicarbonate.

$$CO_2 + OH^- \leftrightarrow HCO_3^- \tag*{R(2.3)}$$

The fast proton transfer reactions (2.4, 2.5 and 2.6) also occur.

Reaction 2.4 describes the ionization of water.

$$H_2O \leftrightarrow H^+ + OH^- \tag*{R(2.4)}$$

Reaction 2.5 describes the deprotonation of carbonic acid. At equilibrium, the concentration of H_2CO_3 is negligible compared to the concentration of free CO_2. In a CO_2 removal process, with a pH normally higher than 8.0 this reaction is often neglected because the concentration of H_2CO_3 becomes very small.

$$H_2CO_3 \leftrightarrow H^+ + HCO_3^- \tag*{R(2.5)}$$

Reaction 2.6 describes the deprotonation of the bicarbonate ion to carbonate ion.

$$HCO_3^- \leftrightarrow H^+ + CO_3^{2-} \tag*{R(2.6)}$$

The absorption of CO_2 into MEA solution can be described by reaction 2.7, where a protonated amine ion ($MEAH^+$) and a carbamate ion ($MEACOO^-$) is formed. A carbamate ion is a product of the reaction of CO_2 and amine, when the amine is MEA the carbamate ion has the formula $HN(C_2H_4OH)COO^-$.

$$2MEA + CO_2 \leftrightarrow MEAH^+ + MEACOO^- \tag*{R(2.7)}$$

Reaction 2.8 describes how a protonated amine ion and bicarbonate (HCO_3^-) is formed.

$$CO_2 + MEA + H_2O \leftrightarrow MEAH^+ + HCO_3^- \tag{R(2.8)}$$

The total concentration of CO_2 is the sum of all the concentrations of the different forms:

$$C_{CO2,TOT} = C_{CO2} + C_{HCO3^-} + C_{CO3^{2-}} + C_{HN(C2H4OH)COO^-} \tag{2.1}$$

The total concentration of amine is the sum of all the concentration of the different forms:

$$C_{MEA,TOT} = C_{MEA} + C_{MEAH^+} + C_{HN(C2H4OH)COO^-} \tag{2.2}$$

2.6 Earlier work

Some of the relevant earlier work that has been done on simulating CO_2 absorption is presented in this subchapter.

- In 2007, Lars Erik Øi (USN) used Aspen HYSYS to simulate CO_2 removal by amine absorption from a gas based power plant. The results showed that adjusting the Murphree Efficiency outside the simulation tool could be a practical approach when using Aspen HYSYS to simulate CO_2 removal. The paper was published at the Conference on Simulation and Modelling SIMS2007 in Gøteborg. [12]

- In 2007, Finn A. Tobiesen, Hallvard F. Svendsen and Olav Juliussen from SINTEF, developed a rigorous rate-based model of acid gas absorption, and a simplified absorber model. They validated the models against mass-transfer data obtained from a 3 month campaign in a laboratory pilot-plant absorber. It was found that the simplified model was satisfactory for lower CO_2 loading, whiles the rigorous model had a better fit for higher CO_2 loading. [13]

- In 2008, Hanne M. Kvamsdal (SINTEF) and Gary T. Rochelle (University of Texas) studied the effects of temperature bulge in CO_2 absorption by MEA. They compared an Aspen Plus rate based absorber with 4 sets of experimental data from a pilot plant at the University of Texas, Austin. Several adjustments were made to the model in order to create a predictable model and to study effects of change in specific parameters. [14]

- In 2009, Luo et al., from NTNU, compared and validated sixteen data sets from four different pilot plant studies, with simulations in four different simulation tools (Aspen Plus equilibrium-based, Aspen Plus rate-based, ProMax, ProTreat^{TM} and CO_2SIM). They concluded that all the simulation tools were able to present reasonable predictions on overall performance of CO_2 absorption rate, while the reboiler duties, concentration and temperature profiles were less predictable. [15]

- In 2011, Espen Hansen worked on his master thesis at USN. Hansen compared Aspen HYSYS, Aspen Plus and ProMAX simulations of CO_2 capture with MEA. He concluded that Aspen HYSYS and Aspen Plus gives similar results, while the results from ProMAX deviated from the Aspen tools. Hansen found that Kent-Eisenberg model in Aspen HYSYS was similar to the Aspen Plus equilibrium-based model for the absorber, but there was a significant difference in the reboiler duties. [16]

- In 2012, Jostein Tvete Bergstrøm worked on his master thesis at USN. Bergstrøm compared Aspen HYSYS (Kent-Esienberg and Li-Mather), Aspen Plus (Rate-based and equilibrium) and ProMAX simulations of CO_2 capture with MEA. Bergstrøm found that the models gave similar results, and that the equilibrium-based model in Aspen Plus and Kent-Eisenberg model in Aspen HYSYS gave coinciding results. [17]

- In 2012, Lars Erik Øi (USN) compared Aspen HYSYS and Aspen Plus (rate-based and equilibrium) simulation of CO_2 capture with MEA. Øi found that there was small deviations in the equilibrium-based model in Aspen HYSYS and Aspen Plus. He found larger deviations between the equilibrium-based calculations and the rate-based calculations. [18]

- In 2013, Ying Zhang and Chau Chyun Chen simulated nineteen data sets of CO_2 absorption in MEA with Aspen rate-based model and the traditional equilibrium-based model. Their result show that rate-based model yields reasonable predictions on all key performance measurements, while equilibrium-based model fails to reliably predict these key performance variables. [19]

- In 2013, Stian Holst Pedersen kvam worked on his master thesis at USN. Kvam compared Aspen Plus (rate based and equilibrium) and Aspen HYSYS (Kent-Eisenberg and Li-mather) simulations of CO_2 capture with MEA. The primary goal was to compare the energy consumption of a standard process, a process with vapour recompression and a vapour recompression with split stream, and not to evaluate the performance of the absorber. [20]

- In 2013, Even Solnes Birkelund worked on his master thesis at UIT. Birkelund compared a standard absorption process, a vapour recompression process and a lean split with vapour recompression process. He simulated the models in Aspen HYSYS and used Kent-Eisenberg as thermodynamic model for the aqueous amine solution, and Peng-Robinson for the vapour phase. All configurations were evaluated due to the energy cost. The results showed that lean split vapour recompression and vapour recompression had the lowest energy cost, while the standard absorption process was simulated to have a much higher energy cost. [21]

- In 2014, Lars Erik Øi et al, simulated different absorption and desorption configurations for 85% amine based CO_2 removal, from a natural gas based power plant using Aspen HYSYS. They simulated a standard process, split-stream, vapour recompressions and different combinations thereof. The simulations were used as a basis for equipment dimensioning, cost estimation and process optimization. [22]

- In 2014, Lars Erik Øi and Stian Holst Pedersen Kvam from USN, simulated different absorption and desorption configurations for 85% CO_2 removal from a natural gas fired combined cycle power plant, with the simulation tools Aspen HYSYS and Aspen Plus. In Aspen Plus, both an equilibrium-based model including Murphree Efficiency and a rate-based model were used. The results show that all simulation models calculate the same trends in the reduction of equivalent heat consumption, when the absorption process configuration were changed from the standard process. [23]

- In 2014, Inga Strømmen Larsen worked on her master thesis at USN. Larsen simulated a rate based Aspen Plus model and compared the results to experimental data from TCM. Larsen found that the Aspen Plus model TCM used was in general agreement with the experimental data. Larsen found temperature and loading profiles similar to the experimental data by adjusting parameters. She also did comparison of mass transfer correlations in Aspen Plus. [24]

- ❖ In 2014 Espen Steinseth Hamborg et al, published a paper with the results from the MEA testing at TCM during the 2013 test campaign. The paper reveals CO_2 removal grade, temperature measurement, and experimental data for the process. [7]

- In 2015 Espen Steinseth Hamborg from TCM presented some of the results from the campaign in 2013 and the results from USN-student Inga Strømmen Larsen's master thesis from 2014, at the PCCC3 in Canada. A v.7.3 Aspen Plus rate-based model was compared to the experimental data. The temperature and loading profile from Aspen Plus presented in this paper gave a good reproduction of the experimental data. [25]

- In 2015, Solomon Aforkoghene Aromada and Lars Erik Øi studied how reduction of energy consumption can be achieved by using alternative configurations. They simulated standard vapour recompression and vapour recompression combined with split stream configurations in Aspen HYSYS, for 85% amine-based CO_2 removal. The results showed that it is possible to reduce energy consumption with both the vapour recompression and the vapor recompression combined with split-stream processes. [26]

- In 2015, Coarlie Desvignes worked on a master thesis at Lyon CPE. Desvignes evaluated 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. Desvignes found that the Aspen Plus model TCM used performed quite well for 30 and 40wt% MEA, but not for higher flue gas temperature and solvent flowrate. [10]

- In 2015, Ye Zhu worked on his master thesis at USN. Zhu simulated an equilibrium model in Aspen HYSYS, 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 found that linear decrease in Murphree efficiency from top to bottom gave good temperature predictions. [27]

- In 2016, Kai Arne Sætre worked on a master's thesis at USN. Sætre simulated seven sets of experimental data from the amine based CO_2 capture process at TCM, with Aspen HYSYS (Kent-Eisenberg and Li-Mather) and Aspen Plus (rate-based and equilibrium). He found that it is possible to fit a rate-based model by adjusting the IAF and equilibrium-based model by adjusting the E_M, both Aspen HYSYS and Aspen Plus will give good results if there are only small changes in the parameters. [28]

- In 2016, Babak Pouladi, Mojtaba Nabipoor Hassankiadeh and Flor Behroozshad, studies the potential to optimize the conditions of CO_2 capture of ethane gas in phase 9 and 10 of south pars in Iran, using DEA as absorbent solvent. They simulated the process in Aspen HYSYS and found the effect of temperature to be significant. [29]

- In 2017, Monica Garcia, Hanna K. Knuutila and Sai Gu, validated a simulation model of the desorption column built in Aspen Plus v8.6. They used four experimental pilot campaigns with 30wt% MEA. The results showed a good agreement between the experimental data and the simulated results. [30]

- In 2017, Mohammad Rehan et al., studied the performance and energy savings of installing an intercooler in a CO_2 capture system based on chemical absorption with MEA as absorption solvent. They used Aspen HYSYS to simulate the CO_2 capture model. The results showed improved CO_2 recovery performance and potential of significant savings in MEA solvent loading and energy requirements, by installing an intercooler in the system. [31]

- In 2017 Leila Faramarzi et al, published a paper with the results from the MEA testing at TCM during the 2015 test campaign. The paper reveals CO_2 removal grade, temperature measurement, and experimental data for the process. [32]

- In 2018, Ole Røsvik worked on his master thesis at USN. Røsvik 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). He found that both Aspen HYSYS and Aspen Plus will give good results if there are only small changes in the parameters. [33]

- In 2018, Lare Erik Øi, Kai Arne Sætre and Espen Steinseth Hamborg, compared four sets of experimental data from the amine based CO_2 capture process at TCM, with different equilibrium-based models in Aspen HYSYS and Aspen Plus, and a rate based model in Aspen Plus. The results show that equilibrium and rate-based models perform equally well in both fitting performance data and in predicting performance at changed conditions. The paper was presented at the Conference on Simulation and Modelling SIMS 59 in Oslo. [34]

2.7 Problem description

Background

TCM is offered to vendors of solvent based CO_2 capture and is mostly running on the vendor's solvents and parameters. TCM does not have permission to publish the results conducted at the vendor's premises. However, TCM have conducted their own test-campaigns in order to publish results.

The results from one scenario from TCM's test-campaign in 2013 was published by Hamborg et al., (2014) [7], and the result from one scenario from the test-campaign in 2015 was published by Faramarzi et al., (2017) [32].

USN and NTNU have produced several papers on amine based CO_2 capture with different simulation tools, throughout the last decade. Performance data from the test-campaigns at TCM have been used in these papers. In addition to the published results some un-published results have been provided to USN by TCM. The repeated conclusion from these papers have been that the rate-based model in Aspen Plus, and the equilibrium-based model in Aspen HYSYS and Aspen Plus perform equally well in both fitting performance data, and in predicting performance at changed conditions. The model with fitted parameters will give a predictable simulation only when there are small changes in process parameters [15] [16] [17] [18] [23] [28] [33] [34].

Another published papers state that the rate-based model yields reasonable predictions on all key performance measurements, while equilibrium-based model fails to predict reliable performance variables [19].

Approach

In this thesis the candidate have simulated 5 scenarios from the test-campaigns at TCM from 2013 and 2015. The candidate have tried to further develop the method of estimating Murphree efficiencies for equilibrium-based models. The candidate have also compared the accuracy of rate-based model and equilibrium-based model in Aspen Plus and Aspen HYSYS.

Aim of Project

The aim of the project was to contribute to achieve predictable models which gives an accurate removal grade and satisfactory temperature- and loading profile. The model should be easy to use for several scenarios with different parameters, and be able to predict reasonable results even when the parameters are changed.

Another aim of the project was to compare if rate-based model and the equilibrium-based model will perform equally well in predicting reliable performance data.

3 Method

In this chapter the method for the simulations, the Murphree efficiency, some necessary calculations methods and decisions is presented and explained. A new E_M-factor is developed. The experimental data from TCM's test campaigns is presented with the input data to the simulations, and specifications of the simulation tools.

3.1 Simulation methodology

The data from TCM is for some cases given in units that needs to be converted to be implemented in Aspen HYSYS and Aspen Plus. Some necessary decisions and fittings needed to be done.

- Only the absorber is simulated
- Experimental data from TCM is converted to units that can be used as parameters in the simulation program
- The pressure loss over the absorber is assumed to be zero
- The main goal is to achieve the same CO_2 removal grade, temperature profile and rich loading as in performance data for the five scenarios.
- The second goal is to compare the reliability in predicting performance data for equilibrium-based model with estimated E_M-profile and rate-based model with estimated IAF.

3.1.1 Simulation tools

Several simulation programs can be used to calculate CO_2 removal by absorption, such as Aspen HYSYS, Aspen Plus, Pro/II, ProTreat and ProMax. In this thesis, the process simulation tool that have been used to perform simulation of CO_2 absorption into amine solution are the equilibrium-based models in Aspen HYSYS and Aspen Plus, and the rate-based model in Aspen Plus. The equilibrium-based models are based on the assumption of equilibrium at each stage. By introducing a Murphree efficiency, the model can be extended. Rate-based models are based on rate expressions for chemical reactions, mass transfer and heat transfer.

3.1.2 Murphree efficiency

There are few tools available for the estimation of stage efficiencies in CO_2 absorption columns. There is a model available for estimation of Murphree efficiency for one plate in a plate column. The estimation model is based on the work of Tomcej et al., (1987) [35], modified later by Rangwala et al., (1992) [36]. This model is based on the assumption that a pseudo first order absorption rate expression is valid. However, there is no model for estimation of Murphree efficiency for a specific packing section height in a structured packing column.

The calculation of necessary column height for CO_2 removal is an important design factor in CO_2 absorption using amine solutions. A simple way to improve the available estimation model is to use Murphree efficiencies for a specific packing height. In a plate column, an efficiency value is estimated for each tray based on the ratio of change in mole fraction from a stage to the next, divided by the change assuming equilibrium. In a packed column, a packing height

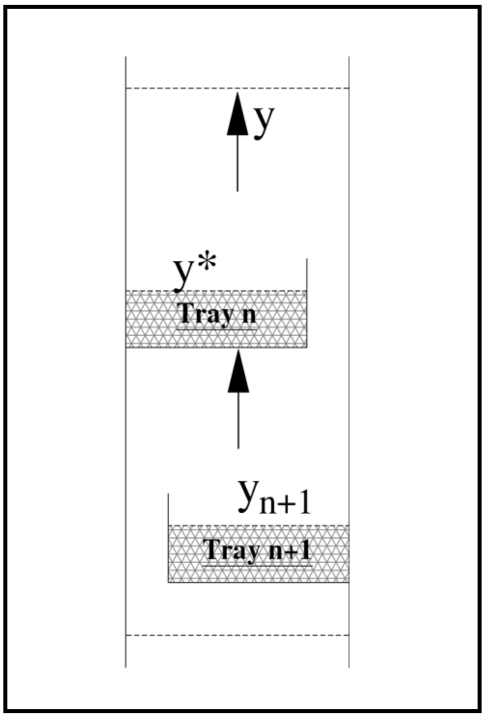


Figure 3.1: Illustration of Murphree efficiency, inspired by Øi (2012) [9].

of e.g. 1 meter could be defined as one tray with a Murphree efficiency. The Murphree efficiencies can be estimated outside the simulation program, before it is implemented to the simulation program. The overall tray efficiency is defined in equation 3.1, as the number of ideal equilibrium trays divided by the actual number of trays.

$$E_O = \frac{N_{IDEAL}}{N_{REAL}} \tag{3.1}$$

The Murphree tray efficiency related to the gas side for tray number "n" is traditionally defined by equation 3.2 [37].

$$E_M = \frac{(y - y_{n+1})}{(y^* - y_{n+1})} \tag{3.2}$$

Where y is the mole fraction in the gas from the tray, y_{n+1} is the mole fraction from the tray below and y* is in equilibrium with the liquid at tray n. This is illustrated in figure 3.1.

Table 3.1 Murphree efficiencies used in this thesis

Murphree efficiencies for each meter of the packed column from top to bottom					
EM	**0,1**	**Zhu**	**Lin**	**SF1**	**SF2**
1	0.1	0.2300	0.17	0,2450	0,2400
2	0.1	0.2192	0.17	0,2425	0,2350
3	0.1	0.2085	0.17	0,2400	0,2300
4	0.1	0.1977	0.17	0,2375	0,2250
5	0.1	0.1869	0.17	0,2350	0,2200
6	0.1	0.1800	0.16	0,2325	0,2150
7	0.1	0.1762	0.15	0,2300	0,2300
8	0.1	0.1546	0.14	0,2000	0,2000
9	0.1	0.1438	0.13	0,1700	0,1700
10	0.1	0.1331	0.12	0,1400	0,1400
11	0.1	0.1223	0.11	0,1100	0,1100
12	0.1	0.1115	0.10	0,0800	0,0800
13	0.1	0.1007	0.09	0,0500	0,0550
14	0.1	0.0900	0.08	0,0475	0,0525
15	0.1	0.0100	0.07	0,0450	0,0500
16	0.1	0.0100	0.06	0,0425	0,0475
17	0.1	0.0100	0.05	0,0400	0,0450
18	0.1	0.0100	0.04	0,0375	0,0425
19	0.1	0.0100	0.03	0,0350	0,0400
20	0.1	0.0100	0.02	0,0001	0,0001
21	0.1	0.0100	0.01	0,0001	0,0001
22	0.1	0.0100	0.01	0,0001	0,0001
23	0.1	0.0100	0.01	0,0001	0,0001
24	0.1	0.0100	0.01	0,0001	0,0001

The Murphree efficiencies of each stage in the 24m high packed column we have at TCM, is estimated for 24 stages of 1m height, the Simulations have been done with both constant and varying efficiency for all stages.

Table 3.1 presents some estimated Murphree efficiency profiles from earlier simulations of TCM data. E_M = 0.1 was simulated in Zhu (2015) [27] to see how constant Murphree efficiency impacts the simulating results. He simulated data from Hamborg et al., (2014) [25], and found that the best fit for removal grade and temperature profile was E_M = Zhu. E_M = Zhu were later used for several scenarios by Sætre (2016) [28]. E_M = Lin, was the best fit, according to Røsvik (2018) [33] where he simulated data from Faramarzi et al., (2017) [32].

The mentioned E_M-profiles have been simulated in this report to verify earlier work, and new E_M-profiles have been estimated based on these results. E_M = SF1 and E_M = SF2 have been estimated in this thesis to fit scenario H14, and also scaled to fit the other scenarios by introducing an E_M-factor.(See 3.2.2)

3.1.3 Converting Sm^3/h to kmol/h

The inlet gas flow is given in Sm^3/h and needs to be given in kmol/h. In 2016, Sætre [28] created a formula to calculate the mole flow, this is given in equation 3.3. The factor 0.023233 is calculated based on standard conditions chosen by TCM to be 15°C and 1 atm, and the ideal gas law.

$$\left[\frac{kmol}{h}\right] = \left[\frac{Sm^3}{h}\right] \times \frac{1}{0{,}023233}\left[\frac{mol}{Sm^3}\right] \tag{3.3}$$

He commented that the results from using this formula deviated from measured data for some of the scenarios, where inlet gas flow was given in both volume flow and molar flow. He concluded that these deviations probably occurred due to uncertainties in the measured data of the experimental data at TCM. Therefore he decided to use the calculated molar flow instead of the measured molar flow, for those scenarios. This decision have also been used for this thesis.

3.1.4 Calculating composition of lean amine

The lean amine is specified in the reports from TCM [7] [32], by the following parameters:

- Lean MEA concentration in water [wt%]
- Lean CO_2 loading [mol CO_2 / mol MEA]
- Lean amine supply flow rate [kg/h]
- Lean amine supply flow temperature [°C]
- Lean amine density [kg/m^3]

To get the most accurate result, it is desired to implement the mole fractions of the lean amine in to the simulations. To accomplish this, some calculation is necessary.

Sætre used a method where he found the molar flow of MEA by using the weight%, mass flow and molar weight, implemented in equation 3.4.

$$\frac{kmol\ MEA}{h} = \frac{MEA\ [wt\%\ in\ water] \times mass\ flow\ rate\ \left[\frac{kg}{h}\right]}{MEA\ molar\ weight\ \left[\frac{kmol}{kg}\right]} \tag{3.4}$$

Following, the H_2O molar flow can be found with the same method, shown in equation 3.5.

$$\frac{kmol\ H_2O}{h} = \frac{(1 - MEA)[wt\%\ in\ \mathrm{water}] \times mass\ flow\ rate\ \left[\frac{kg}{h}\right]}{H_2O\ molar\ weight\ \left[\frac{kmol}{kg}\right]} \tag{3.5}$$

Finally, the CO_2 molar flow can be found by implementing the MEA molar flow and Lean CO_2 loading into equation 3.6.

$$\frac{kmol\ CO_2}{h} = MEA\ molar\ flow\ rate\ \left[\frac{kmol}{h}\right] \times CO_2\ loading\ \left[\frac{kmol\ CO_2}{kmol\ MEA}\right] \tag{3.6}$$

When all the tree molar flows are found the molar fractions is easily calculated and can be implemented to the simulations.

3.1.5 Calculating CO_2 removal grade

The CO_2 capture efficiency can be quantified in four ways as described in Thimsen et al., (2014) [8] and shown in table 3.2, in addition CO_2 recovery calculation is given in table 3.2, and is a measure of the CO_2 mass balance [7].

Table 3.2: Methods for calculating CO_2 removal grade and CO_2 recovery

Method 1	**Method 2**	**Method 3**	**Method 4**	**CO_2 Recovery**
$\frac{P}{S}$	$\frac{P}{P+D}$	$\frac{S-D}{S}$	$1 - \frac{O_{CO2}}{1-O_{CO2}}\ \frac{(1-I_{CO2})}{I_{CO2}}$	$\frac{D+P}{S}$

S = Flue gas supply

D = Depleted flue gas

P = Product CO_2

OCO_2 = Depleted flue gas CO_2 content, dry basis

ICO_2 = Flue gas supply CO_2 content, dry basis

In this report method 3, from table 3.2, is used to calculate removal grade. This method is only dependent on the CO_2 flow in the flue gas supply and the depleted flue gas, the CO_2 flow from the desorber is not included in these calculations. The uncertainty of this method was calculated to be 2,8% in Hamborg et al., (2014) [7], but it was stated that it might be even higher.

3.2 Suggested method for estimating Murphree efficiency

3.2.1 Estimating E_M-profile by calculating overall removal efficiency

To calculate an estimated Murphree efficiency profile the overall removal grade based on the efficiency of each stage, was calculated with equation 3.7. Where y is the CO_2 removal efficiency of each stage in the absorber packing and n is the number of stages.

$$removal\ grade = 100\% - \left(100\% \cdot \left((1-y_1)\cdot(1-y_2)\cdot(\ \dots\ )\cdot(1-y_n)\right)\right) \tag{3.7}$$

The calculated efficiency was compared with the simulated efficiency. The results showed that an E_M-profile calculated to ≈94% gave a simulated result close to 90% for scenario H14. For scenario 2B5 an E_M-profile calculated to ≈89.4% gave a simulated result close to 87.3%. For scenario 6w an E_M-profile calculated to ≈81.1% gave a simulated result close to 83.7%. For scenario Goal1 an E_M-profile calculated to ≈92.3% gave a simulated result close to 90.1%. For scenario F17 an E_M-profile calculated to ≈85.3% gave a simulated result close to 83.7%. When the required overall efficiency was estimated, the Murphree efficiency of each stage was adjusted to fit the temperature profile of the performance data. This was performed in excel, by adjusting the efficiencies of each stage while keeping the overall removal efficiency close to the estimated required overall efficiency level.

3.2.2 Fitting E_M to several scenarios by introducing an E_M-factor

This method evolves around the idea that two similar scenarios with different removal grade might fit the same E_M-profile. If one E_M-profile provides a good fit to the temperature profile of one scenario with high removal grade, the idea is that the E_M-profile can be scaled down to fit the temperature profile of another scenario with lower removal grade, or scaled up to fit a scenario with even higher removal grade. The method is given by equation 3.8.

$$\begin{bmatrix} \underline{E_M} \\ y_1 \\ y_2 \\ \dots \\ y_n \end{bmatrix} \cdot k = \begin{matrix} \underline{E_M(k)} \\ ky_1 \\ ky_2 \\ \dots \\ ky_n \end{matrix} \tag{3.8}$$

Where y is the Murphree efficiency of each stage, n is the number of stages, k is a constant, from now on known as the E_M-factor, estimated by guessing a value of k, and adjusting the value until the requested removal grade for the new scenario is achieved by equation 3.7. Here e.g. the bisection method could be used to converge to the correct E_M-factor.

3.3 Scenarios

This subchapter contains the most important data from all five scenarios used in this report. These scenarios are used as performance data for the simulations in this report, and are all taken from test-campaigns at TCM in 2013 and 2015. All scenarios were run with amine concentrations close to 30 wt% MEA in water. The scenarios are given in tables with performance data and tables with converted data implemented to the simulations.

3.3.1 Scenario H14

Scenario H14 is data from the report published by Hamborg et al., (2014) [7]. This report was produced during the 2013-test campaign at TCM. The scenario was a part of an independent verification protocol, it had low MEA-emissions and MEA-related degradation, and was within all emission limits set by the Norwegian Environment Agency [28].

This scenario has been used in several Master theses at USN earlier, and some of the results are verified in sub-chapter 4.1 and 4.2.

Table 3.3 shows the experimental and measured data from TCM and table 3.4 shows the input data to the simulation. The complete data set is attached in appendix B.

Table 3.3: Experimental and measured data from TCM for scenario H14

TCM data for scenario H14					
Amine inlet			**Flue gas inlet**		
Flow rate	[kg/h]	54900	Flow rate	[Sm^3/h]	46970
Temperature	[C]	36.5	Temperature	[C]	25.0
MEA (CO_2 free)	[wt%]	30.00	CO_2	[vol%]	3.70
loading	[mol CO_2/ molMEA]	0.23	O_2	[vol%]	13.60

Table 3.4: Input data to simulations for scenario H14

Input data for scenario H14					
Amine inlet			**Flue gas inlet**		
Flow rate	[kg/h]	54900	Flow rate	[kmol/h]	2022
Temperature	[C]	36.5	Temperature	[C]	25.0
MEA	[mol%]	10.94	CO_2	[mol%]	3.70
H_2O	[mol%]	86.54	H_2O	[mol%]	2.95
CO_2	[mol%]	2.52	O_2	[mol%]	13.60
Pressure	[bara]	1.0313	N_2	[mol%]	79.75
			Pressure	[bara]	1.0630

The removal grade is given to be close to 90.0% in Hamborg et al., (2014) [7].

The inlet flue gas molar flow is calculated by equation 3.3 in chapter 3.1.3, and the mole fractions of the lean amine is found by using the method in chapter 3.1.4. The flue gas compositions is given in vol% for O_2 and CO_2 but is used as mol% in the simulations. The fraction of H_2O is assumed from similar scenarios like 6w in Sætre (2016) [28]. The implemented parameters are the same parameters as used in Øi, Sætre and Hamborg (2018) [34].

The pressure in the absorber is assumed to be the same as the pressure in the inlet flue gas flow, 106.3 kPa, and there is assumed no pressure drop over the packed section.

3.3.2 Scenario 2B5

Scenario 2B5 is data from the 2015-campaign at TCM, that was supplied to USN from TCM.

This scenario were used in Sætre's Master thesis from USN (2016) [28], some of the results are verified in this report in sub-chapter 4.1 and 4.2.

Table 3.5 shows the experimental and measured data from TCM and table 3.6 shows the input data to the simulation. Different from scenario H14 and F17, this scenario is given with four different measured sets of temperature profiles, with an average removal grade for all sets. The complete data set from appendix J in Sætre (2016) [28] is attached in appendix D.

Table 3.5: Experimental and measured data from TCM for scenario 2B5

TCM data for scenario 2B5					
Amine inlet			**Flue gas inlet**		
Flow rate	[kg/h]	49485	Flow rate	[Sm^3/h]	46982
Temperature	[C]	36.8	Temperature	[C]	28.2
MEA (CO_2 free)	[wt%]	31.60	CO_2	[mol%]	3.57
loading	[mol CO_2/ molMEA]	0.20	O_2	[mol%]	14.60
			H_2O	[mol%]	3.70
			N_2	[mol%]	77.20
			Ar	[mol%]	0.90

Table 3.6: Input data to simulations for scenario 2B5

Input data for scenario 2B5					
Amine inlet			**Flue gas inlet**		
Flow rate	[kg/h]	49485	Flow rate	[kmol/h]	2022
Temperature	[C]	36.8	Temperature	[C]	28.2
MEA	[mol%]	11.67	CO_2	[mol%]	3.57
H_2O	[mol%]	85.65	H_2O	[mol%]	3.70
CO_2	[mol%]	2.68	O_2	[mol%]	14.60
Pressure	[bara]	1.0313	N_2	[mol%]	78.08
			Pressure	[bara]	1.0630

The average removal grade is given to be 87.3% in the data set from TCM. The implemented parameters to the simulation are the same parameters as used in Øi, Sætre and Hamborg (2018) [34].

The pressure in the absorber is assumed to be the same as the pressure in the inlet flue gas flow, 106.3 kPa, and there is assumed no pressure drop over the packed section.

3.3.3 Scenario 6w

Scenario 6w is data from the 2013-campaign at TCM, the data is collected from appendix D in the master's thesis of Sætre (2016) [28].

This scenario have earlier been used in the USN master's theses of Larsen (2014) [24], Desvignes (2015) [10] and Sætre (2016) [28]. Some of the results from Sætre's theses are verified in this report in sub chapter 4.1 and 4.2.

Table 3.7 shows the experimental and measured data from TCM and table 3.8 shows the input data to the simulation. Like scenario 2B5, this scenario is given with four different measured sets of temperature profiles, with an average removal grade for all sets. The complete data set from appendix D in Sætre (2016) [28] is attached in appendix D.

Table 3.7: Experimental and measured data from TCM for scenario 6w

TCM data for scenario 6w					
Amine inlet			**Flue gas inlet**		
Flow rate	[kg/h]	54915	Flow rate	[Sm^3/h]	46602
Temperature	[C]	36.9	Temperature	[C]	25.0
MEA (CO_2 free)	[wt%]	30.40	CO_2	[mol%]	3.57
loading	[mol CO_2/ molMEA]	0.25	O_2	[mol%]	13.60
			H_2O	[mol%]	3.00
			N_2	[mol%]	79.83
			Ar	[mol%]	0.00

Table 3.8: Input data to simulations for scenario 6w

Input data for scenario 6w					
Amine inlet			**Flue gas inlet**		
Flow rate	[kg/h]	54915	Flow rate	[kmol/h]	2005
Temperature	[C]	36.9	Temperature	[C]	25.0
MEA	[mol%]	11.13	CO_2	[mol%]	3.57
H_2O	[mol%]	86.37	H_2O	[mol%]	3.00
CO_2	[mol%]	2.50	O_2	[mol%]	13.60
Pressure	[bara]	1.0313	N_2	[mol%]	79.83
			Pressure	[bara]	1.0630

The average removal grade is given to be 79.0% in the data set from TCM. The implemented parameters to the simulation are equal to the parameters used in Øi, Sætre and Hamborg (2018) [34].

The pressure in the absorber is assumed to be the same as the pressure in the inlet flue gas flow, 106.3 kPa, and there is assumed no pressure drop over the packed section.

3.3.4 Scenario Goal1

Scenario Goal1 is data from the 2015-campaign at TCM, that was supplied to USN from TCM. The data is collected from appendix K in the master's thesis of Sætre (2016) [28].

This scenario were used in Sætre's Master thesis from USN (2016) [28], some of the results are verified in this report in sub chapter 4.1.

Table 3.9 shows the experimental and measured data from TCM and table 3.10 shows the input data to the simulation. Just like for Scenario 2B5 and 6w, this scenario is given with four different measured sets of temperature profiles, with an average removal grade for all sets. The complete data set from appendix K in Sætre (2016) [28] is attached in appendix E.

Table 3.9: Experimental and measured data from TCM for scenario Goal1

TCM data for scenario Goal1					
Amine inlet			**Flue gas inlet**		
Flow rate	[kg/h]	44391	Flow rate	[Sm^3/h]	46868
Temperature	[C]	36.5	Temperature	[C]	25.0
MEA (CO_2 free)	[wt%]	32.40	CO_2	[mol%]	3.62
loading	[mol CO_2/ molMEA]	0.20	O_2	[mol%]	14.30
			H_2O	[mol%]	3.10
			N_2	[mol%]	78.10
			Ar	[mol%]	0.90

Table 3.10: Input data to simulations for scenario Goal1

Input data for scenario Goal1					
Amine inlet			**Flue gas inlet**		
Flow rate	[kg/h]	44391	Flow rate	[kmol/h]	2017
Temperature	[C]	36.5	Temperature	[C]	25.0
MEA	[mol%]	11.57	CO_2	[mol%]	3.62
H_2O	[mol%]	86.29	H_2O	[mol%]	3.10
CO_2	[mol%]	2.14	O_2	[mol%]	14.30
Pressure	[bara]	1.0313	N_2	[mol%]	79.00
			Pressure	[bara]	1.0630

The average removal grade is given to be 90.1% in the data set from TCM. The implemented parameters to the simulation are the same parameters as used in Øi, Sætre and Hamborg (2018) [34]. Except for the lean amine temperature, which was 28.6 °C in Sætre (2016) and Øi, Sætre and Hamborg (2018). From appendix K in Sætre (2016) the lean amine temperature was found to be 36.5 °C, while the rich amine temperature was 28.6 °C. The mole fraction composition of amine was also adjusted to fit the MEA wt% from performance data.

The pressure in the absorber is assumed to be the same as the pressure in the inlet flue gas flow, 106.3 kPa, and there is assumed no pressure drop over the packed section.

3.3.5 Scenario F17

Scenario F17 is data from the report published by Faramarzi et al, (2017) [32]. This report was produced during the 2015- test campaign at TCM. The scenario was part of an independent verification protocol, Emission levels of MEA, NH_3, aldehydes, nitrosamines and other compounds were also measured and were all below the permissible levels set by the Norwegian Environment Agency.

This scenario was used in the USN master thesis of Røsvik (2018) [33]. Some of the results are verified in sub chapter 4.1 and 4.2.

Table 3.11 shows the experimental and measured data from TCM and table 3.12 shows the input data to the simulation. The complete data set is attached in appendix F.

Table 3.11: Experimental and measured data from TCM for scenario F17

TCM data for scenario F17					
Amine inlet			**Flue gas inlet**		
Flow rate	[kg/h]	57434	Flow rate	[Sm^3/h]	59430
Temperature	[C]	37.0	Temperature	[C]	29.8
MEA (CO_2 free)	[wt%]	31.00	CO_2	[vol%]	3.70
loading	[mol CO_2/ molMEA]	0.20	O_2	[vol%]	14.60

Table 3.12: Input data to simulations for scenario F17

Input data for scenario F17					
Amine inlet			**Flue gas inlet**		
Flow rate	[kg/h]	57434	Flow rate	[kmol/h]	2558
Temperature	[C]	37.0	Temperature	[C]	29.8
MEA	[mol%]	11.44	CO_2	[mol%]	3.70
H_2O	[mol%]	86.27	H_2O	[mol%]	3.70
CO_2	[mol%]	2.29	O_2	[mol%]	14.60
Pressure	[bara]	1.0313	N_2	[mol%]	78.00
			Pressure	[bara]	1.0100

The removal grade is given to be close to 83.5% in Faramarzi et al., (2017) [32].

The inlet flue gas molar flow is calculated by equation 3.3 in chapter 3.1.3, and the mole fractions of the lean amine is found by using the method in chapter 3.1.4, just like for scenario H14. The flue gas compositions is given in vol% for O_2 and CO_2 but is used as mol% in the simulations. The implemented parameters are the same parameters as used in Røsvik (2018) [33].

The pressure in the absorber is assumed to be the same as the pressure in the inlet flue gas flow, 101 kPa, and there is assumed no pressure drop over the packed section.

3.4 Specifications of the simulation tools

3.4.1 Equilibrium-based model

The Aspen HYSYS equilibrium-based file used in this thesis is named "KaiHamborgABSver.HSC"

Properties of the file is given in table 3.13 below.

Table 3.13: Specification for Aspen HYSYS Equilibrium-based model

Specifications - Aspen HYSYS Equilibrium	
Properties	
Amine package	Kent-Eisenberg
(Amine packages used for comparison in chapter 4.7)	*(Li-Mather)* *(Acid Gas - Liquid Treating)*
Absorber	
Number of stages	24
Nominal pressure	106.3 [kPa]
Rating	
Uniform section	Yes
Internal type	Sieve
Diameter	3m
Tray space	0.5
Weeping factor	1000

The Aspen Plus equilibrium-based file used in this thesis is named "Aspenpluseq6w.apwz".

Properties of the file is given in table 3.14 below.

Table 3.14: Specification for Aspen Plus Equilibrium-based model

Specifications - Aspen Plus Equilibrium	
Properties	
Method	ElecNRTL
Henry comp ID	MEA
Chemistry ID	MEA
Configuration	
Calculation type	Equilibrium
Number of stages	24
Valid phases	Vapor-Liquid
Pressure stage 1	1.04 bara
Efficiencies	
Efficiency type	Murphree Efficiency
Method	Individual comp.
Rating	
Not specified	

3.4.2 Rate-based model

The Aspen Plus rate-based file used in this thesis is named “TCM2B5Rev6-4_abs.apw”.

The specifications in this file is provided in the table below.

Table 3.15: Specification of the model used for rate-based simulation

Specifications - Aspen Plus Rate-based	
Calculation type	Rate-based
Number of stages	50
Efficiency type	Vaporization efficiencies
Reaction ID	MEA-NEW
Holdup	0.0001 stage 1 to 50
Reaction conduction factor	0.9
Packing type	Koch metal 2x
Section diameter [m]	3
Section packed height [m]	24
Flow model	Countercurrent
Interfacial area factor	0.29 to 1
Film Liquid phase	Discrxn
Film Vapor phase	Film
Mass transfer coeff method	Bravo et al., (1985)
Heat transfer coeff method	Chilton and Colburn
Interfacial area method	Bravo et al., (1985)
Holdup method	Bravo et al., (1992)
Add. Discretize points liquid	5

The files used in both Aspen HYSYS and Aspen Plus have been provided to me by my supervisor, these files were created and used by Sætre (2016) [28], for his master thesis. These files are the basis for figure 3 and 4 in Øi, Sætre and Hamborg (2018) [34].

4 Results

This chapter presents the results from the simulations of all scenarios in Aspen Plus and Aspen HYSYS. The five scenarios have been used for earlier master theses:

- Scenario H14 have been simulated in both Aspen HYSYS and Aspen Plus in earlier master thesis's at USN. In 2015 Ye Zhu simulated the scenario in Aspen HYSYS, for his master thesis. Then in 2016 and 2018, Kai Arne Sætre and Ole Røsvik, respectively, simulated the same scenario in both Aspen HYSYS and Aspen Plus.
- Scenario 2B5 have been simulated in both Aspen HYSYS and Aspen Plus in Kai Arne Sætre's master thesis from 2016.
- Scenario 6w have been simulated in both Aspen HYSYS and Aspen Plus in earlier USN master's theses by Larsen (2014), Desvignes (2015) and Sætre (2016).
- Scenario Goal1 have been simulated in both Aspen HYSYS and Aspen Plus in Kai Arne Sætre's master thesis from 2016.
- Scenario F17 have been simulated in both Aspen HYSYS and Aspen Plus in Ole Røsvik's master thesis from 2018.

An introduction and description of the simulations in each sub-chapter is given below:

- 4.1 Verification of earlier work in Aspen HYSYS

  This sub-chapter presents the simulation of the five scenarios compared with results from earlier work and performance data. All data in this sub-chapter is simulated in equilibrium-based model in Aspen HYSYS with Kent Eisenberg as amine package.

  The simulated temperature profile from Aspen HYSYS compared with simulated results from earlier theses is attached in appendix G.

- 4.2 Verification of earlier work in Aspen Plus

  This sub-chapter presents the simulation of the five scenarios compared with results from earlier work and performance data. All scenarios have been simulated in rate-based model and equilibrium-based model in Aspen Plus with e-NRTL.

  The simulated temperature profile from Aspen Plus compared with simulated results from earlier theses is attached in appendix H.

- 4.3 Simulation in Aspen HYSYS with estimated E_M

  Earlier studies have focused on the packed section as one packing with Murphree efficiencies from top to bottom. The results from these studies showed that a linear decrease in Murphree efficiency from the top to the lower middle of the packing, followed by a low constant efficiency for the bottom part of the packing have given the best fit to the temperature profile, e.g. E_M=Zhu.

During this project several combinations of Murphree efficiencies have been tested, some of them based on the idea that the three separated packing sections in the column might have higher efficiencies at the top of each section, because fresh amine enters at the top of each section. Based on this theory, two new E_M-profiles were estimated with equation 3.7, E_M=SF1 and E_M=SF2. Both with linearly decreasing efficiency in each packing section in the packed column. These two sets was first estimated for Scenario H14, and later scaled to fit the other scenarios, by introducing the E_M-factor in equation 3.8.

In this sub-chapter the five E_M-profiles given in table 3.1 in sub chapter 3.1.2, have been scaled for each scenario to produce requested removal grade in simulation. All simulations in this sub-chapter have been simulated in equilibrium-based model in Aspen HYSYS with Kent Eisenberg.

The estimated Murphree efficiency profiles is attached in appendix I, along with the simulated temperature profiles and important data from simulation.

Some interesting connections between E_M-factor and performance data was seen in the results from these simulations, which led to the calculations in chapter 5.

- 4.4 Simulation in Aspen Plus with estimated E_M and IAF

In this sub-chapter all the E_M-profiles used in sub-chapter 4.3 have been scaled to achieve requested removal grade for all E_M-profiles in all five scenarios in Aspen Plus, by adjusting the E_M-factor. The simulations have been simulated in equilibrium-based model in Aspen Plus with e-NRTL.

The interfacial area factor have been adjusted to achieve requested removal grade for all scenarios in rate-based model in Aspen plus.

The estimated IAF is attached in appendix J, along with the simulated temperature profiles and important data from simulation.

- 4.5 Comparison of Rate-based and Equilibrium-based model

In this sub-chapter the simulated results from sub-chapter 4.3 and 4.4 have been compared.

The simulated temperature profiles and important data from simulation is attached in appendix K.

- 4.6 Simulation with default E_M in Aspen HYSYS

There is a possibility to get Aspen HYSYS to estimate the Murphree efficiencies, these efficiencies is from now on called default efficiencies. The method that was used to achieve the requested removal grade with default efficiencies, was to vary the amount of stages in the packed column. In this sub chapter the simulations of each scenario with default efficiencies have been compared with the results from the estimated simulation of E_M=SF1 for each scenario.

The default E_M-profiles estimated by Aspen HYSYS is attached in appendix L, along with the simulated temperature profiles and important data from simulation.

- 4.7 Comparison of Kent-Eisenberg, Li-Mather and Acid-Gas

  There is three equilibrium-based amine packages available for simulation of absorption in Aspen HYSYS. In earlier master theses from USN, Kent-Eisenberg and Li-Mather have been compared. In this sub-chapter all three amine packages are compared for all scenarios with all the E_M-profiles used in the simulation chapter.

  In this sub-chapter each scenario is presented with a figure that compares the temperature profiles for each set of Murphree efficiency simulated with each of the three amine packages. Each scenario is also presented with a table that compares the key data for each set of Murphree efficiency simulated with each of the three amine packages.

  The simulated temperature profiles and important data for all simulations in this sub-chapter is attached in appendix M.

Comments on the results from all simulations can be found in chapter 6.

4.1 Verification of earlier work in Aspen HYSYS

4.1.1 Verification of scenario H14 in Aspen HYSYS

In the first simulation the Murphree efficiency was adjusted to 0,1 and was constant for all stages. Figure 4.1 shows the temperature profiles for performance data and simulated data, compared with simulated data from Zhu (2015) [27], Sætre (2016) [28] and Røsvik (2018) [33]. Table 4.1 shows the key results from simulation compared with performance data, and data from earlier simulations of the same scenario.

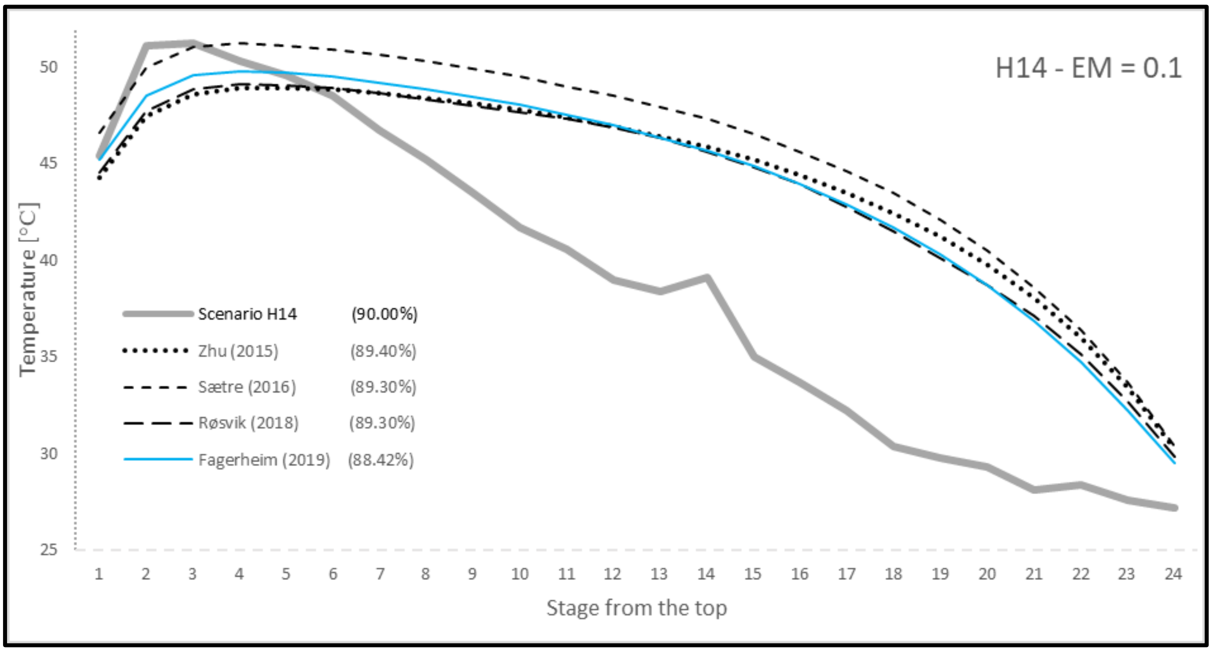


Figure 4.1: Verification of Scenario H14 with E_M = 0.1 (HYSYS)

Table 4.1: Key results from simulation of scenario H14 with $E_M = 0.1$ (HYSYS)

	TCM data	Zhu (2015)	Sætre (2016)	Røsvik (2018)	Fagerheim (2019)
Removal grade	90.00%	89.40%	87,00%	89.30%	88.42%
Rich loading	0.4800	0.4870	0.4920	-	0.4885
Ttop [˚C]	45.40	44.29	46.60	44,52	45.20
Tmax [˚C]	51.20	48.93	51.20	49,10	49.79
Tbtm [˚C]	27.20	30.26	30.40	29,84	29,48

In 2015 Zhu [27] simulated scenario H14 and adjusted the Murphree efficiency to fit the temperature profiles. He achieved the best fit, for both removal grade and temperature profile when he adjusted the first stages (1-14) linearly from 0.23-0.09, the remaining stages (15-24) were set constant to 0.01 for each stage. In this thesis, this E_M-profile is called Zhu.

Figure 4.2 presents the temperature profiles with E_M adjusted according to Zhu.

Table 4.2 provide the key results from simulation compared with performance data, and data from earlier simulations of the same scenario.

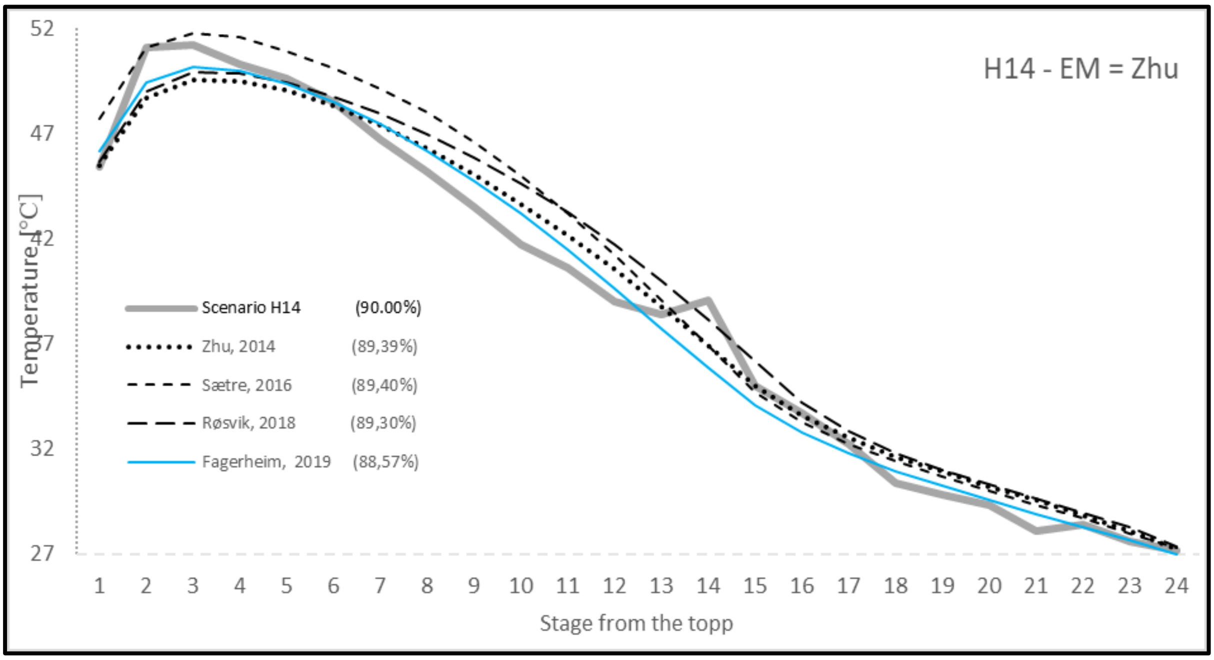


Figure 4.2: Verification of Scenario H14 with E_M = Zhu (HYSYS)

Table 4.2: Key results from simulation of scenario H14 with E_M = Zhu (HYSYS)

	TCM data	Zhu (2015)	Sætre (2016)	Røsvik (2018)	Fagerheim (2019)
Removal grade	90.00%	89.39%	86.90%	89.30%	88.57%
Rich loading	0.4800	0.4789	0.4910	-	0.4890
Ttop [˚C]	45.40	45.48	47.70	45.66	46.14
Tmax [˚C]	51.20	49.56	51.80	49.94	50.16
Tbtm [˚C]	27.20	27.22	27.30	27.38	27.00

4.1.2 Verification of scenario 2B5 in Aspen HYSYS

Figure 4.3 presents the results from the simulation of data for scenario 2B5 with $E_M = 0.1$. Scenario 2B5 consist of a data set with four sets of temperature measurements, the thick blue line in figure 4.3 is the average temperature values of each stage from the data set.

Table 4.3 provides the key results from the simulation compared with performance data and results from Sætre (2016) [28].

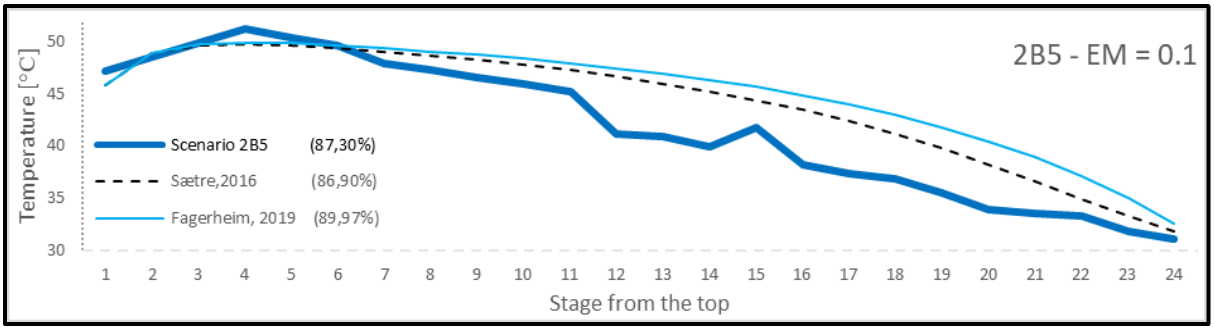


Figure 4.3: Verification of Scenario 2B5 with $E_M = 0.1$ (HYSYS)

Table 4.3: Key results from simulation of scenario 2B5 with $E_M = 0.1$ (HYSYS)

	TCM data	**Sætre (2016)**	**Fagerheim (2019)**
Removal grade	87.30%	86.90%	89.97%
Rich loading	0.5000	0.4900	0.4715
Ttop [˚C]	47.09	45.80	45.80
Tmax [˚C]	51.47	49.70	49.89
Tbtm [˚C]	30.99	31.80	32.51

Figure 4.4 and table 4.4 below, presents the results from the simulation of data for scenario 2B5 with E_M = Zhu.

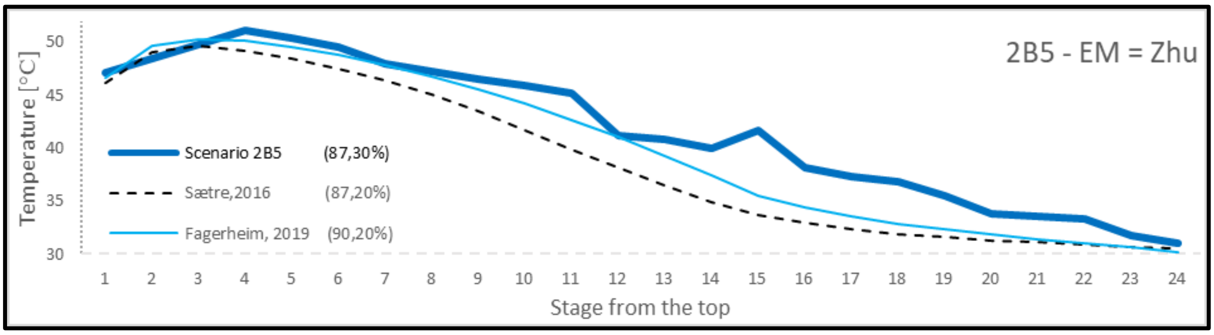


Figure 4.4: Verification of Scenario 2B5 with E_M = Zhu (HYSYS)

Table 4.4: Key results from simulation of scenario 2B5 with E_M = Zhu (HYSYS)

	TCM data	**Sætre (2016)**	**Fagerheim (2019)**
Removal grade	87.30%	87.20%	90.20%
Rich loading	0.5000	0.4901	0.4722
Ttop [˚C]	47.09	46.20	47.09
Tmax [˚C]	51.47	49.10	51.16
Tbtm [˚C]	30.99	30.50	30.74

4.1.3 Verification of scenario 6w in Aspen HYSYS

Figure 4.5 presents the results from the simulation of data for scenario 6w with E_M = 0.1. Scenario 6w also consist of a data set with four sets of temperature measurements, the thick purple line in figure 4.5 is the average temperature values of each stage from the data set.

Table 4.5 provides the key results from the simulation compared with performance data and results from Sætre (2016) [28].

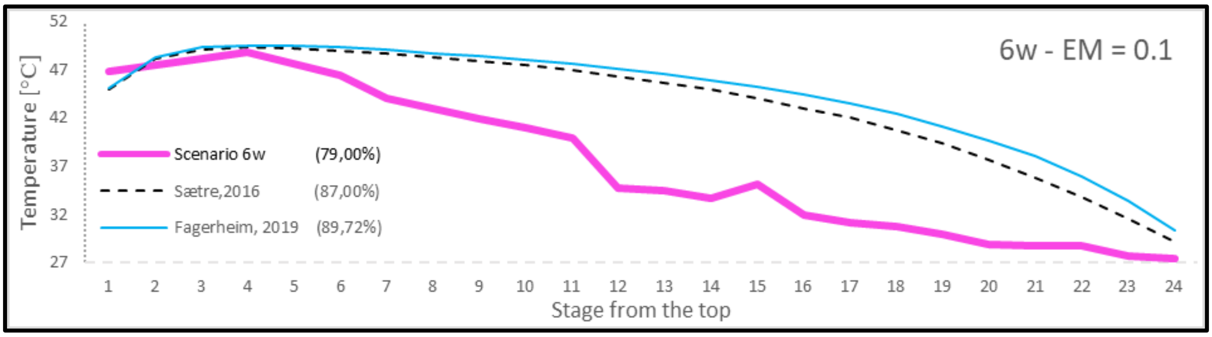


Figure 4.5: Verification of Scenario 6w with E_M = 0.1 (HYSYS)

Table 4.5: Key results from simulation of scenario 6w with E_M = 0.1 (HYSYS)

	TCM data	Sætre (2016)	Fagerheim (2019)
Removal grade	79.00%	87.00%	89.72%
Rich loading	0.4600	0.4920	0.4721
Ttop [˚C]	46.10	45.00	45.04
Tmax [˚C]	49.35	49.30	49.52
Tbtm [˚C]	27.33	29.10	30.33

Figure 4.6 and table 4.6 below, presents the results from the simulation of data for scenario 6w with E_M = Zhu.

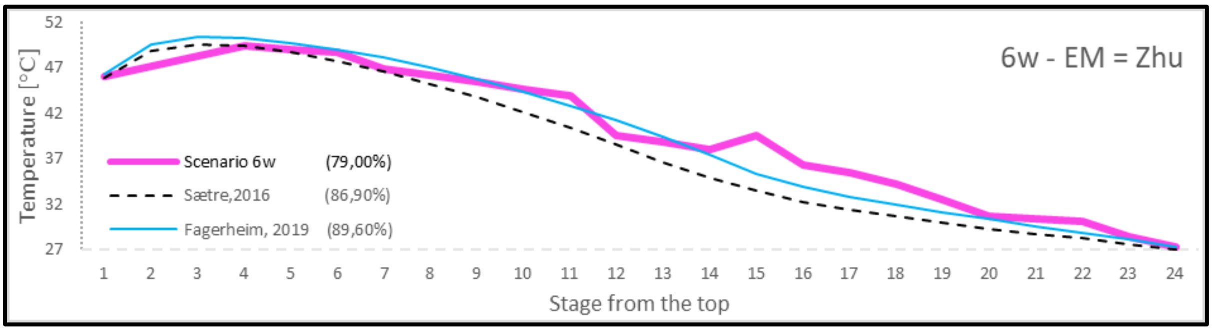


Figure 4.6: Verification of Scenario 6w with E_M = Zhu (HYSYS)

Table 4.6: Key results from simulation of scenario 6w with E_M = Zhu (HYSYS)

	TCM data	Sætre (2016)	Fagerheim (2019)
Removal grade	79.00%	86.90%	89.60%
Rich loading	0.4600	0.4910	0.4721
Ttop [˚C]	46.10	45.80	46.24
Tmax [˚C]	49.35	49.50	50.29
Tbtm [˚C]	27.33	27.00	27.30

4.1.4 Verification of scenario Goal1 in Aspen HYSYS

Figure 4.7 presents the results from the simulation of data for scenario Goal1 with $E_M = 0.1$. Scenario Goal1 does also consist of a data set with four sets of temperature measurements, the thick gray line in figure 4.7 is the average temperature values of each stage from the data set.

Table 4.7 provides the key results from the simulation compared with performance data and results from Sætre (2016) [28].

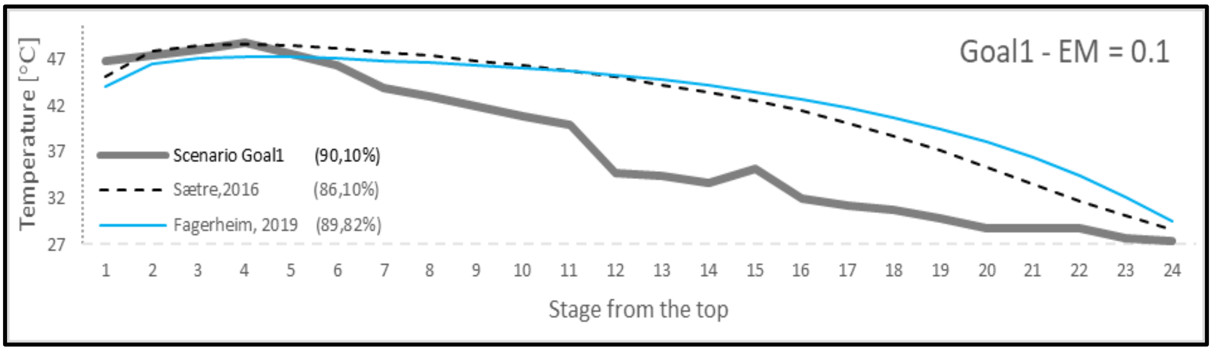


Figure 4.7: Verification of Scenario Goal1 with $E_M = 0.1$ (HYSYS)

Table 4.7: Key results from simulation of scenario Goal1 with $E_M = 0.1$ (HYSYS)

	TCM data	**Sætre (2016)**	**Fagerheim (2019)**
Removal grade	90.10%	86.10%	89.82%
Rich loading	0.5000	0.5000	0.4863
Ttop [˚C]	46.81	45.10	44.03
Tmax [˚C]	48.81	48.70	47.30
Tbtm [˚C]	27.31	28.50	29.55

Figure 4.8 and table 4.8 below, presents the results from the simulation of data for scenario Goal 1 with E_M = Zhu.

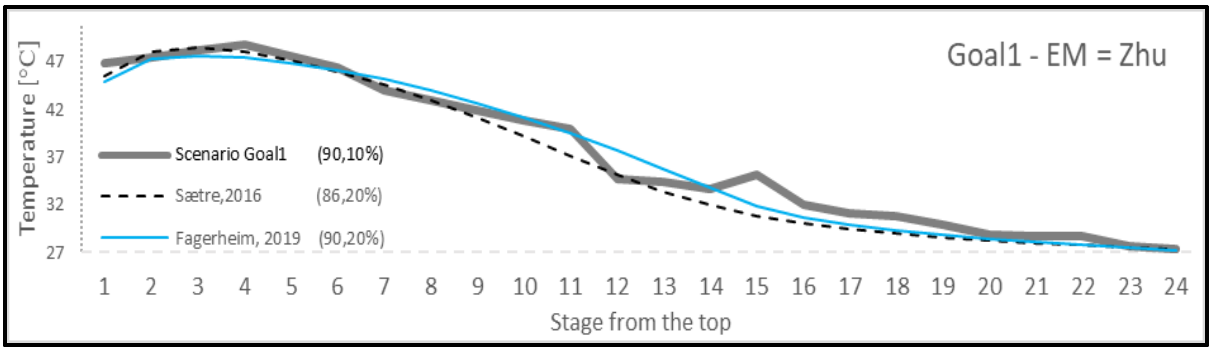


Figure 4.8: Verification of Scenario Goal1 with E_M = Zhu (HYSYS)

Table 4.8: Key results from simulation of scenario Goal1 with E_M = Zhu (HYSYS)

	TCM data	**Sætre (2016)**	**Fagerheim (2019)**
Removal grade	90.10%	86.20%	90.20%
Rich loading	0.5000	0.5000	0.4876
Ttop [˚C]	46.81	45.50	44.83
Tmax [˚C]	48.81	48.50	47.64
Tbtm [˚C]	27.31	27.30	27.20

4.1.5 Verification of scenario F17 in Aspen HYSYS

Figure 4.9 underneath presents the temperature profiles of performance data and simulated data for scenario F17 with $E_M = 0.1$, the thick black line in figure 4.9 is the temperature values of each stage from the data set.

Table 4.9 provides the key results from the simulation compared with performance data and results from Røsvik (2018) [33].

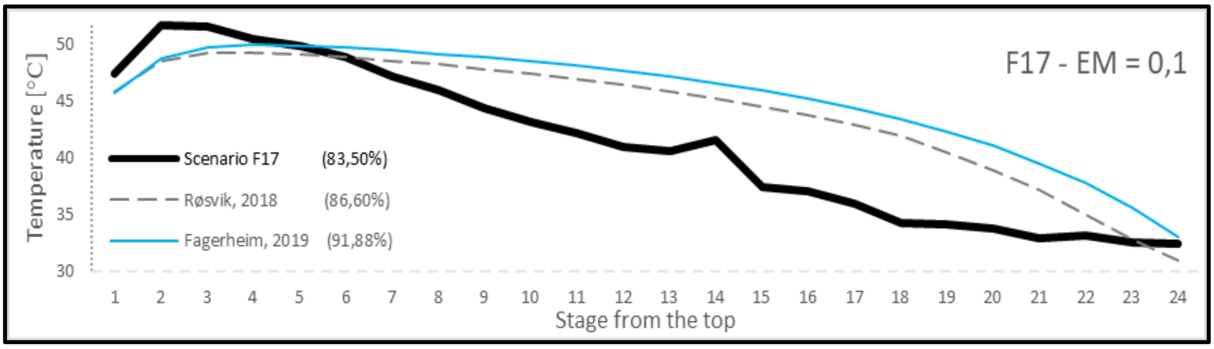


Figure 4.9: Verification of Scenario F17 with $E_M = 0.1$ (HYSYS)

Table 4.9: Key results from simulation of scenario F17 with $E_M = 0.1$ (HYSYS)

	TCM data	Røsvik (2018)	Fagerheim (2019)
Removal grade	83.50%	86.60%	91.88%
Rich loading	0.4800	-	0.3554
Ttop [˚C]	47.40	45.84	45.72
Tmax [˚C]	51.70	49.31	49.96
Tbtm [˚C]	32.40	30.98	33.00

Figure 4.10 underneath presents the temperature profiles for performance data and simulated data for scenario F17 with E_M = Zhu, and table 4.10 provides the key results from the simulation compared with performance data and results from Røsvik (2018) [33].

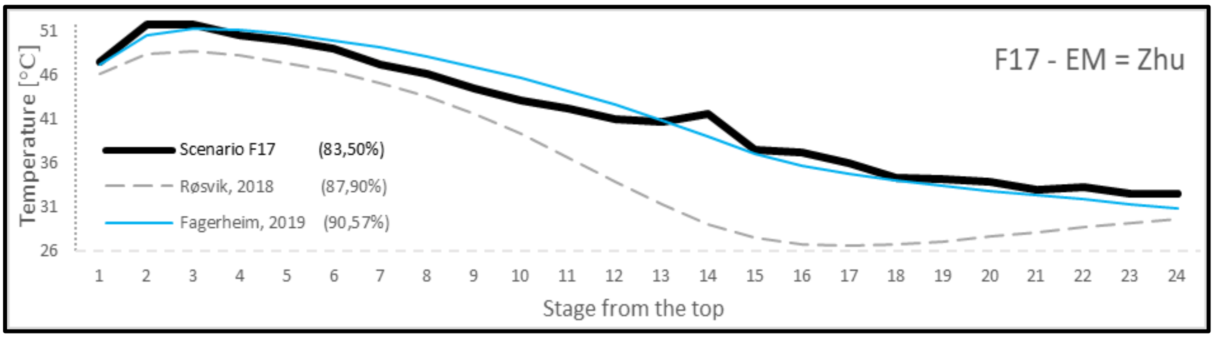


Figure 4.10: Verification of Scenario F17 with E_M = Zhu (HYSYS)

Table 4.10: Key results from simulation of scenario F17 with E_M = Zhu (HYSYS)

	TCM data	Røsvik (2018)	Fagerheim (2019)
Removal grade	83.50%	87.90%	90.57%
Rich loading	0.4800	-	0.4552
Ttop [˚C]	47.40	46.04	47.09
Tmax [˚C]	51.70	48.63	51.16
Tbtm [˚C]	32.40	29.59	30.75

Figure 4.11 and table 4.11 underneath, shows the results from the simulation of data for scenario F17 with E_M = Lin, which was concluded to be the best fit in Røsvik's master's thesis from 2018 [33].

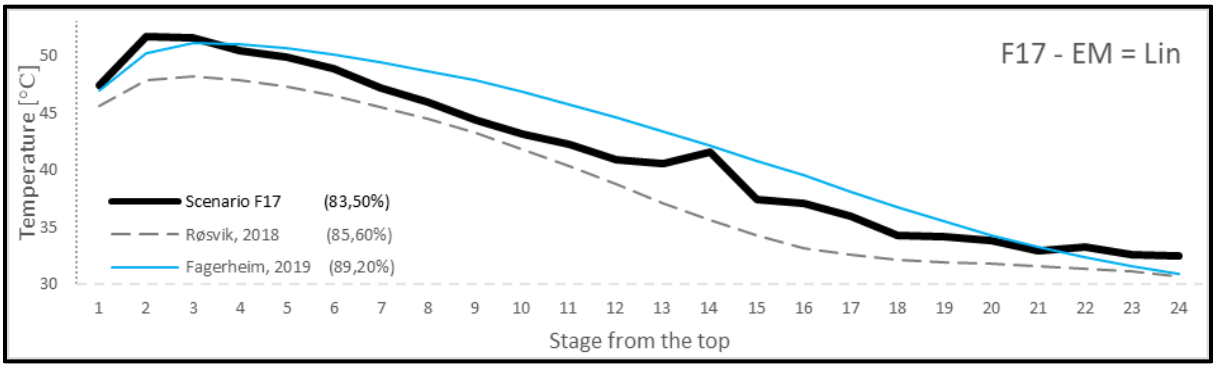


Figure 4.11: Verification of Scenario F17 with E_M = Lin (HYSYS)

Table 4.11: Key results from simulation of scenario F17 with E_M = Lin (HYSYS)

	TCM data	Røsvik (2018)	Fagerheim (2019)
Removal grade	83.50%	85.60%	89.20%
Rich loading	0.4800	-	0.4514
Ttop [˚C]	47.40	45.60	46.92
Tmax [˚C]	51.70	48.19	51.09
Tbtm [˚C]	32.40	30.64	30.88

4.2 Verification of earlier work in Aspen Plus

4.2.1 Verification of scenario H14 in Aspen Plus

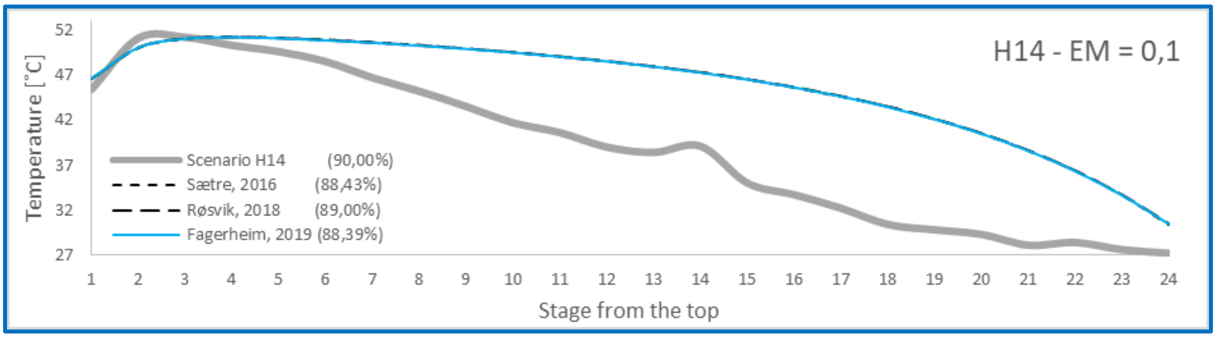


Figure 4.12: Verification of Scenario H14 with E_M = 0.1 (Plus)

Table 4.12: Key results from simulation of scenario H14 with E_M = 0.1 (Plus)

	TCM data	Sætre (2016)	Røsvik (2018)	Fagerheim (2019)
Removal grade	90.00%	87.20%	88.40%	88.40%
Rich loading	0.4800	0.4910	-	0.4880
Ttop [˚C]	45.40	46.50	46.65	46.60
Tmax [˚C]	51.20	50.90	51.28	51.19
Tbtm [˚C]	27.20	30.20	30.50	30.43

Figure 4.12 presents the temperature profiles of performance data and data simulated in Aspen Plus for scenario H14 with $E_M = 0.1$, Table 4.12 provides the key results from the simulation compared with performance data and results from Sætre (2016) [28] and Røsvik (2018) [33].

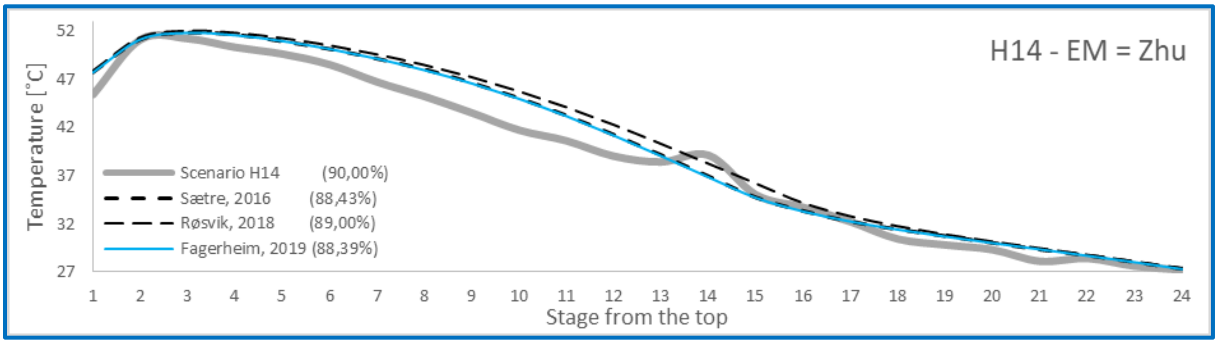


Figure 4.13: Verification of Scenario H14 with E_M = Zhu (Plus)

Table 4.13: Key results from simulation of scenario H14 with E_M = Zhu (Plus)

	TCM data	Sætre (2016)	Røsvik (2018)	Fagerheim (2019)
Removal grade	90.00%	86.90%	89.00%	88.39%
Rich loading	0.4800	0.4900	-	0.4880
Ttop [˚C]	45.40	47.40	47.83	47.69
Tmax [˚C]	51.20	51.20	52.03	51.79
Tbtm [˚C]	27.20	27.50	27.33	27.29

Figure 4.13 presents the temperature profiles of performance data and simulated data for scenario H14 with E_M = Zhu, Table 4.13 provides the key results from the simulation compared with performance data and results from Sætre and Røsvik.

Figure 4.14 presents the temperature profiles of performance data and simulated data, simulated with Aspen Plus rate-based model for scenario H14, Table 4.14 provides the key results from the simulation compared with performance data and results from Sætre and Røsvik.

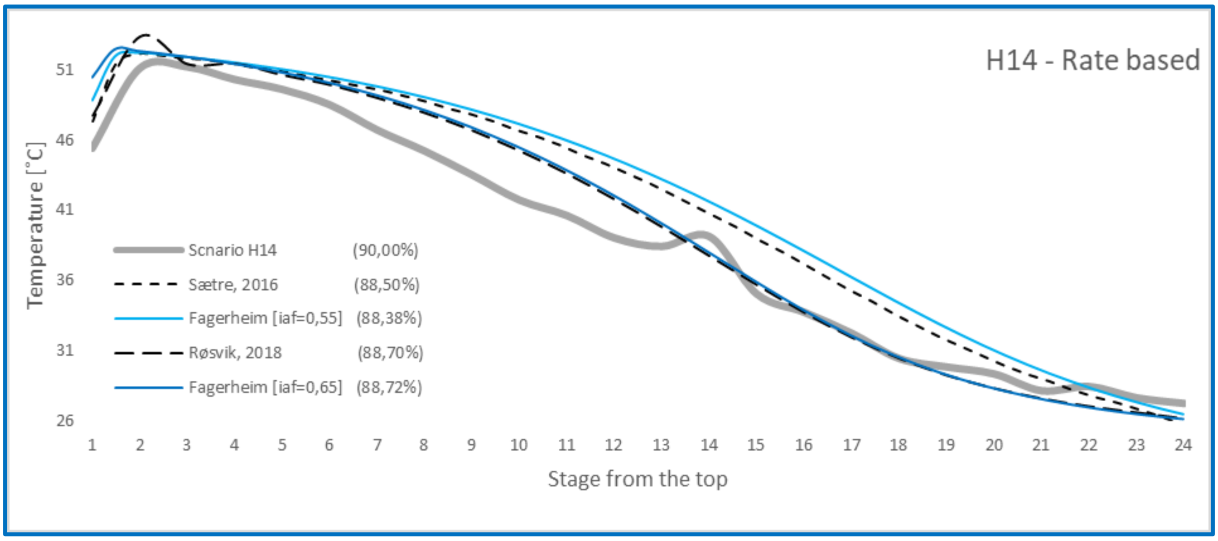


Figure 4.14: Verification of Scenario H14 rate-based model (Plus)

Table 4.14: Key results from simulation of scenario H14 rate-based model (Plus)

	TCM data	Sætre (2016)	Røsvik (2018)	Fagerheim (2019)	
				IAF=0.55	IAF=0.65
Removal grade	90.00%	88.50%	88.70%	88.38%	88.72%
Rich loading	0.4800	0.4880	-	0.4881	0.4891
Ttop [˚C]	45.40	48.10	47.73	48.82	50.46
Tmax [˚C]	51.20	52.10	51.45	52.21	52.45
Tbtm [˚C]	27.20	26.10	26.07	26.43	26.09

4.2.2 Verification of scenario 2B5 in Aspen Plus

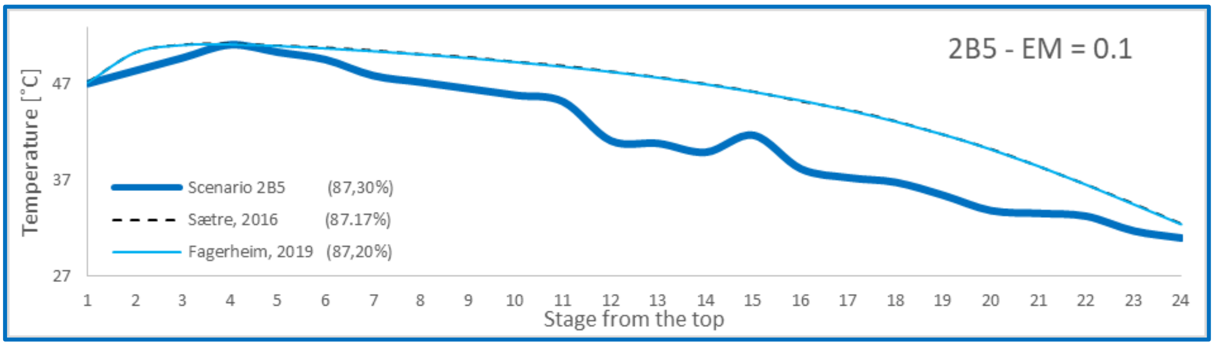


Figure 4.15: Verification of Scenario 2B5 with E_M = 0.1 (Plus)

Table 4.15: Key results from simulation of scenario 2B5 with E_M = 0.1 (Plus)

	TCM data	Sætre (2016)	Fagerheim (2019)
Removal grade	87.30%	87.20%	87.20%
Rich loading	0.5000	0.4900	0,4887
Ttop [˚C]	47.09	47.20	47.19
Tmax [˚C]	51.47	51.20	51.17
Tbtm [˚C]	30.99	32.40	32.41

Figure 4.15 presents the temperature profiles of performance data and simulated data for scenario 2B5 with E_M = 0.1, Table 4.15 provides the key results from the simulation compared with performance data and results from Sætre (2016) [28].

Figure 4.16 and table 4.16 presents the results from the simulation, compared with performance data and results from Sætre, for scenario 2B5 with E_M=Zhu.

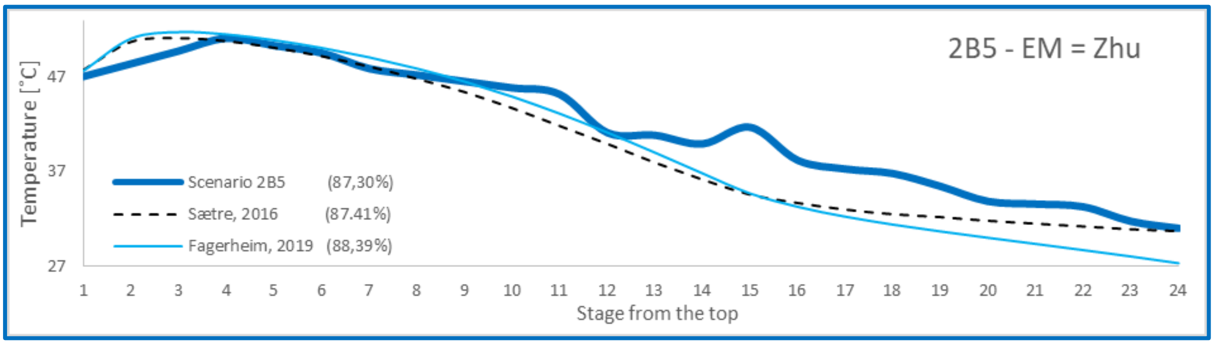


Figure 4.16: Verification of Scenario 2B5 with E_M = Zhu (Plus)

Table 4.16: Key results from simulation of scenario 2B5 with E_M = Zhu (Plus)

	TCM data	**Sætre (2016)**	**Fagerheim (2019)**
Removal grade	87.30%	87.40%	88.39%
Rich loading	0.5000	0.4900	0.4880
Ttop [˚C]	47.09	47.80	47.69
Tmax [˚C]	51.47	51.20	51.78
Tbtm [˚C]	30.99	30.70	27.28

Figure 4.17 presents the temperature profiles of performance data and simulated data, simulated with Aspen Plus rate-based model for scenario 2B5. Table 4.17 provides the key results from the simulation compared with performance data and results from Sætre.

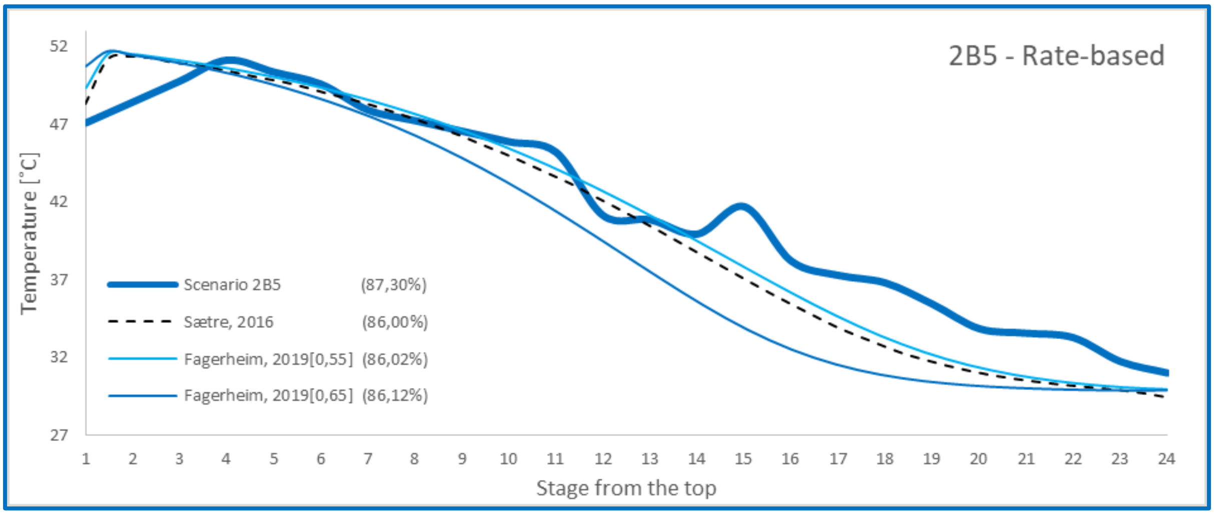


Figure 4.17: Verification of Scenario 2B5 rate-based model (Plus)

Table 4.17: Key results from simulation of scenario 2B5 rate-based model (Plus)

	TCM data	**Sætre (2016)**	**Fagerheim (2019)**	
			IAF=0.55	**IAF=0.65**
Removal grade	87.30%	86.00%	86.02%	86.12%
Rich loading	0.5000	0.4900	0.4854	0.4856
Ttop [˚C]	47.09	48.30	49.35	50.75
Tmax [˚C]	51.47	51.50	51.54	51.71
Tbtm [˚C]	30.99	29.50	29.94	29.87

4.2.3 Verification of scenario 6w in Aspen Plus

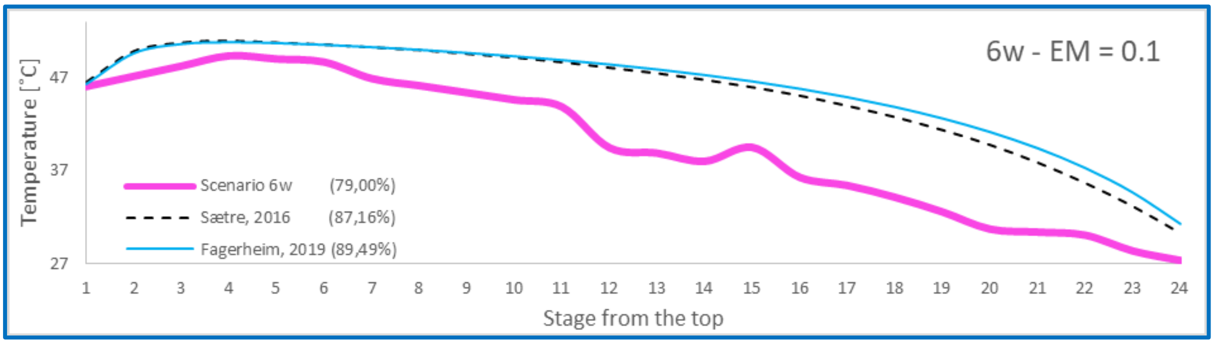


Figure 4.18: Verification of Scenario 6w with E_M = 0.1 (Plus)

Table 4.18: Key results from simulation of scenario 6w with E_M = 0.1 (Plus)

	TCM data	**Sætre (2016)**	**Fagerheim (2019)**
Removal grade	79.00%	87.20%	89.49%
Rich loading	0.4600	0.4910	0.4707
Ttop [˚C]	46.10	46.50	46.31
Tmax [˚C]	49.35	50.90	50.80
Tbtm [˚C]	27.33	30.20	31.26

Figure 4.18 and table 4.18 presents the results from the simulation, compared with performance data and results from Sætre, for scenario 6w with E_M=0.1.

Figure 4.19 and table 4.19 presents the results from the simulation, compared with performance data and results from Sætre, for scenario 6w with E_M=Zhu.

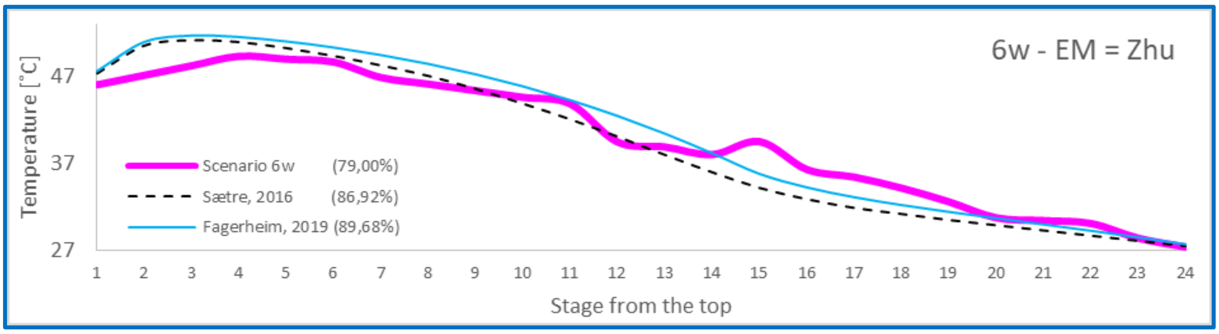


Figure 4.19: Verification of Scenario 6w with E_M = Zhu (Plus)

Table 4.19: Key results from simulation of scenario 6w with E_M = Zhu (Plus)

	TCM data	**Sætre (2016)**	**Fagerheim (2019)**
Removal grade	79.00%	86.90%	89.68%
Rich loading	0.4600	0.4900	0.4702
Ttop [˚C]	46.10	47.40	47.62
Tmax [˚C]	49.35	51.20	51.73
Tbtm [˚C]	27.33	27.50	27.64

Figure 4.20 and table 4.20 presents the results from the simulation, compared with performance data and results from Sætre, for scenario 6w with rate-based model.

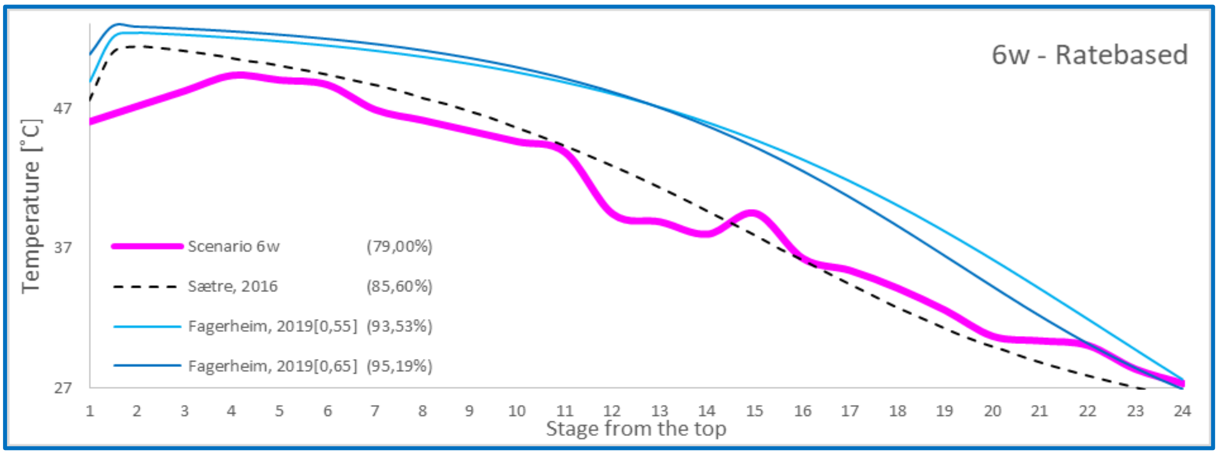


Figure 4.20: Verification of Scenario 6w rate-based model (Plus)

Table 4.20: Key results from simulation of scenario 6w rate-based model (Plus)

	TCM data	Sætre (2016)	Fagerheim (2019)	
			IAF=0.55	**IAF=0.65**
Removal grade	79.00%	86.10%	93.53%	95.19%
Rich loading	0.4600	0.4880	0.4819	0.4865
Ttop [˚C]	46.10	47.57	48.92	50.86
Tmax [˚C]	49.35	51.33	52.38	52.86
Tbtm [˚C]	27.33	26.17	27.63	26.94

4.2.4 Verification of scenario Goal1 in Aspen Plus

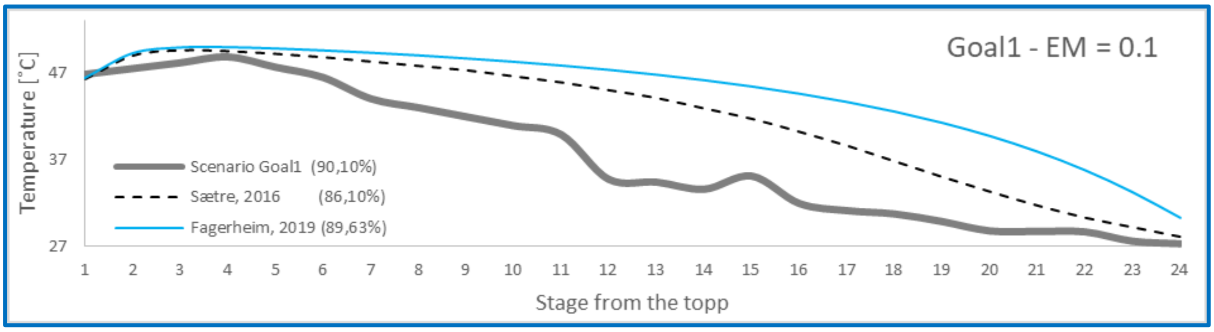


Figure 4.21: Verification of Scenario Goal1 with E_M = 0.1 (Plus)

Table 4.21: Key results from simulation of scenario Goal1 with E_M = 0.1 (Plus)

	TCM data	Sætre (2016)	Fagerheim (2019)
Removal grade	90.10%	82.70%	89.63%
Rich loading	0.5000	0.5000	0.4854
Ttop [˚C]	46.81	46.30	46.39
Tmax [˚C]	48.81	49.60	49.93
Tbtm [˚C]	27.31	28.10	30.29

Figure 4.21 and table 4.21 presents the results from the simulation, compared with performance data and results from Sætre, for scenario Goal1 with E_M=0.1.

Figure 4.22 and table 4.22 presents the results from the simulation, compared with performance data and results from Sætre, for scenario Goal1 with E_M=Zhu.

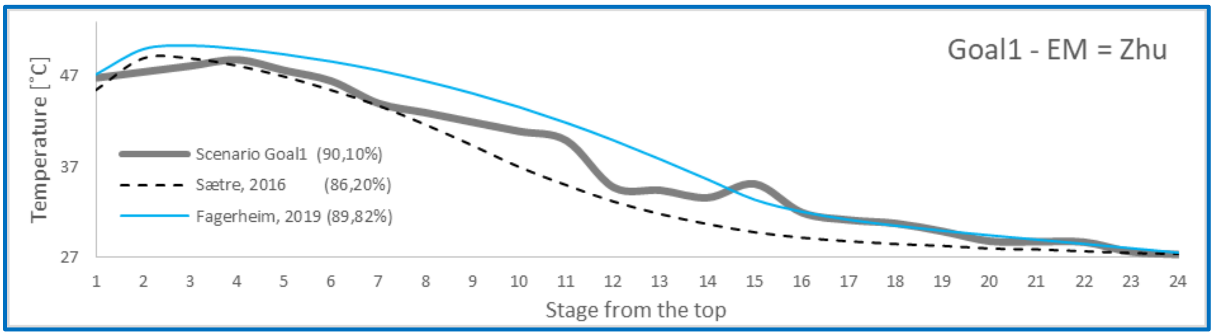


Figure 4.22: Verification of Scenario Goal1 with E_M = Zhu (Plus)

Table 4.22: Key results from simulation of scenario Goal1 with E_M = Zhu (Plus)

	TCM data	Sætre (2016)	Fagerheim (2019)
Removal grade	90.10%	82.70%	89.82%
Rich loading	0.5000	0.5000	0.4860
Ttop [˚C]	46.81	46.50	47.22
Tmax [˚C]	48.81	49.00	50.37
Tbtm [˚C]	27.31	27.40	27.52

Figure 4.23 and table 4.23 presents the results from the simulation, compared with performance data and results from Sætre, for scenario Goal1 with rate-based model.

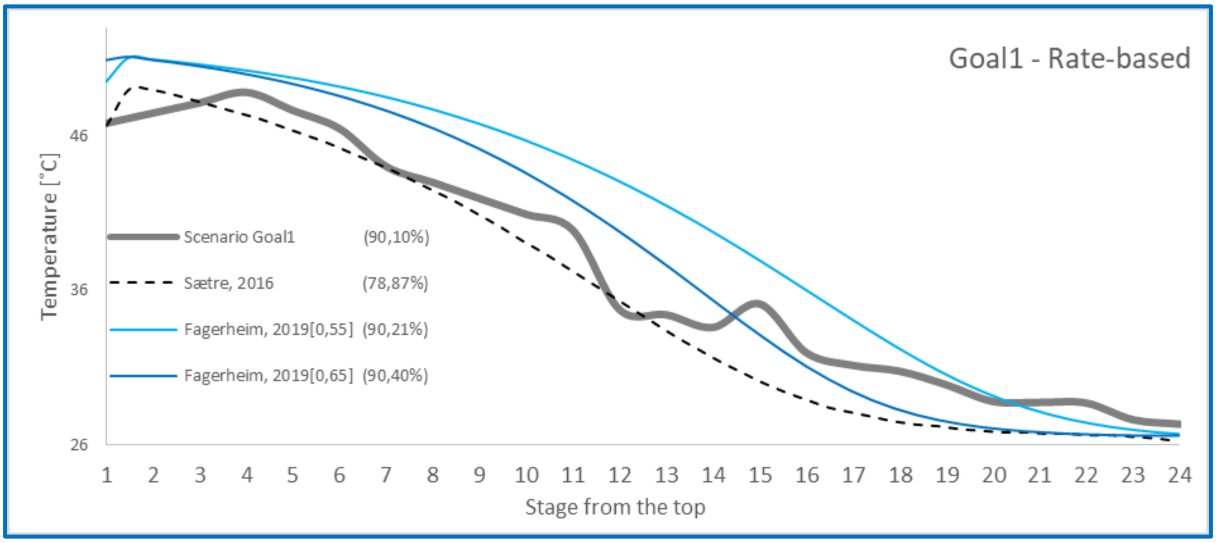


Figure 4.23: Verification of Scenario Goal1 rate-based model (Plus)

Table 4.23: Key results from simulation of scenario Goal1 rate-based model (Plus)

	TCM data	Sætre (2016)	Fagerheim (2019)	
			IAF=0.55	**IAF=0.65**
Removal grade	90.10%	78.90%	90.21%	90.40%
Rich loading	0.5000	0.4900	0.4877	0.4880
Ttop [˚C]	46.81	46.70	49.51	50.90
Tmax [˚C]	48.81	49.00	51.05	51.11
Tbtm [˚C]	27.31	26.20	26.68	26.57

4.2.5 Verification of scenario F17 in Aspen Plus

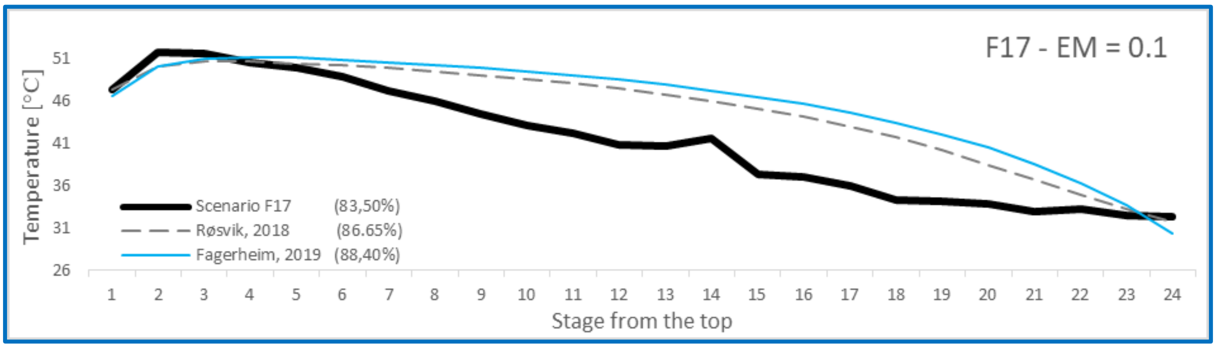


Figure 4.24: Verification of Scenario F17 with E_M = 0.1 (Plus)

Table 4.24: Key results from simulation of scenario F17 with E_M = 0.1 (Plus)

	TCM data	**Røsvik (2018)**	**Fagerheim (2019)**
Removal grade	83.50%	86.65%	88.40%
Rich loading	0.4800	-	0.4880
Ttop [˚C]	47.40	47.34	46.59
Tmax [˚C]	51.70	50.69	51.19
Tbtm [˚C]	32.40	31.74	30.43

Figure 4.24 and table 4.24 presents the results from the simulation, compared with performance data and results from Røsvik (2018) [33], for scenario F17 with E_M=0.1.

Figure 4.25 and table 4.25 presents the results from the simulation, compared with performance data and results from Røsvik, for scenario F17 with E_M=Zhu.

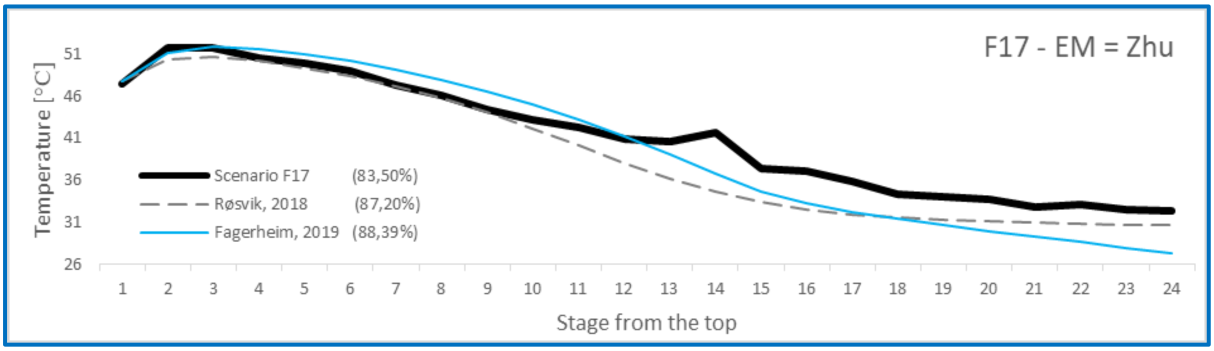


Figure 4.25: Verification of Scenario F17 with E_M = Zhu (Plus)

Table 4.25: Key results from simulation of scenario F17 with E_M = Zhu (Plus)

	TCM data	**Røsvik (2018)**	**Fagerheim (2019)**
Removal grade	83.50%	87.20%	88.39%
Rich loading	0.4800	-	0.4880
Ttop [˚C]	47.40	47.72	47.69
Tmax [˚C]	51.70	50.55	51.79
Tbtm [˚C]	32.40	30.63	27.28

Figure 4.26 and table 4.26 presents the results from the simulation, compared with performance data and results from Røsvik, for scenario F17 with E_M=Lin, which was presented as the best result for scenario F17 in his thesis.

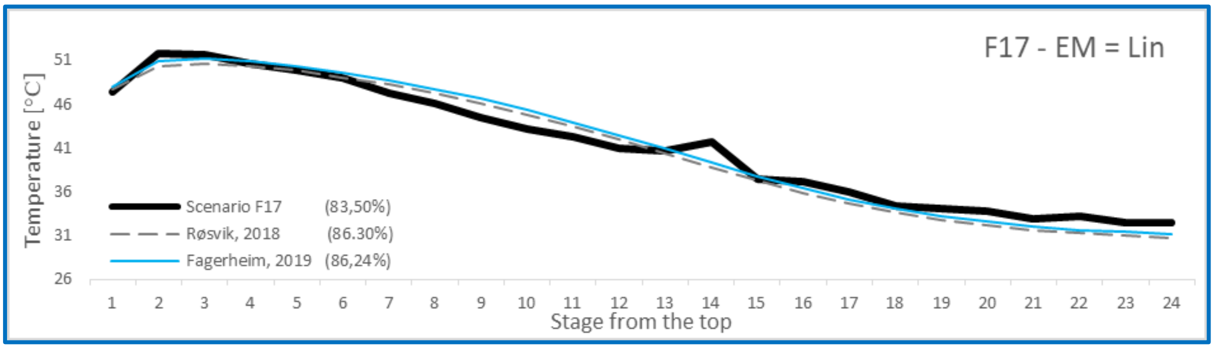


Figure 4.26: Verification of Scenario F17 with E_M = Lin (Plus)

Table 4.26: Key results from simulation of scenario F17 with E_M = Lin (Plus)

	TCM data	Røsvik (2018)	Fagerheim (2019)
Removal grade	83.50%	86.30%	86.24%
Rich loading	0.4800	-	0.4929
Ttop [˚C]	47.40	47.58	47.97
Tmax [˚C]	51.70	50.63	51.19
Tbtm [˚C]	32.40	30.71	31.11

Figure 4.27 presents the temperature profiles of performance data and simulated data, simulated with Aspen Plus rate-based model for scenario F17, Table 4.27 provides the key results from the simulation compared with performance data and results from Røsvik.

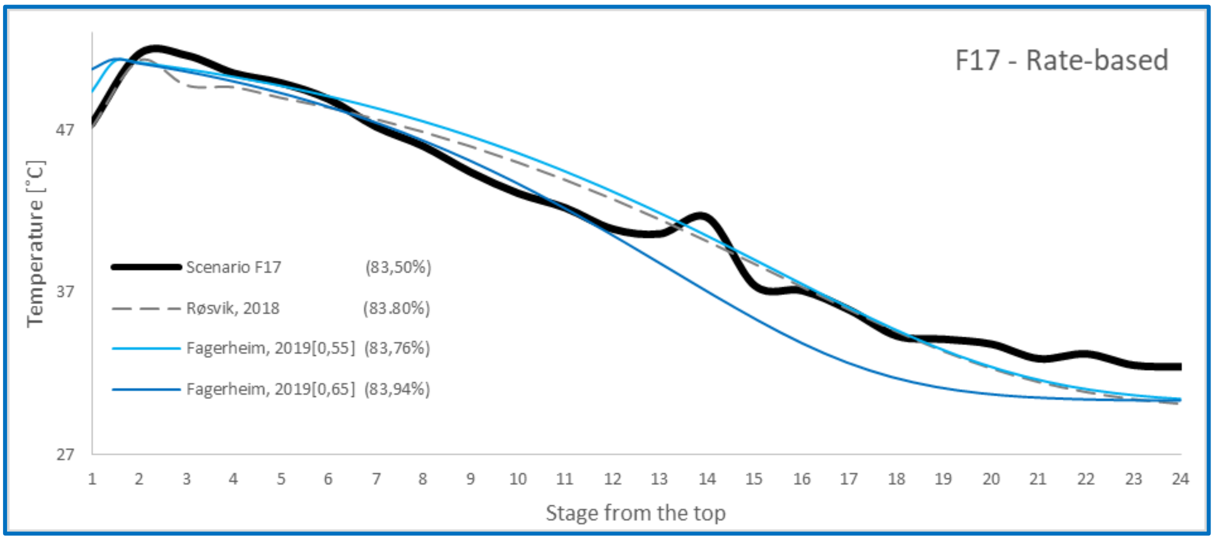


Figure 4.27: Verification of Scenario F17 rate-based model (Plus)

Table 4.27: Key results from simulation of scenario F17 rate-based model (Plus)

	TCM data	Røsvik (2018)	Fagerheim (2019)	
			IAF=0.55	**IAF=0.65**
Removal grade	83.50%	83.80%	83.76%	83.94%
Rich loading	0.4800	-	0.4845	0.4852
Ttop [˚C]	47.40	47.13	49.38	50.74
Tmax [˚C]	51.70	51.27	51.23	51.37
Tbtm [˚C]	32.40	30.08	30.42	30.32

4.3 Simulation in Aspen HYSYS with estimated E_M

4.3.1 Simulation of H14 with estimated E_M

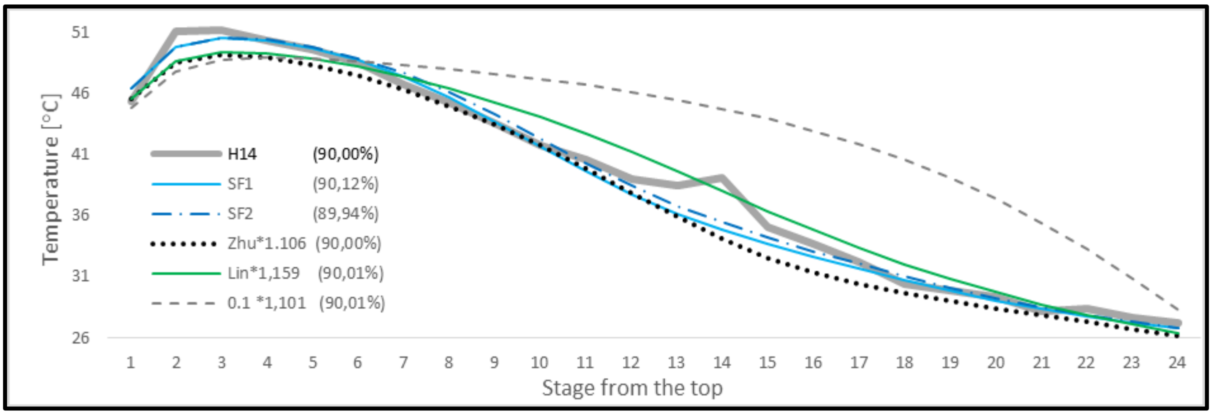


Figure 4.28: Simulated results for scenario H14 with estimated E_M (HYSYS)

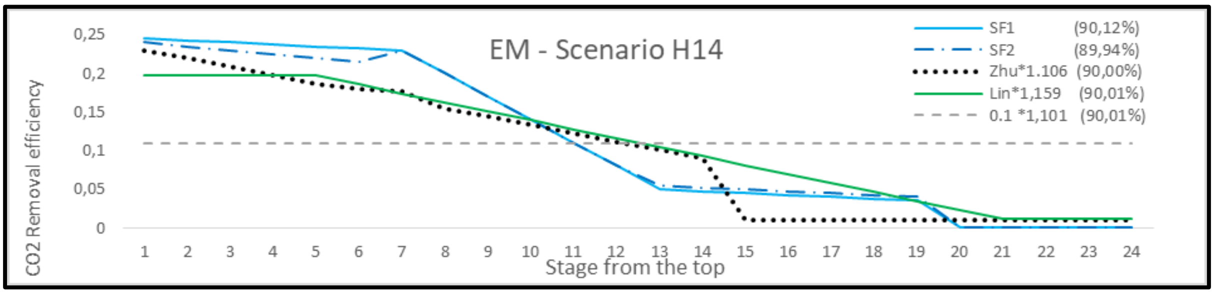


Figure 4.29: Estimated E_M sets for scenario H14 (HYSYS)

Table 4.28: Key results from simulation of scenario H14 with estimated E_M (HYSYS)

E_M	**TCM data**	**SF1**	**SF2**	**Zhu*1.106**	**Lin*1.159**	**0.1*1.101**
Removal grade	90.00%	90.12%	89.94%	90.00%	90.01%	90.01%
Rich loading	0.4800	0.4936	0.4931	0.4932	0.4933	0.4932
Ttop [˚C]	45.4	46.4	46.4	45.6	45.5	44.8
Tmax [˚C]	51.2	50.6	50.6	49.2	49.4	48.9
Tbtm [˚C]	27.2	26.7	26.8	26.1	26.3	28.3

Figure 4.28 illustrates the results from the simulation with the new estimated E_M-profiles compared with some of the E_M-profiles used in earlier theses, scaled to give requested removal grade.

Figure 4.29 shows the slope of the E_M-profiles, which illustrates that E_M=SF1, have highest efficiency at the top of the packing section, with a soft decreasing slope (-0.002) from stage 1-7. Continued with a steeper decreasing slope (-0.025) from stage 7-13, again followed by a soft decreasing slope (0.002) from stage 13-19 before the efficiency remains constant at 0.0001 for step stages 20-24. E_M=SF2, have a curve similar to E_M=SF1, except from stage 1-6, which have a decreasing slope twice as steep (-0.004), followed by an increase (+0.015) from 6-7. From stage 7-24 the curve follows E_M=SF1, except from stage 13-19, where the slope is the same as for SF1, but the efficiencies are lower.

4.3.2 Simulation of 2B5 with estimated E_M

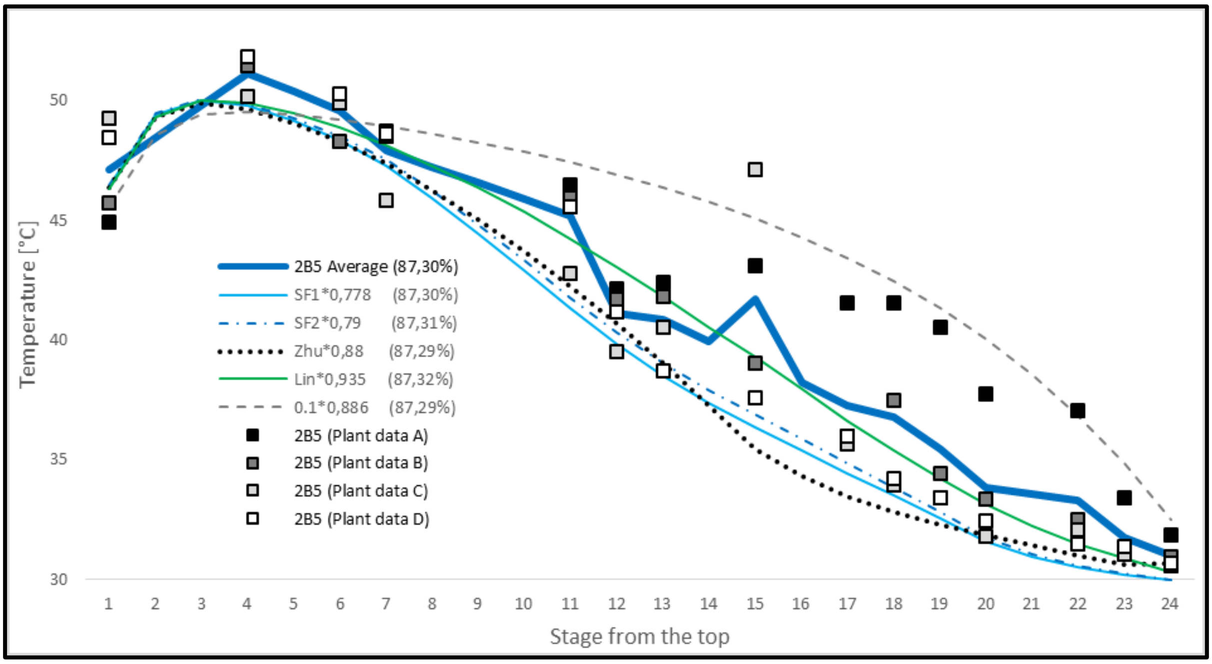


Figure 4.30: Simulated results for scenario 2B5 with downscaled estimated E_M for H14 (HYSYS)

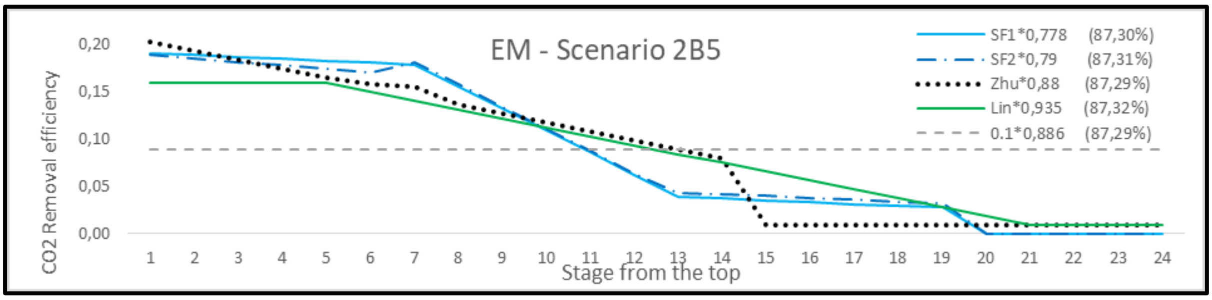


Figure 4.31: Estimated E_M sets for scenario 2B5 (HYSYS)

Table 4.29: Key results from simulation of scenario 2B5 with estimated E_M (HYSYS)

E_M	TCM data	SF1*0.778	SF2*0.79	Zhu*0.88	Lin*0.935	0.1*0.886
Removal grade	87.30%	87.30%	87.31%	87.29%	87.32%	87.29%
Rich loading	0.5000	0.4635	0.4635	0.4634	0.4635	0.4634
Ttop [˚C]	47.09	46.44	46.45	46.36	46.31	45.55
Tmax [˚C]	51.47	50.02	50.05	49.88	50.01	49.54
Tbtm [˚C]	30.99	29.96	29.97	30.67	30.32	32.51

Figure 4.30 present the results from simulation of scenario 2B5, with all the different E_M-profiles scaled down to produce simulations with removal grade close to 87.3%. Scenario 2B5 have four sets of measurement, the individual measurements are given as points in the graph while the thick blue line illustrates the average values of these measurements.

Figure 4.31 illustrates the slopes of the scaled E_M-profiles, which is equal to Scenario H14, but the values are lower.

4.3.3 Simulation of 6w with estimated E_M

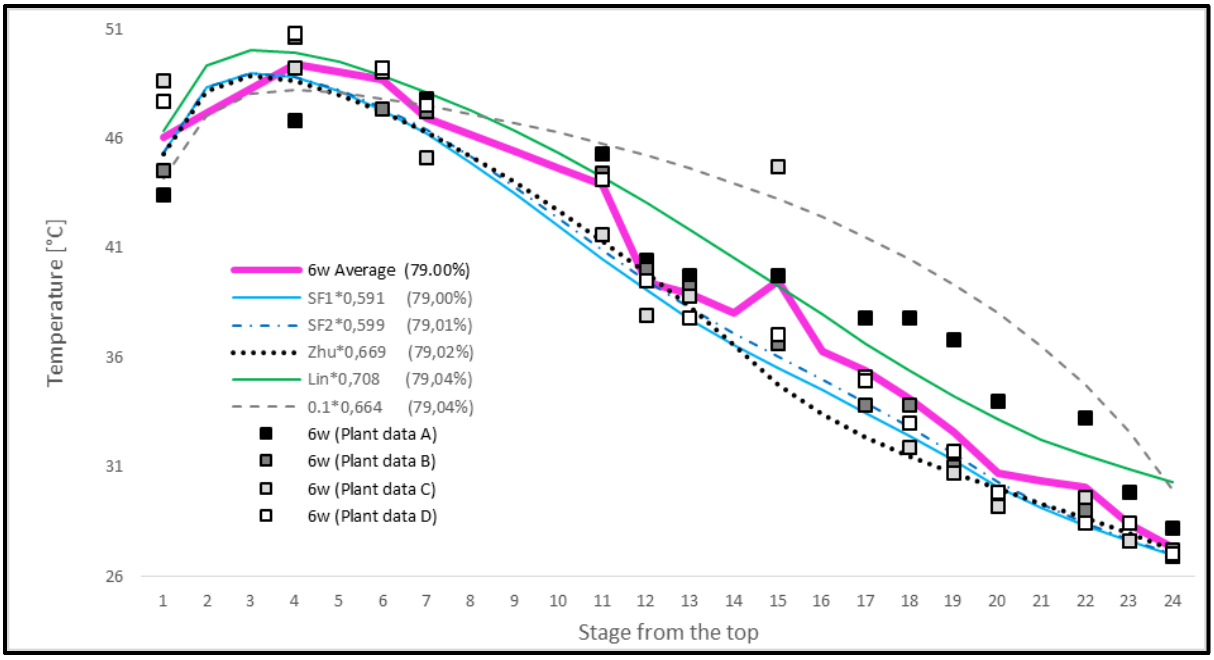


Figure 4.32: Simulated results for scenario 6w with downscaled estimated E_M for H14 (HYSYS)

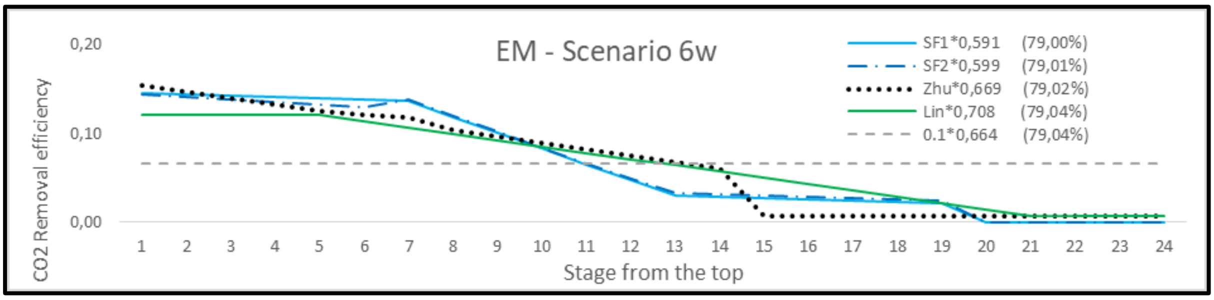


Figure 4.33: Estimated E_M sets for scenario 6w (HYSYS)

Table 4.30: Key results from simulation of scenario 6w with estimated E_M (HYSYS)

E_M	**TCM data**	**SF1*0.591**	**SF2*0.599**	**Zhu*0.669**	**Lin*0.708**	**0.1*0.664**
Removal grade	79.00%	79.00%	79.01%	79.02%	79.04%	79.04%
Rich loading	0.4600	0.4426	0.4426	0.4426	0.4427	0.4426
Ttop [˚C]	46.10	45.34	45.33	45.26	46.31	44.16
Tmax [˚C]	49.35	48.99	48.99	48.82	50.01	48.19
Tbtm [˚C]	27.33	26.97	27.01	27.21	30.32	29.92

Figure 4.32 presents the results for scenario 6w. Just like for Scenario 2B5, the E_M-profiles used for scenario H14 have been scaled down to produce simulations with removal grade close to 79.0%. Scenario 6w have four sets of measurement, the individual measurements are given as points in the graph while the thick purple line illustrates the average values of these measurements.

Figure 4.33 illustrates the slopes of the scaled E_M-profiles, which is equal to Scenario H14 and 2B5, but the values are lower.

4.3.4 Simulation of Goal1 with estimated E_M

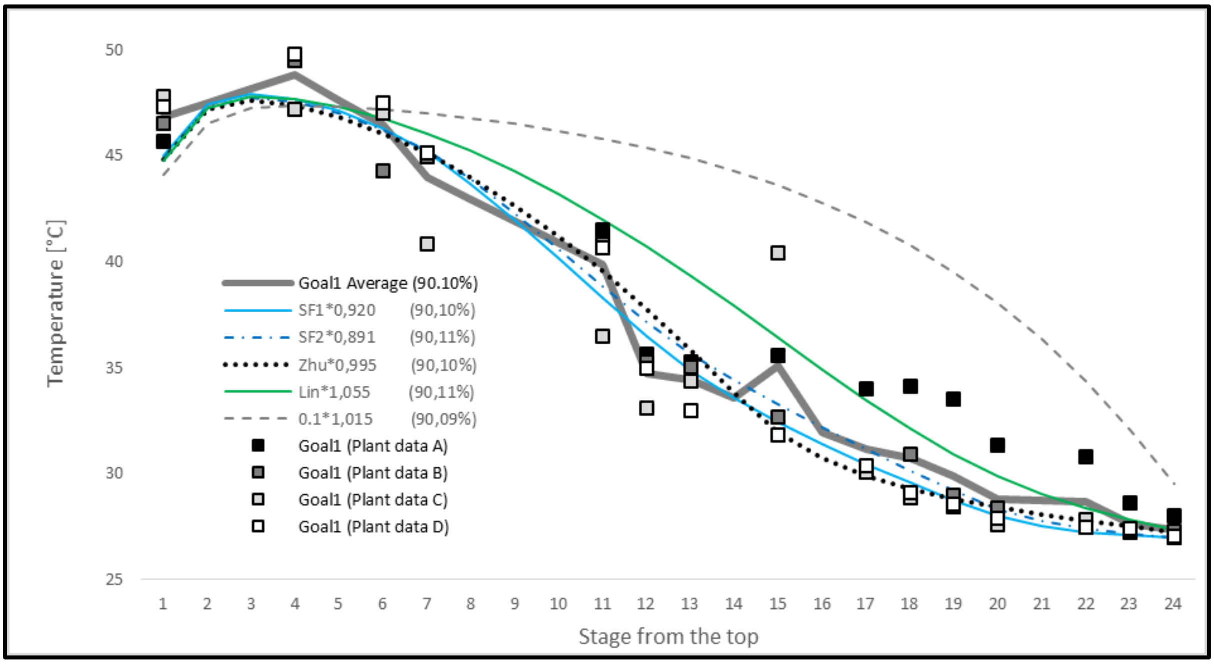


Figure 4.34: Simulated results for scenario Goal1 with downscaled estimated E_M for H14 (HYSYS)

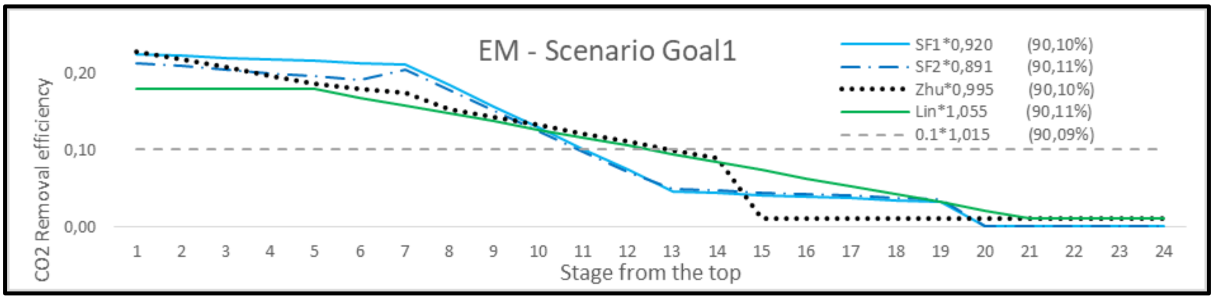


Figure 4.35: Estimated E_M sets for scenario Goal1 (HYSYS)

Table 4.31: Key results from simulation of scenario Goal1 with estimated E_M (HYSYS)

E_M	TCM data	SF1*0.920	SF2*0.891	Zhu*0.995	Lin*1.055	0.1*1.015
Removal grade	90.10%	90.10%	90.11%	90.10%	90.11%	90.09%
Rich loading	0.5000	0.4904	0.4874	0.4873	0.4875	0.4872
Ttop [˚C]	46.81	44.98	44.88	44.82	44.78	44.07
Tmax [˚C]	48.81	47.89	47.75	47.62	47.78	47.36
Tbtm [˚C]	27.31	26.95	26.98	27.20	27.34	29.51

Figure 4.34 presents the result from the simulation of scenario Goal1 with all E_M-profiles scaled to produce simulations with removal grade close to 90.1 %. Just like for Scenario 2B5 and 6w, scenario goal1 have four sets of measurement, the individual measurements are given as points in the graph while the thick gray line illustrates the average values of these measurements.

Figure 4.35 illustrates the slopes of the scaled E_M-profiles, here the values are higher than for scenario 2B5 and 6w, which is natural since the removal grade is higher. But the values are lower than for scenario H14, the assumed reason for this is discussed in chapter 5.

4.3.5 Simulation of F17 with estimated E_M

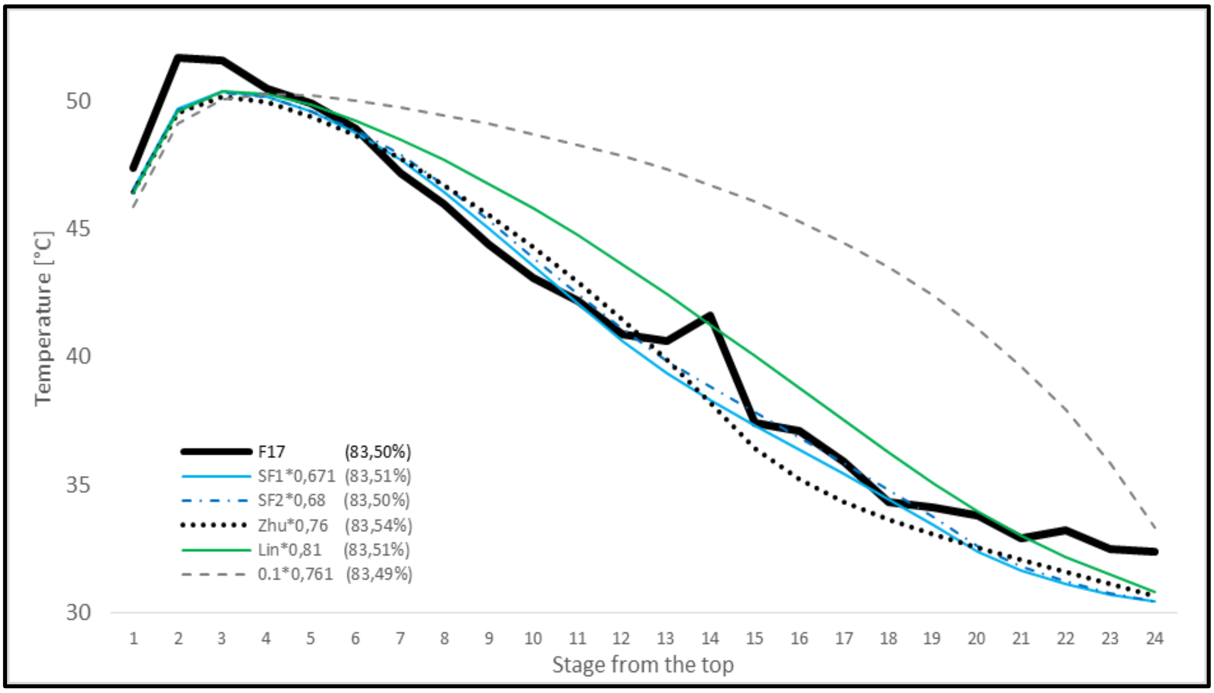


Figure 4.36: Simulated results for scenario F17 with downscaled estimated E_M for H14 (HYSYS)

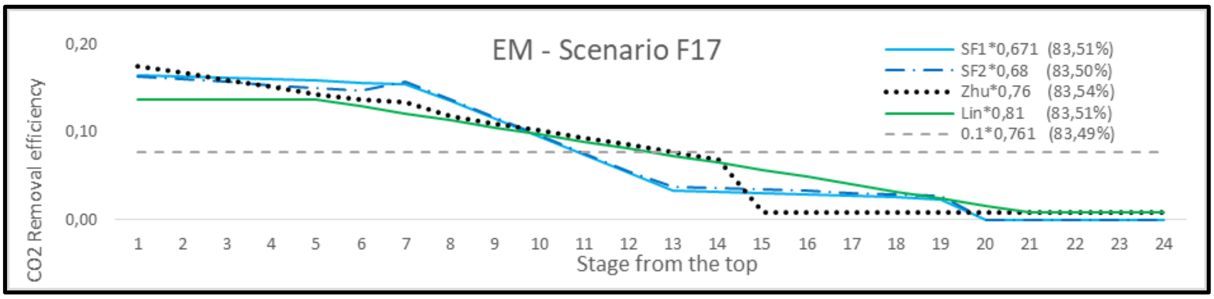


Figure 4.37: Estimated E_M sets for scenario F17 (HYSYS)

Table 4.32: Key results from simulation of scenario F17 with estimated E_M (HYSYS)

E_M	**TCM data**	**SF1*0.671**	**SF2*0.68**	**Zhu*0.76**	**Lin*0.81**	**0.1*0.761**
Removal grade	83.70%	83.51%	83.50%	83.54%	83.51%	83.49%
Rich loading	0.4800	0.4354	0.4353	0.4354	0.4353	0.4353
Ttop [˚C]	47.40	46.56	46.54	45.46	46.41	45.88
Tmax [˚C]	51.70	50.38	50.35	50.20	50.35	50.28
Tbtm [˚C]	32.40	30.42	30.44	30.67	30.82	33.33

Figure 4.36 illustrates the results from the simulations of scenario F17 with all E_M-profiles scaled down to produce simulations with removal grade close to 83.5 %.

Figure 4.37 shows the slopes of the E_M-profiles, here the values are higher than for scenario 6w and lower than for scenario 2B5, which is natural since the removal grade is in between these two scenarios.

4.4 Simulation in Aspen Plus with estimated E_M and IAF

4.4.1 Simulation of H14 with estimated E_M and IAF

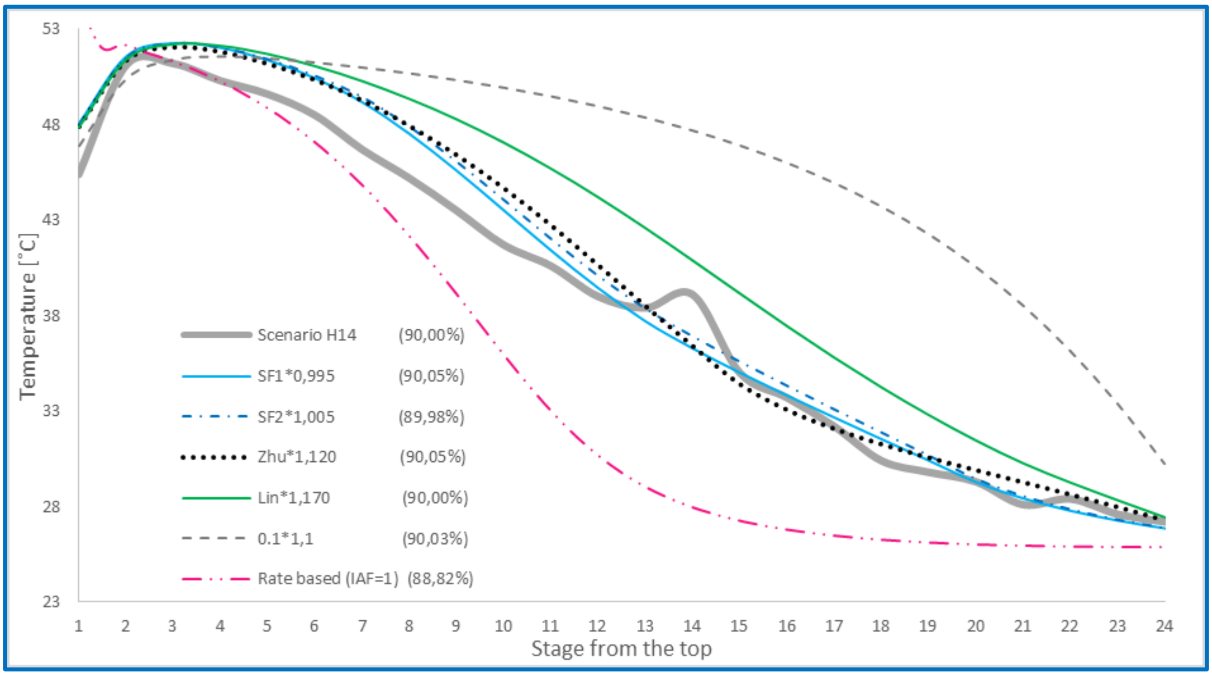


Figure 4.38: Simulated results for scenario H14 with estimated E_M and IAF (Plus)

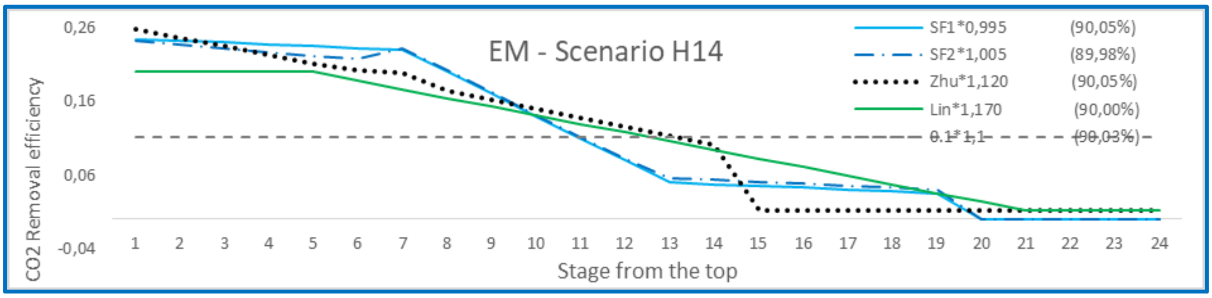


Figure 4.39: Estimated E_M sets for scenario H14 (Plus)

Table 4.33: Key results from simulation of scenario H14 with estimated E_M and IAF (Plus)

E_M	**TCM data**	**SF1*0,995**	**SF2*1,005**	**Zhu*1,12**	**Lin*1,17**	**0.1*1,1**	**RB (IAF=1)**
Removal grade	90.00%	90.05%	89.98%	90.05%	90.00%	90.03%	88.82%
Rich loading	0.4800	0.4929	0.4929	0.4929	0.4928	0.4928	0.4894
Ttop [˚C]	45.40	48.05	48.03	47.91	47.85	46.89	54.40
Tmax [˚C]	51.20	52.27	52.26	52.06	52.21	51.58	54.40
Tbtm [˚C]	27.20	26.86	26.88	27.27	27.44	30.21	25.91

Figure 4.38 illustrates the results from the simulations of scenario H14 with all E_M-profiles scaled to produce simulations in Aspen Plus equilibrium-based model with removal grade close to 90%. The pink line is simulated in Aspen Plus rate-based model with IAF adjusted to get the removal grade as near 90% as possible.

Figure 4.39 shows the slopes of the Murphree efficiency profiles.

4.4.2 Simulation of 2B5 with estimated E_M and IAF

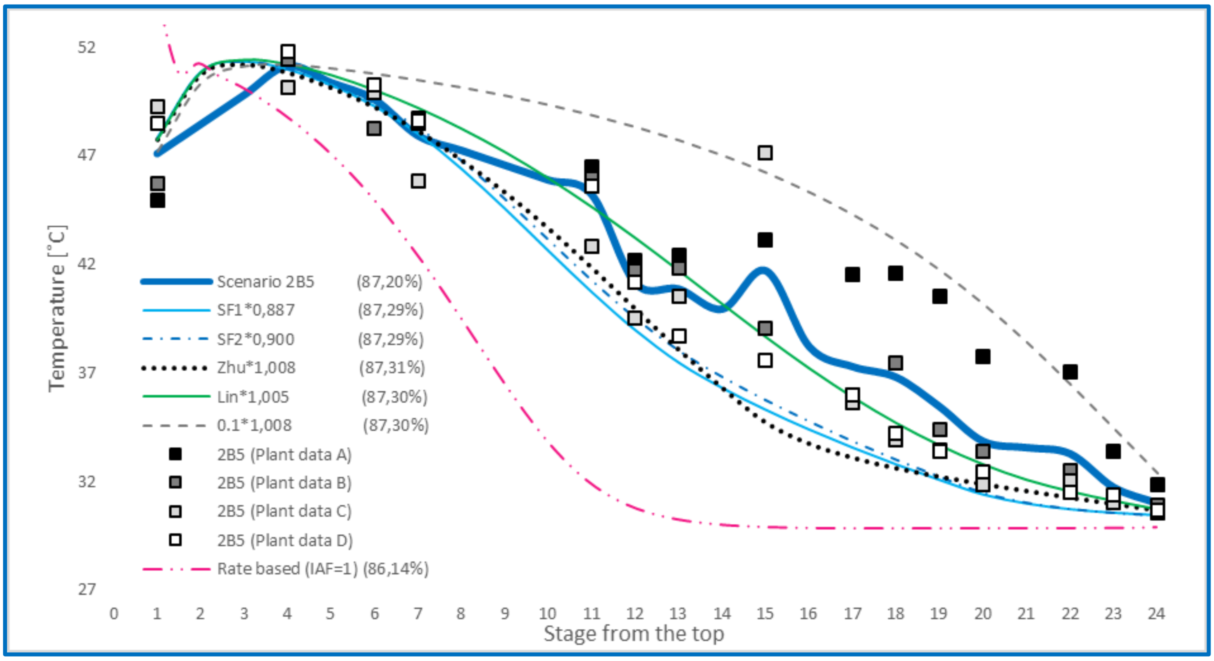


Figure 4.40: Simulated results for scenario 2B5 with estimated E_M and IAF (Plus)

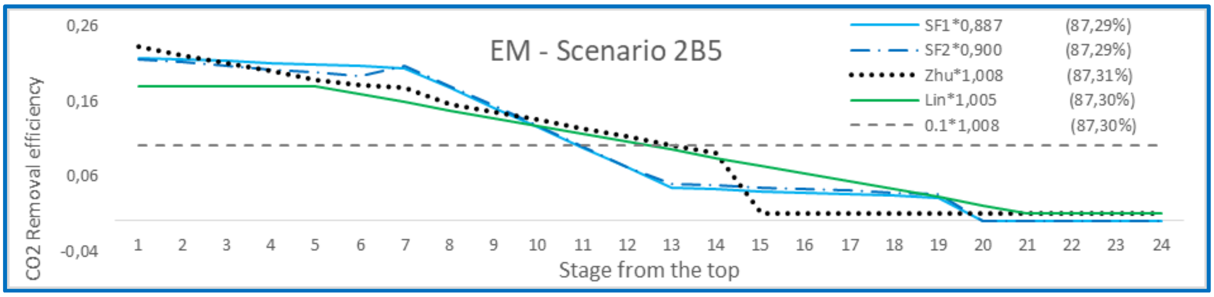


Figure 4.41: Estimated E_M sets for scenario 2B5 (Plus)

Table 4.34: Key results from simulation of scenario 2B5 with estimated E_M and IAF (Plus)

E_M	**TCM data**	**SF1*0.887**	**SF2*0.900**	**Zhu*1.008**	**Lin*1.005**	**0.1*1.008**	**RB(IAF=1)**
Removal grade	87.30%	87.29%	87.29%	87.31%	87.30%	87.30%	86.14%
Rich loading	0.5000	0.4891	0.4891	0.4892	0.4891	0.4891	0.4857
Ttop [˚C]	47.09	47.82	47.81	47.75	47.73	47.21	54.26
Tmax [˚C]	51.47	51.32	51.33	51.19	51.41	51.19	54.26
Tbtm [˚C]	30.99	30.44	30.45	30.66	30.72	32.38	29.87

Figure 4.40 illustrates the results from the simulations of scenario 2B5 with all E_M-profiles scaled to produce simulations in Aspen Plus equilibrium-based model with removal grade close to 87,20%. The pink line is simulated in Aspen Plus rate-based model with IAF adjusted to get the removal grade as near 87.20% as possible.

Figure 4.41 shows the slopes of the Murphree efficiency profiles.

4.4.3 Simulation of 6w with estimated E_M and IAF

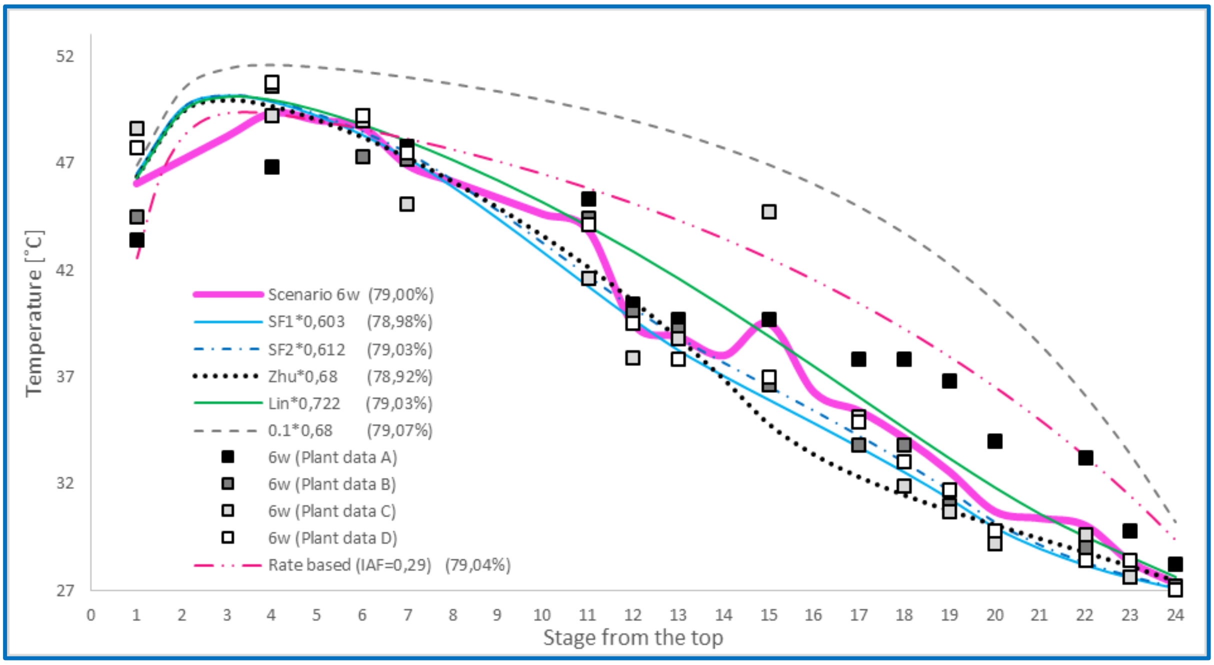


Figure 4.42: Simulated results for scenario 6w with estimated E_M and IAF (Plus)

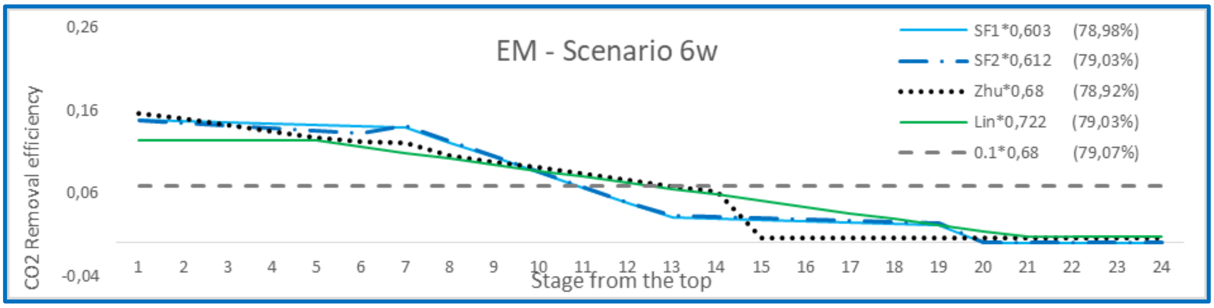


Figure 4.43: Estimated E_M sets for scenario 6w (Plus)

Table 4.35: Key results from simulation of scenario 6w with estimated E_M and IAF (Plus)

E_M	TCM data	SF1*0.603	SF2*0.612	Zhu*0.680	Lin*0.722	0.1*0.680	RB(IAF=0.29)
Removal grade	79.00%	78.98%	79.03%	78.92%	79.03%	79.07%	79.04%
Rich loading	0.4600	0.4418	0.4420	0.4413	0.4419	0.4420	0.4870
Ttop [˚C]	46.10	46.49	46.49	46.37	46.31	45.22	42.55
Tmax [˚C]	49.35	50.16	50.17	49.94	50.10	49.25	49.39
Tbtm [˚C]	27.33	27.10	27.13	27.43	27.63	30.53	29.41

Figure 4.42 illustrates the results from the simulations of scenario 6w with all E_M-profiles scaled to produce simulations in Aspen Plus equilibrium-based model with removal grade close to 79%. The pink line is simulated in Aspen Plus rate-based model with IAF adjusted to get the removal grade as near 79% as possible.

Figure 4.43 shows the slopes of the Murphree efficiency profiles.

4.4.4 Simulation of Goal1 with estimated E_M and IAF

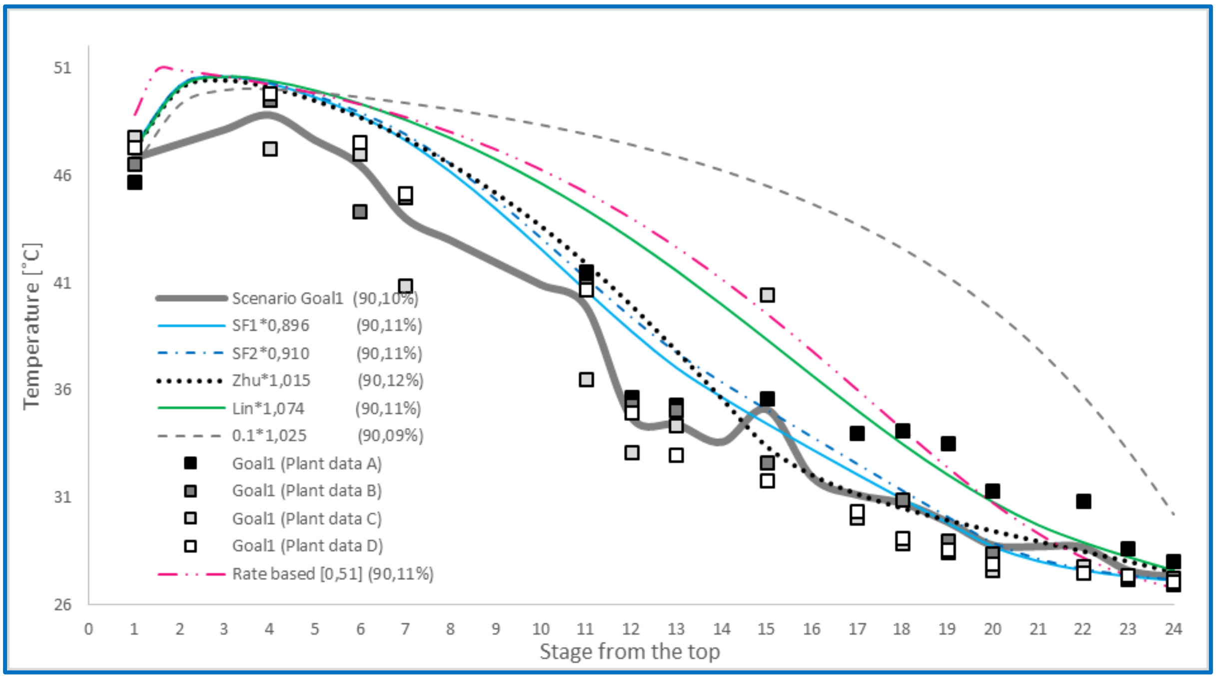


Figure 4.44: Simulated results for scenario Goal1 with estimated E_M and IAF (Plus)

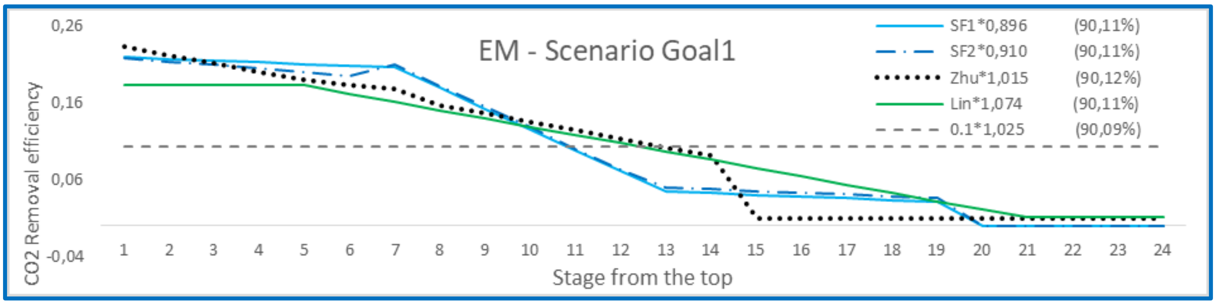


Figure 4.45: Estimated E_M sets for scenario Goal1 (Plus)

Table 4.36: Key results from simulation of scenario Goal1 with estimated E_M and IAF (Plus)

E_M	TCM data	SF1*0.896	SF2*0.910	Zhu*1.015	Lin*1.074	0.1*1.025	RB(IAF=0.51)
Removal grade	90.10%	90.11%	90.11%	90.12%	90.11%	90.09%	90.11%
Rich loading	0.5000	0.4870	0.4870	0.4871	0.4871	0.4869	0.4870
Ttop [˚C]	46.81	47.36	47.36	47.26	47.23	46.47	48.83
Tmax [˚C]	48.81	50.59	50.59	50.43	50.59	50.04	50.91
Tbtm [˚C]	27.31	27.15	27.16	27.52	27.61	30.24	44.73

Figure 4.44 illustrates the results from the simulations of scenario Goal1 with all E_M-profiles scaled to produce simulations in Aspen Plus equilibrium-based model with removal grade close to 90.1%. The pink line is simulated in Aspen Plus rate-based model with IAF adjusted to get the removal grade as near 90.1% as possible.

Figure 4.45 shows the slopes of the Murphree efficiency profiles.

4.4.5 Simulation of F17 with estimated E_M and IAF

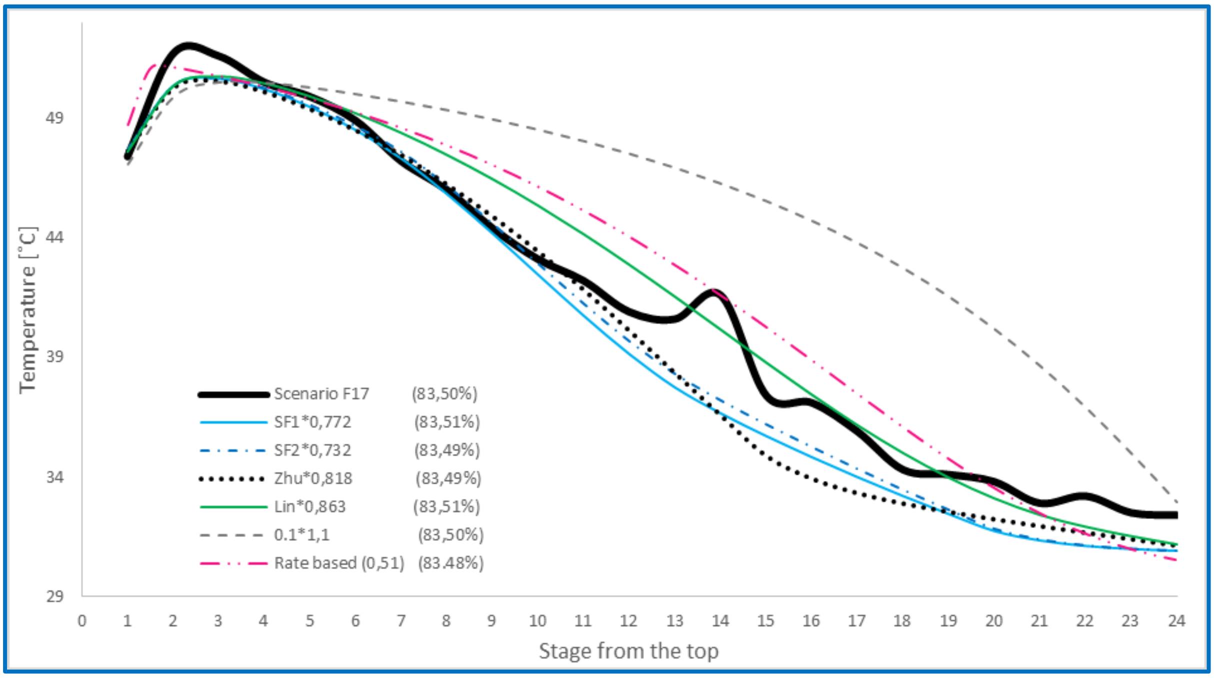


Figure 4.46: Simulated results for scenario F17 with estimated E_M and IAF (Plus)

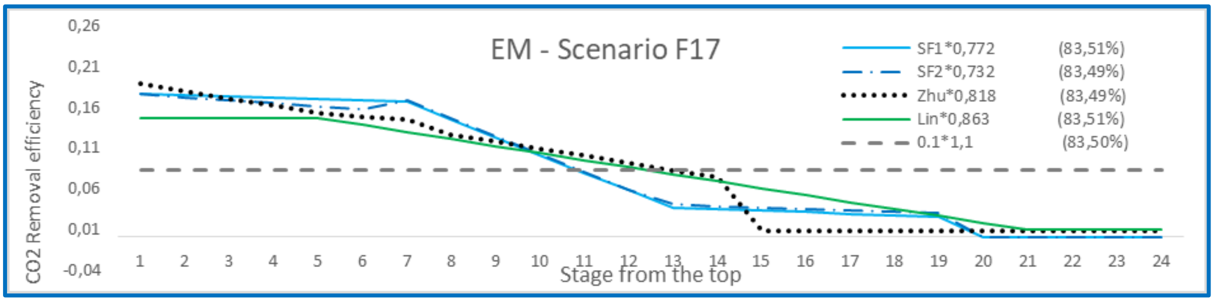


Figure 4.47: Estimated E_M sets for scenario F17 (Plus)

Table 4.37: Key results from simulation of scenario F17 with estimated E_M and IAF (Plus)

E_M	TCM data	SF1*0.772	SF2*0.732	Zhu*0.818	Lin*0.863	0.1*1.1	RB(IAF=0.51)
Removal grade	83.70%	83.51%	83.49%	83.49%	83.51%	83.50%	83.48%
Rich loading	0.4800	0.4837	0.4836	0.4836	0.4837	0.4836	0.4836
Ttop [˚C]	47.40	47.67	47.68	47.61	47.59	47.59	48.72
Tmax [˚C]	51.70	50.64	50.66	50.51	50.74	50.74	51.12
Tbtm [˚C]	32.40	30.91	30.91	31.14	31.18	31.18	44.73

Figure 4.46 illustrates the results from the simulations of scenario F17 with all E_M-profiles scaled to produce simulations in Aspen Plus equilibrium-based model with removal grade close to 83.5%. The pink line is simulated in Aspen Plus rate-based model with IAF adjusted to get the removal grade as near 83.5% as possible.

Figure 4.47 shows the slopes of the Murphree efficiency profiles.

4.5 Comparison of Rate-based and Equilibrium-based model

4.5.1 Comparison of Rate-based and Equilibrium for Scenario H14

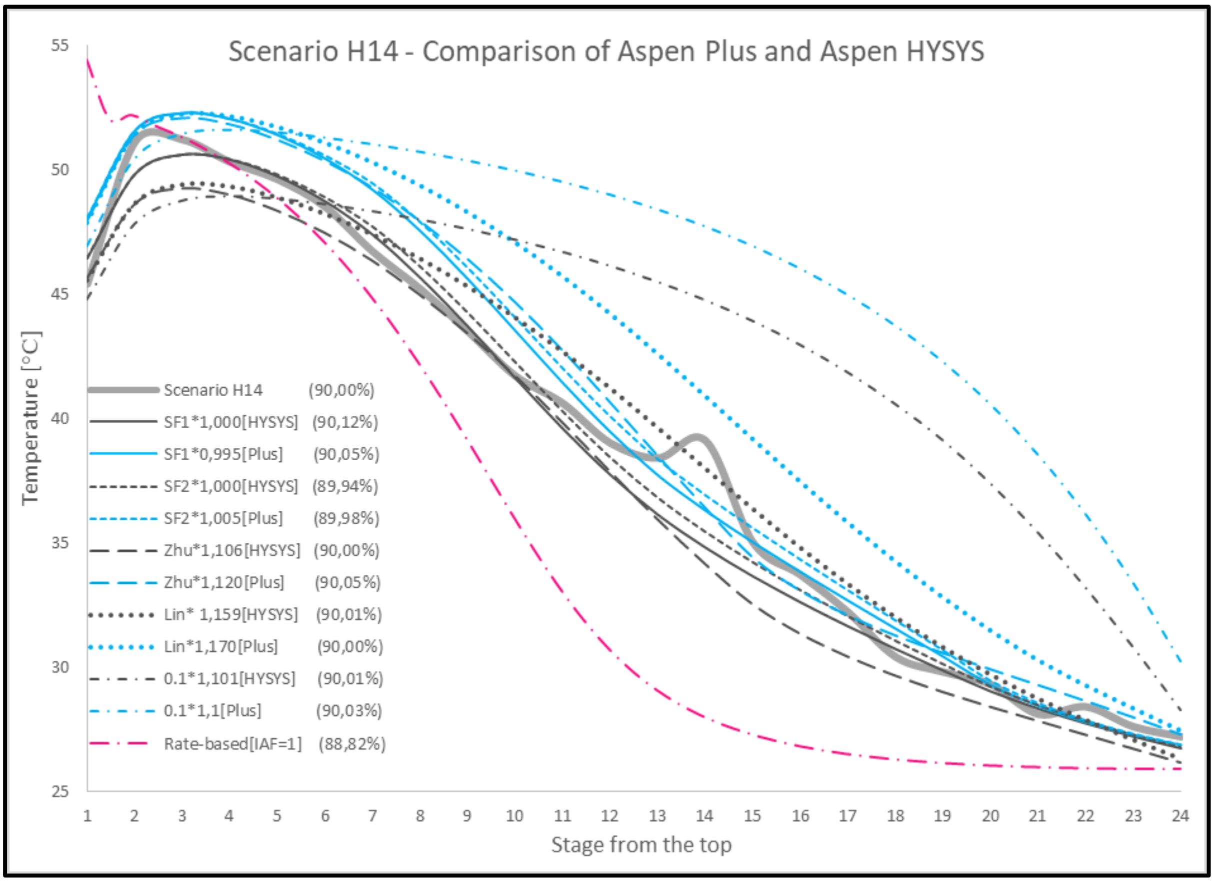


Figure 4.48: Comparison of Rate-based and Equilibrium for Scenario H14

Table 4.38: Key results from comparison of Rate-based and Equilibrium for Scenario H14

Comparison HYSYS and Plus - Scenario H14												
	TCM Data Scenario H14	**SF1**		**SF2**		**Zhu**		**Lin**		**0.1**		**Rate-based**
		HYSYS	**Plus**	**HYSYS**	**Plus**	**HYSYS**	**Plus**	**HYSYS**	**Plus**	**HYSYS**	**Plus**	**Plus**
EM-Factor		1.000	0.995	1.000	1.005	1.106	1.120	1.159	1.170	1.101	1.100	IAF = 1
Removal grade	**90.00%**	90.12	90.05	89.94	89.98	90.00	90.05	90.01	90.00	90.01	90.03	88.82
Rich loading	**0.4800**	0.4936	0.4929	0.4931	0.4929	0.4932	0.4929	0.4933	0.4928	0.4932	0.4928	0.4894
Ttop	**45.40**	46.43	48.05	46.41	48.03	45.59	47.91	45.53	47.85	44.79	46.90	54.40
Tmax	**51.20**	50.59	51.56	50.58	51.54	48.58	52.06	48.60	52.21	48.93	51.58	54.40
Tbtm	**27.20**	26.73	26.86	26.76	26.88	26.14	27.27	26.31	27.44	28.29	30.21	24.73

Figure 4.48 presents the simulated temperature results of scenario H14 from sub-chapter 4.3.1 and 4.4.1. The thick gray line illustrates the performance temperature profile. The thin gray lines are simulated in equilibrium-based model in Aspen HYSYS, thin blue lines are simulated in equilibrium-based model in Aspen Plus and the pink line is simulated in rate-based model in Aspen Plus. Table 4.38 provides the key results from the simulation of scenario H14 in Aspen plus and Aspen HYSYS compared with performance data.

4.5.2 Comparison of Rate-based and Equilibrium-based for Scenario 2B5

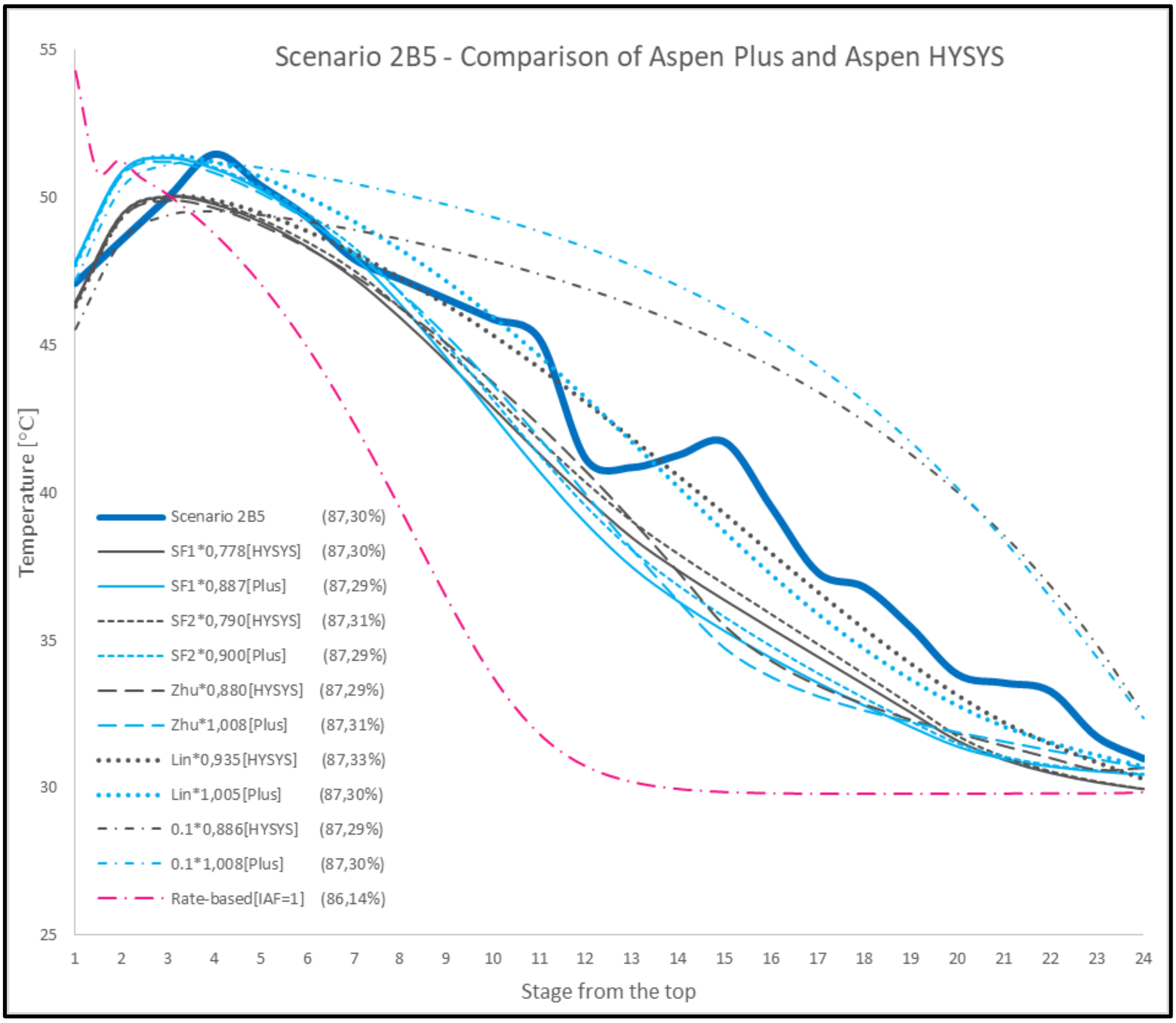


Figure 4.49: Comparison of Rate-based and Equilibrium for Scenario 2B5

Table 4.39: Key results from comparison of Rate-based and Equilibrium for Scenario 2B5

Comparison HYSYS and Plus - Scenario 2B5												
	TCM Data Scenario 2B5	SF1		SF2		Zhu		Lin		0.1		Rate-based
		HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	Plus
EM-Factor		0.778	0.887	0.790	0.900	0.880	1.008	0.935	1.005	0.886	1.008	IAF = 1
Removal grade	**87.30%**	87.30	87.29	87.31	87.29	87.29	87.31	87.32	87.30	87.29	87.30	86.14
Rich loading	**0.5000**	0.4635	0.4891	0.4635	0.4891	0.4534	0.4892	0.4635	0.4891	0.4634	0.4891	0.4857
Ttop	**47.09**	46.44	47.82	46.45	47.81	46.36	47.75	46.31	47.37	45.55	47.21	54.27
Tmax	**51.47**	50.02	51.33	50.05	51.34	49.88	51.20	50.02	51.41	49.41	51.19	51.25
Tbtm	**30.99**	29.96	30.44	29.97	30.45	30.67	30.66	30.32	30.72	32.51	32.38	29.87

Figure 4.49 presents the simulated temperature results of scenario 2B5 from sub-chapter 4.3.2 and 4.4.2.

Table 4.39 provides the key results from the simulation of scenario 2B5 in Aspen plus and Aspen HYSYS compared with performance data.

4.5.3 Comparison of Rate-based and Equilibrium-based for Scenario 6w

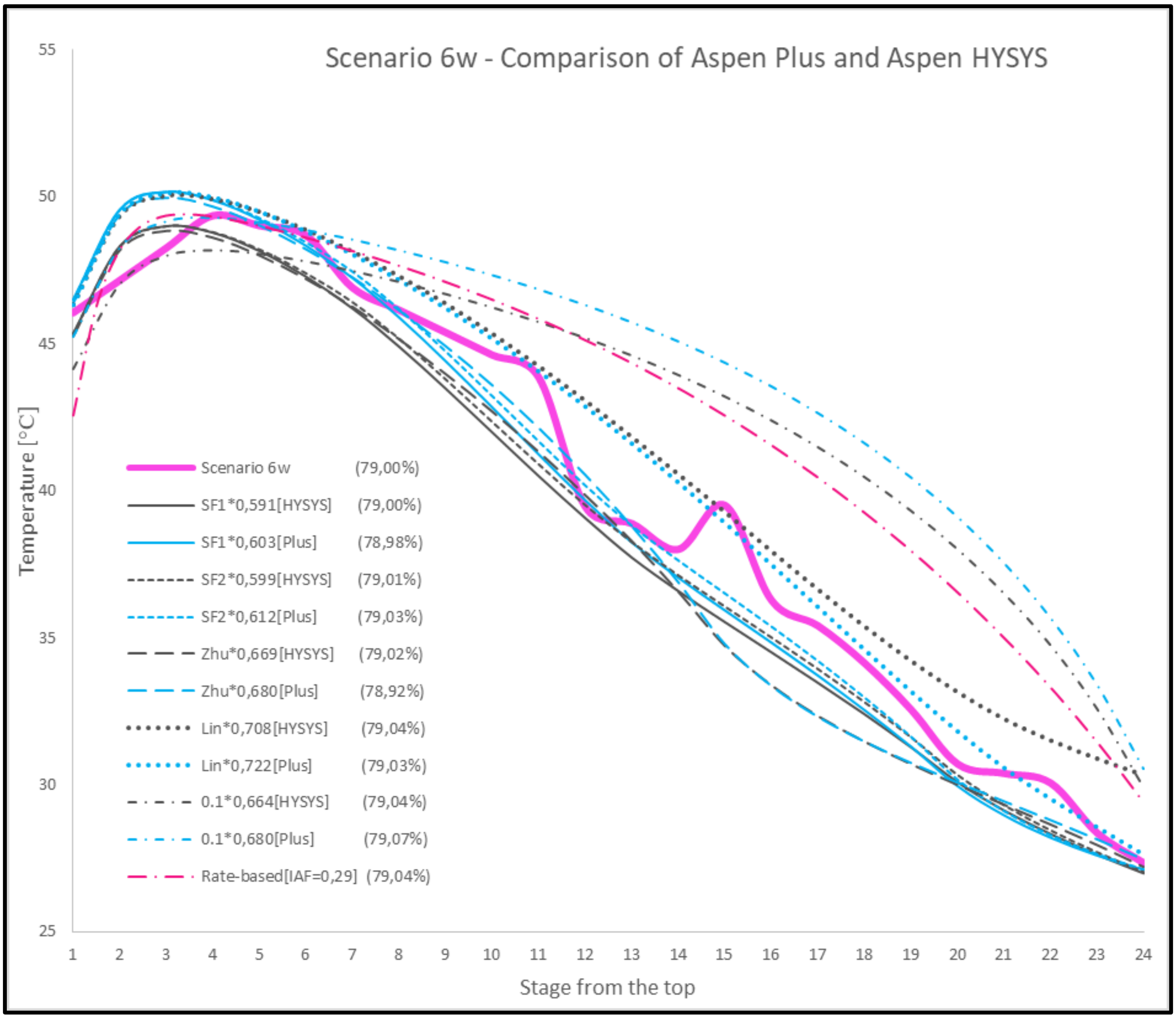


Figure 4.50: Comparison of Rate-based and Equilibrium for Scenario 6w

Table 4.40: Key results from comparison of Rate-based and Equilibrium for Scenario 6w

Comparison HYSYS and Plus - Scenario 6w												
	TCM Data Scenario 6w	SF1		SF2		Zhu		Lin		0.1		Rate-based
		HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	Plus
EM-Factor		0.591	0.603	0.599	0.612	0.669	0.680	0.708	0.722	0.664	0.680	IAF = 0.29
Removal grade	**79.00%**	79.00	78.98	79.01	79.03	79.02	78.92	79.04	79.03	79.04	79.07	79.04
Rich loading	**0.4600**	0.4426	0.4418	0.4426	0.4420	0.4426	0.4413	0.4427	0.4419	0.4426	0.4420	0.4870
Ttop	**46.10**	45.34	47.00	45.33	46.49	45.25	46.36	46.31	46.30	44.16	45.22	42.55
Tmax	**49.35**	48.99	50.16	48.99	50.16	48.82	49.94	50.02	50.10	48.19	49.26	49.39
Tbtm	**27.33**	26.98	27.10	27.01	27.13	27.21	27.43	30.32	27.64	29.92	30.53	29.41

Figure 4.50 presents the simulated temperature results of scenario 6w from sub-chapter 4.3.3 and 4.4.3.

Table 4.40 provides the key results from the simulation of scenario 6w in Aspen plus and Aspen HYSYS compared with performance data.

4.5.4 Comparison of Rate-based and Equilibrium-based for Scenario Goal1

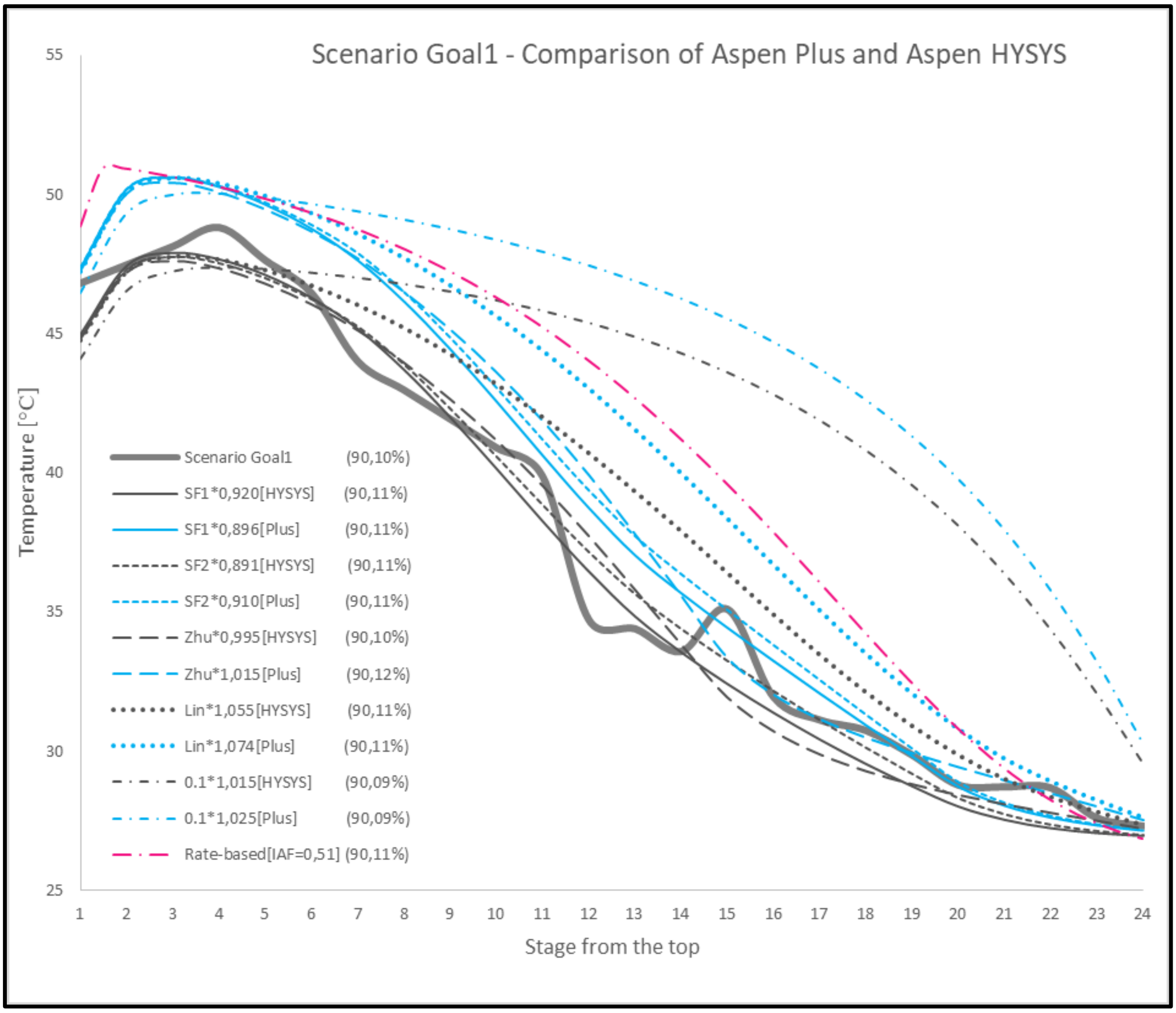


Figure 4.51: Comparison of Rate-based and Equilibrium for Scenario Goal1

Table 4.41: Key results from comparison of Rate-based and Equilibrium for Scenario Goal1

Comparison HYSYS and Plus - Scenario Goal1											
	TCM Data Scenario Goal1	**SF1**		**SF2**		**Zhu**		**Lin**		**0.1**	**Rate-based**
		HYSYS	**Plus**	**HYSYS**	**Plus**	**HYSYS**	**Plus**	**HYSYS**	**Plus**	**HYSYS**	**Plus**	**Plus**
EM-Factor		0.920	0.896	0.891	0.910	0.995	1.015	1.055	1.074	1.015	1.025	IAF = 0.51
Removal grade	**90.10%**	90.10	90.11	90.11	90.11	90.10	90.12	90.11	90.11	90.09	90.09	90.11
Rich loading	**0.5000**	0.4904	0.4870	0.4874	0.4870	0.4873	0.4871	0.4875	0.4871	0.4872	0.4869	0.4870
Ttop	**46.81**	46.44	47.82	46.45	47.81	46.36	47.75	46.31	47.73	45.55	47.21	54.27
Tmax	**48.81**	50.02	51.33	50.05	51.34	49.88	51.20	50.02	51.41	49.41	51.19	51.25
Tbtm	**27.31**	29.96	30.44	29.97	30.45	30.67	30.66	30.32	30.72	32.51	32.38	29,87

Figure 4.51 presents the simulated temperature results of scenario Goal1 from sub-chapter 4.3.4 and 4.4.4.

Table 4.41 provides the key results from the simulation of scenario Goal1 in Aspen plus and Aspen HYSYS compared with performance data.

4.5.5 Comparison of Rate-based and Equilibrium-based for Scenario F17

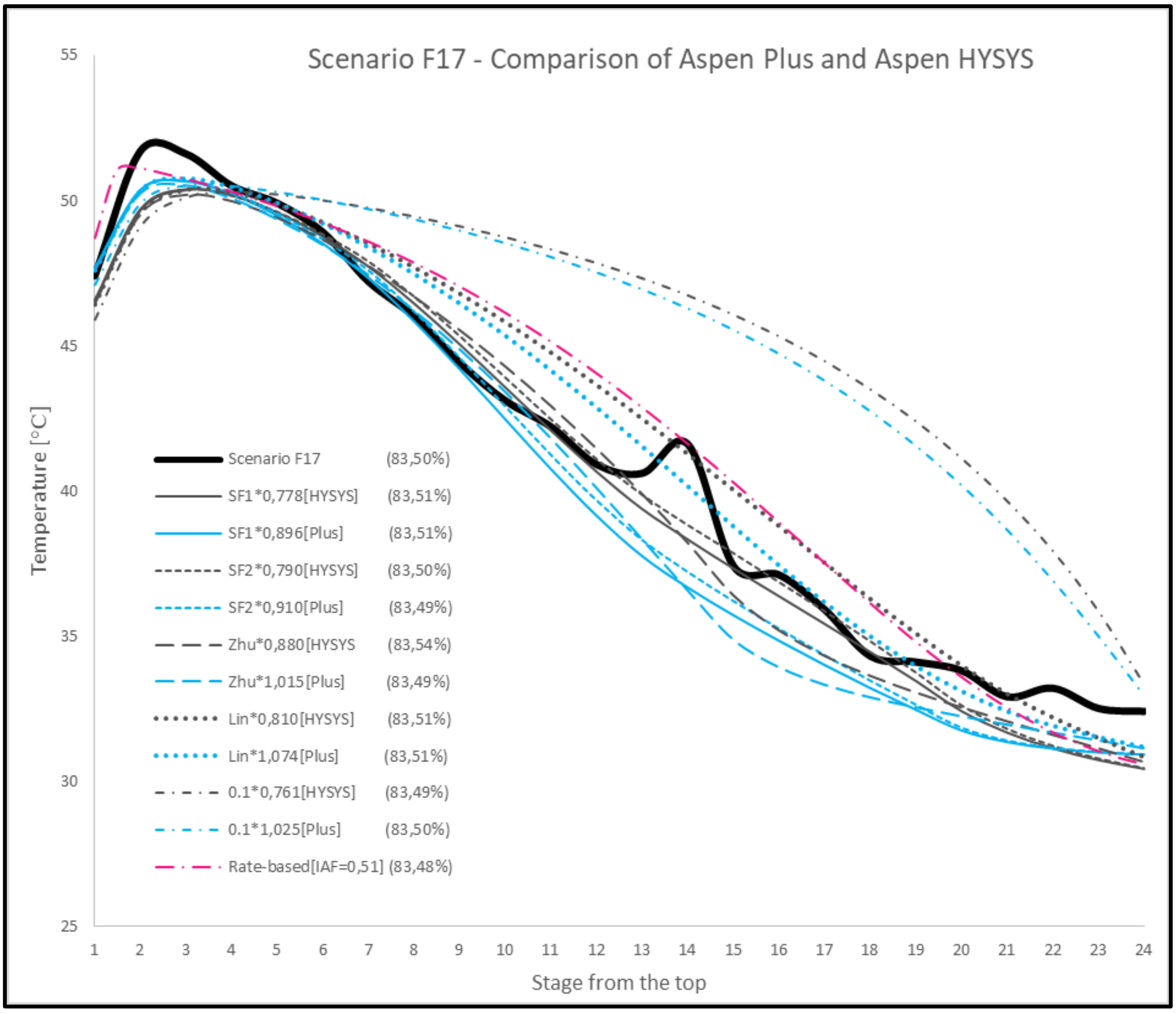


Figure 4.52: Comparison of Rate-based and Equilibrium for Scenario F17

Table 4.42: Key results from comparison of Rate-based and Equilibrium for Scenario F17

Comparison HYSYS and Plus - Scenario F17												
	TCM Data Scenario F17	SF1		SF2		Zhu		Lin		0.1		Rate-based
		HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	Plus
EM-Factor		0.920	0.896	0.891	0.910	0.995	1.015	1.055	1.074	1.015	1.025	IAF = 0.51
Removal grade	**83.50%**	83.51	83.51	83.50	83.49	83.54	83.49	83.51	83.51	83.49	83.50	83.48
Rich loading	**0.4800**	0.4354	0.4837	0.4353	0.4836	0.4354	0.4836	0.4353	0.4837	0.4353	0.4836	0.4836
Ttop	**47.40**	46.56	47.67	46.54	47.67	46.46	47.60	46.41	47.59	45.88	47.08	48.72
Tmax	**51.70**	50.38	50.65	50.35	50.66	50.20	50.51	50.36	50.74	50.29	50.50	51.13
Tbtm	**32.40**	30.42	30.91	30.44	30.91	30.67	31.13	30.82	31.18	33.33	32.95	30.55

Figure 4.52 presents the simulated temperature results of scenario F17 from sub-chapter 4.3.5 and 4.4.5.

Table 4.42 provides the key results from the simulation of scenario F17 in Aspen plus and Aspen HYSYS compared with performance data.

4.6 Simulation with default E_M in Aspen HYSYS

4.6.1 Default VS Estimated E_M for scenario H14

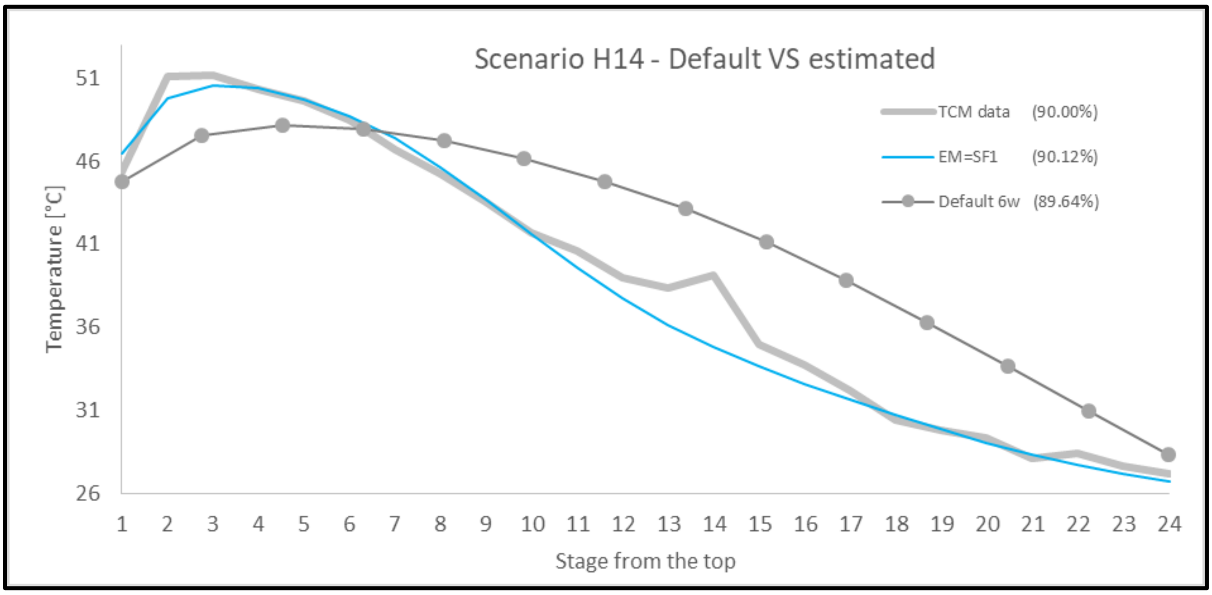


Figure 4.53: Simulated results for scenario H14 with default E_M

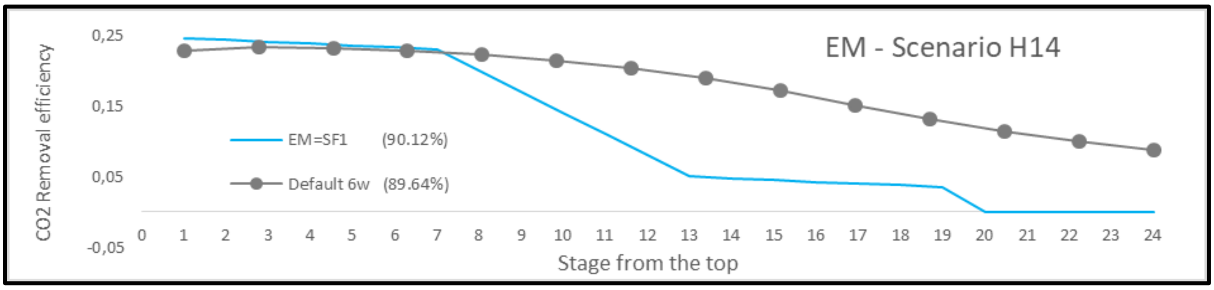


Figure 4.54: Estimated E_M=SF1 VS default E_M for scenario H14

Table 4.43: Key results from simulation of scenario H14 with estimated E_M

E_M	TCM data	SF1	Default 6w
Removal grade	90.00%	90.12%	89.64%
Rich loading	0.4800	0.4936	0.4921
Ttop [˚C]	45.4	46.4	44.74
Tmax [˚C]	51.2	50.6	48.19
Tbtm [˚C]	27.2	26.7	28.33

Figure 4.53 illustrates the temperature profile of the simulation of scenario H14 with a default Murphree efficiency profile compared with performance data and simulation with estimated E_M=SF1. The pointed line illustrates the default temperature profile, the simulation produced the removal grade closest to performance data with 14 stages, the 14 points on the line is the simulated measurements.

Figure 4.54 illustrates the slopes of the default Murphree efficiency profile compared with the slope of E_M=SF1. Table 4.43 provides the key results from simulation.

4.6.2 Default VS Estimated E_M for scenario 2B5

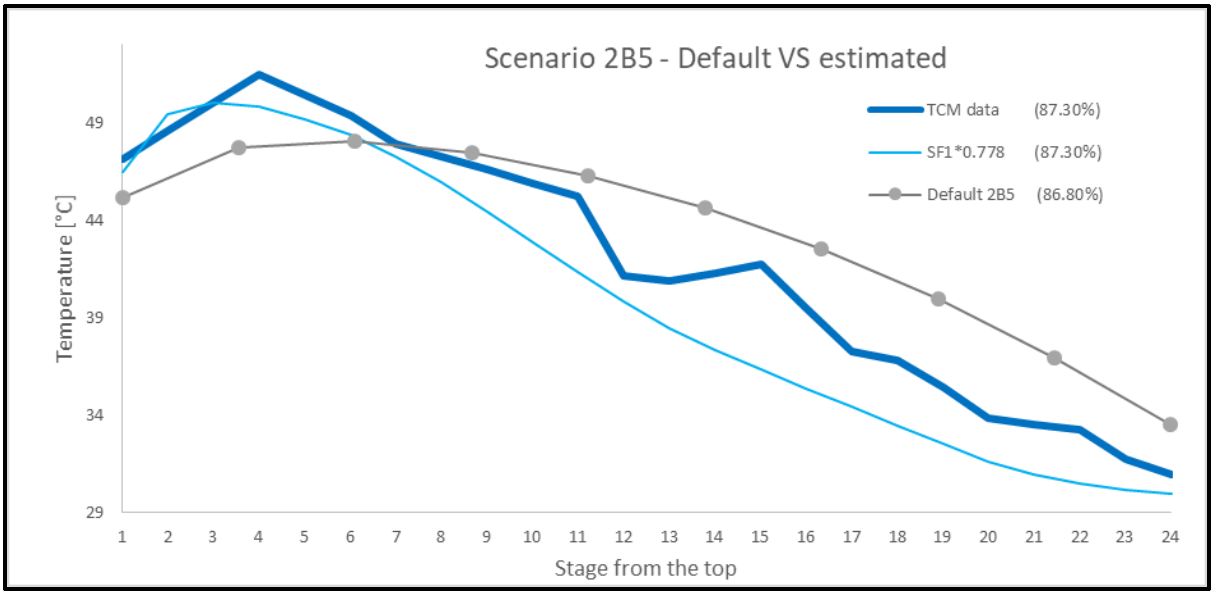


Figure 4.55: Simulated results for scenario 2B5 with default E_M

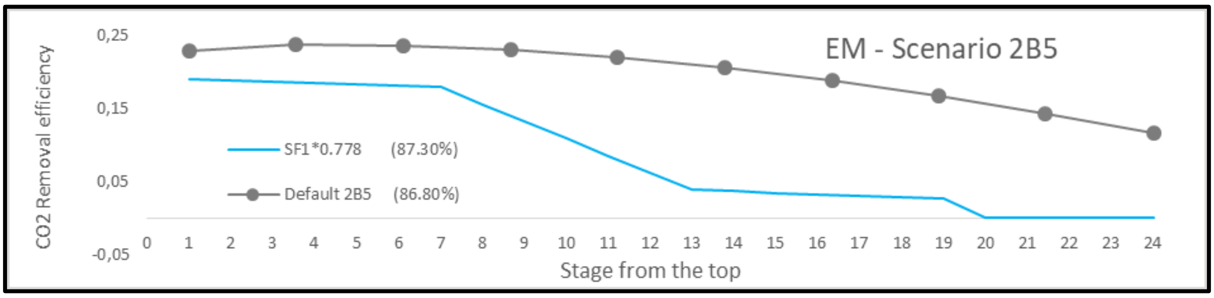


Figure 4.56: Estimated E_M=SF1 VS default E_M for scenario 2B5

Table 4.44: Key results from simulation of scenario 2B5 with estimated E_M

E_M	TCM data	SF1*0.778	Default 2B5
Removal grade	87.30%	87.30%	86.80%
Rich loading	0.5000	0.4635	0.4619
Ttop [˚C]	47.09	46.44	45.12
Tmax [˚C]	51.47	50.02	48.05
Tbtm [˚C]	30.99	29.96	33.53

Figure 4.55 illustrates the temperature profile of the simulation of scenario 2B5 with default Murphree efficiencies compared with performance data and simulation with estimated E_M=SF1*0.778. The pointed line illustrates the default temperature profile, the simulation produced the removal grade closest to performance data with 10 stages, the 10 points on the line is the simulated measurements.

Figure 4.56 illustrates the slopes of the default Murphree efficiency profile compared with the slope of E_M=SF1*0.778. Table 4.44 provides the key results from simulation.

4.6.3 Default VS Estimated E_M for scenario 6w

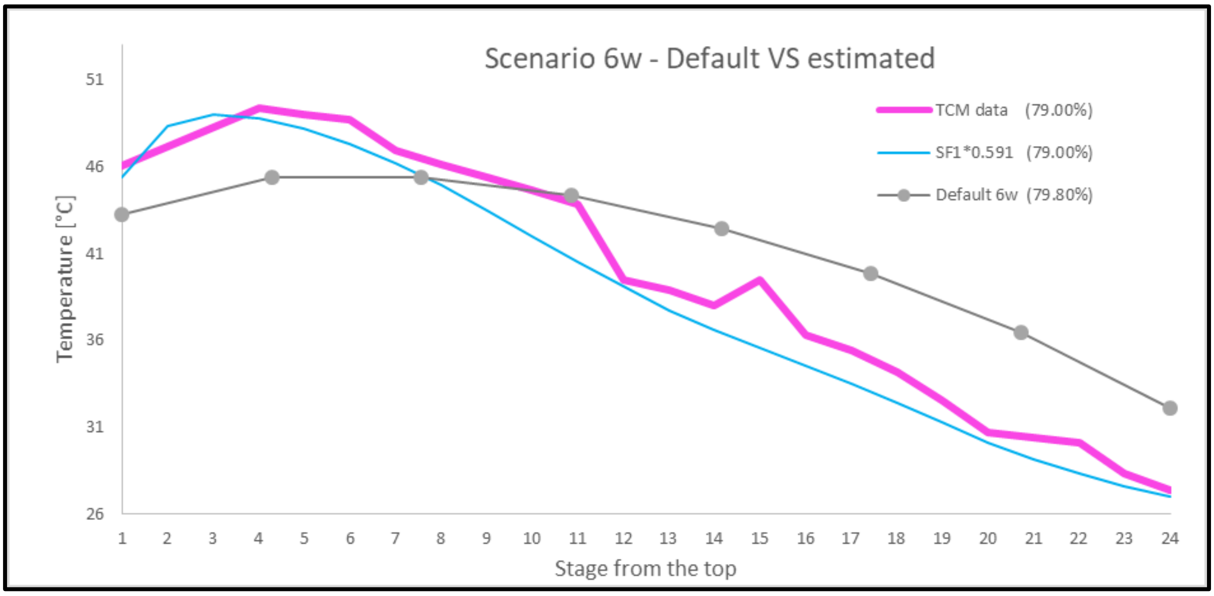


Figure 4.57: Simulated results for scenario 6w with default E_M

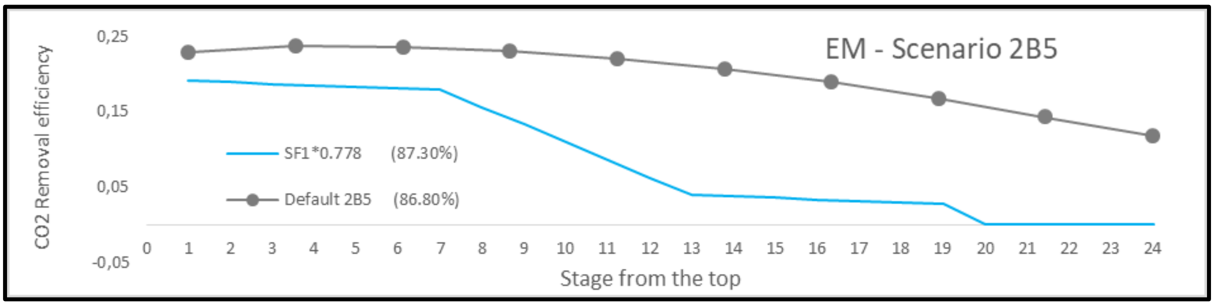


Figure 4.58: Estimated E_M=SF1 VS default E_M for scenario 6w

Table 4.45: Key results from simulation of scenario 6w with estimated E_M

E_M	TCM data	SF1*0.591	Default 6w
Removal grade	79.00%	79.00%	79.80%
Rich loading	0.4600	0.4426	0.4446
Ttop [˚C]	46.10	45.34	43.26
Tmax [˚C]	49.35	48.99	45.40
Tbtm [˚C]	27.33	26.97	32.11

Figure 4.57 illustrates the temperature profile of the simulation of scenario 6w with a default Murphree efficiency profile compared with performance data and simulation with estimated E_M=SF1*0.591. The pointed line illustrates the default temperature profile, the simulation produced the removal grade closest to performance data with 8 stages, the 8 points on the line is the simulated measurements.

Figure 4.45 illustrates the slopes of the default Murphree efficiency profile compared with the slope of E_M=SF1*0.591. Table 4.45 provides the key results from simulation.

4.6.4 Default VS Estimated E_M for scenario Goal1

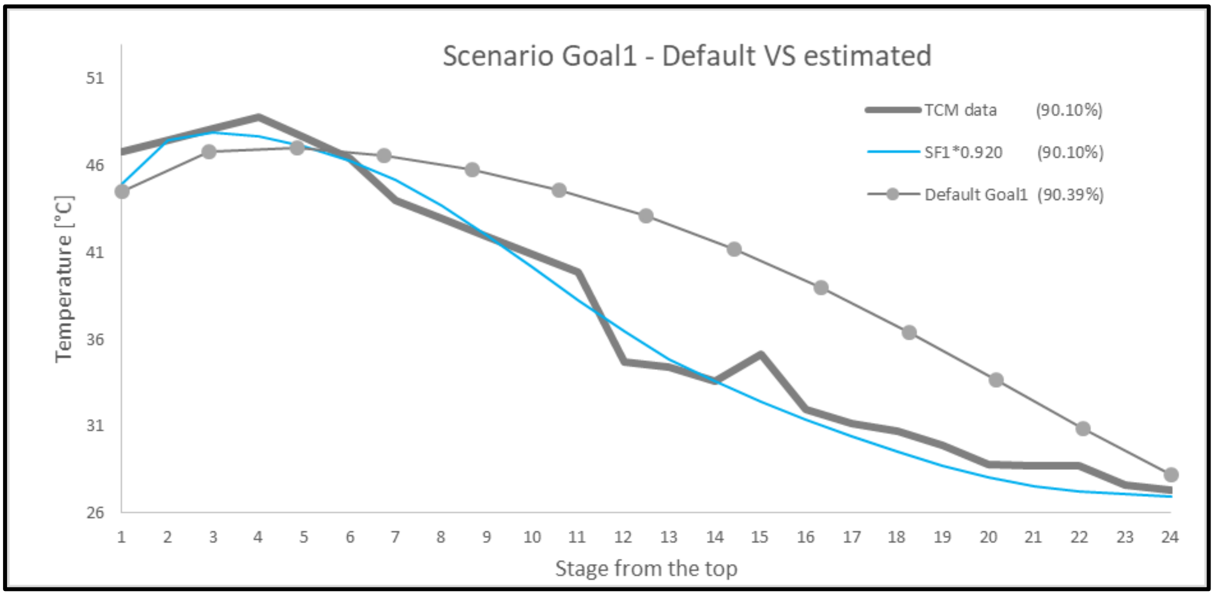


Figure 4.59: Simulated results for scenario Goal1 with default E_M

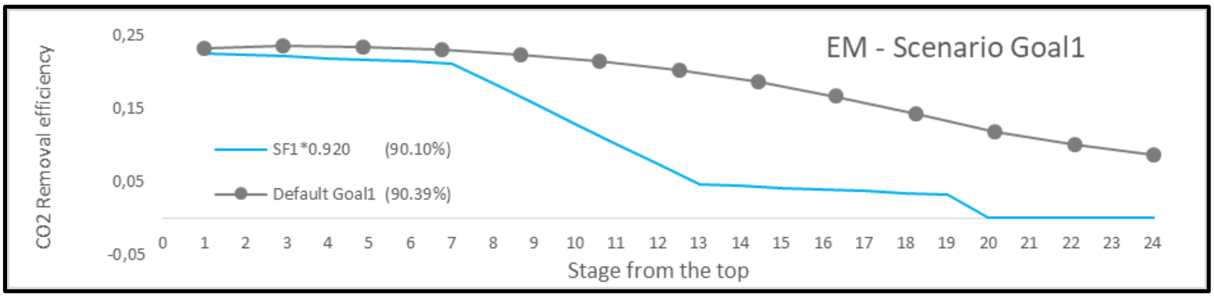


Figure 4.60: Estimated E_M=SF1 VS default E_M for scenario Goal1

Table 4.46: Key results from simulation of scenario Goal1 with estimated E_M

E_M	TCM data	SF1*0.920	Default Goal1
Removal grade	90.10%	90.10%	90.39%
Rich loading	0.5000	0.4904	0.4883
Ttop [˚C]	46.81	44.98	44.53
Tmax [˚C]	48.81	47.89	47.06
Tbtm [˚C]	27.31	26.95	28.20

Figure 4.59 illustrates the temperature profile of the simulation of scenario Goal1 with default Murphree efficiency profile compared with performance data and simulation with estimated E_M=SF1*0.920. The pointed line illustrates the default temperature profile, the simulation produced the removal grade closest to performance data with 13 stages, the 13 points on the line is the simulated measurements.

Figure 4.60 illustrates the slopes of the default Murphree efficiency profile compared with the slope of E_M=SF*0.920. Table 4.46 provides the key results from simulation.

4.6.5 Default VS Estimated E_M for scenario F17

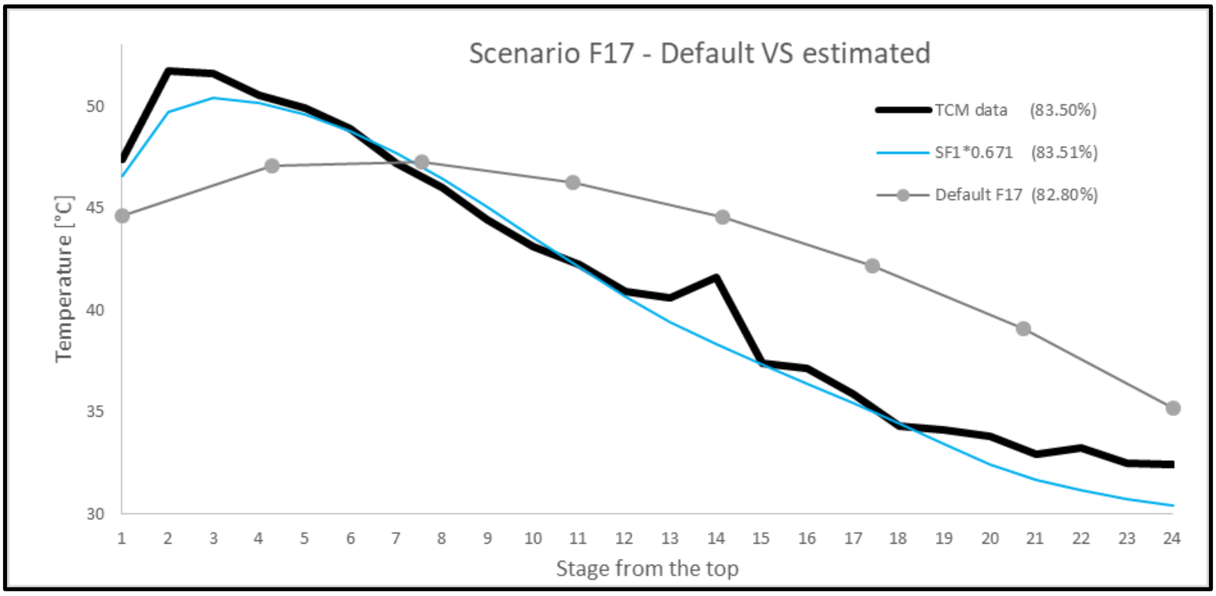


Figure 4.61: Simulated results for scenario F17 with default E_M

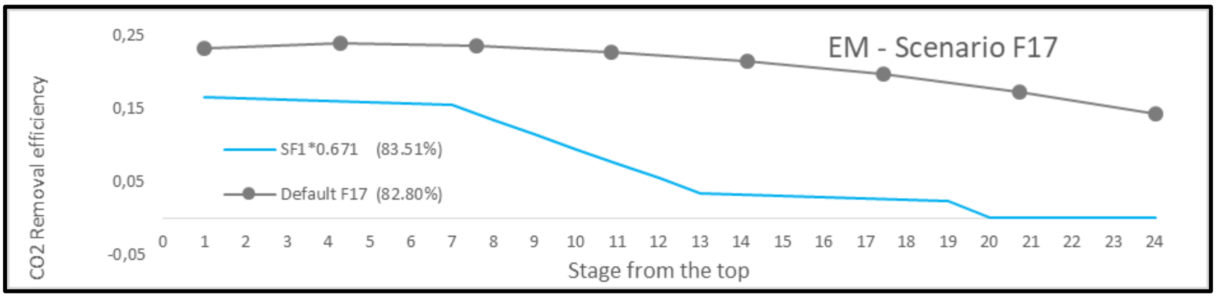


Figure 4.62: Estimated E_M=SF1 VS default E_M for scenario F17

Table 4.47: Key results from simulation of scenario F17 with estimated E_M

E_M	**TCM data**	**SF1*0.671**	**Default F17**
Removal grade	83.50%	83.51%	82.80%
Rich loading	0.4800	0.4354	0.4332
Ttop [˚C]	47.4	46.56	44.63
Tmax [˚C]	51.7	50.38	47.24
Tbtm [˚C]	32.4	30.42	35.15

Figure 4.61 illustrates the temperature profile of the simulation of scenario F17 with default Murphree efficiency profiles compared with performance data and simulation with estimated E_M=SF1*0.671. The pointed line illustrates the default temperature profile, the simulation produced the removal grade closest to performance data with 8 stages, the 8 points on the line is the simulated measurements.

Figure 4.62 illustrates the slopes of the default Murphree efficiency profile compared with the slope of E_M=SF1*0.671. Table 4.47 provides the key results from simulation.

4.7 Comparison of Amine package in Aspen HYSYS

4.7.1 Comparison of amine packages for scenario H14

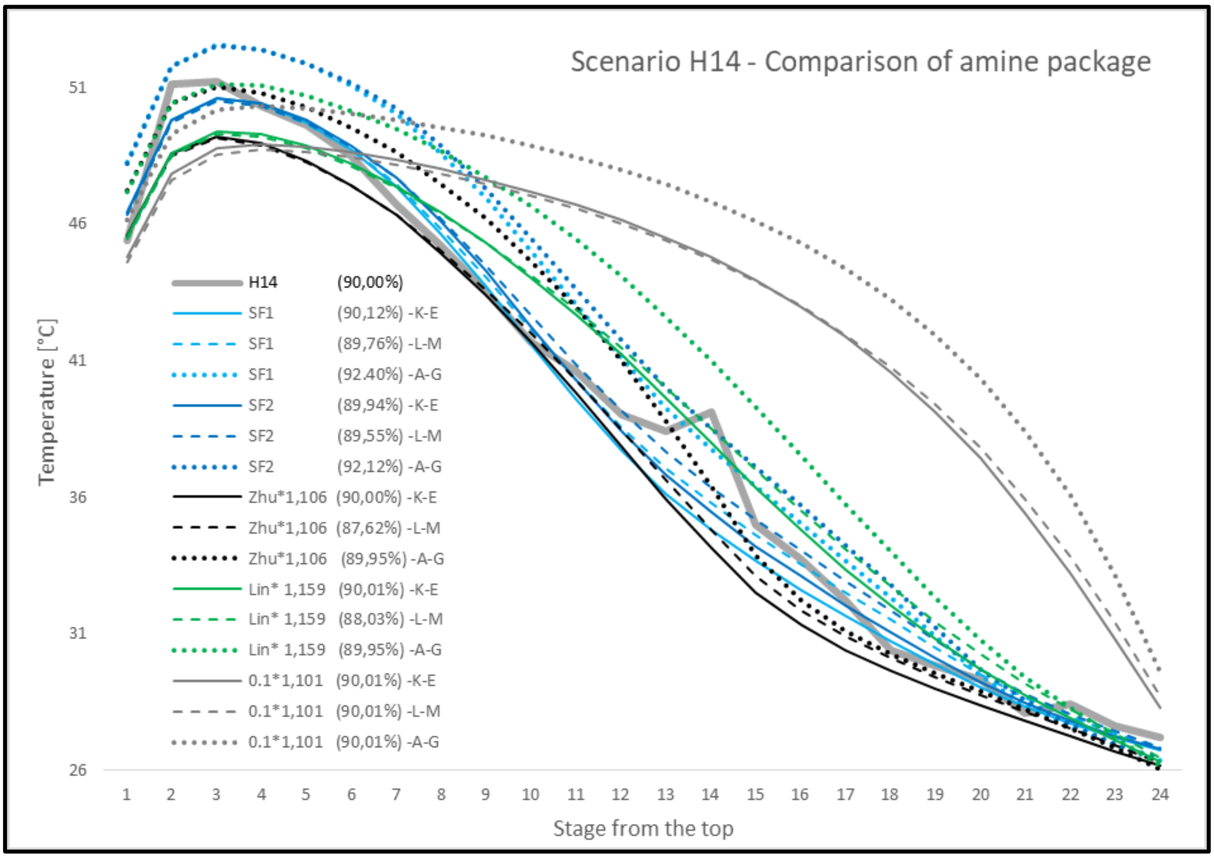


Figure 4.63: Comparison of Amine fluid packages for Scenario H14

Table 4.48: Comparison of key results from simulation with different amine packages for scenario H14

Comparison of amine Packages in Aspen HYSYS										
Scenario H14		**Zhu*1,106**			**Lin*1,159**			**0.1*1,101**		
		K-E	**L-M**	**A-G**	**K-E**	**L-M**	**A-G**	**K-E**	**L-M**	**A-G**
Capture rate	[%]	90.00	89.64	92.14	90.01	89.63	91.85	90.01	89.87	91.92
Rich loading		0.4932	0.4922	0.4986	0.4933	0.4922	0.4977	0.4932	0.4928	0.4980
Ttop	[°C]	45.59	45.52	47.24	45.53	45.45	47.19	44.79	44.62	46.14
Tmax	[°C]	49.21	49.13	51.00	49.37	49.27	51.14	48.93	48.73	50.33
Tbtm	[°C]	26.14	26.25	26.02	26.31	26.44	26.17	28.29	28.69	29.57
		SF1			**SF2**					
		K-E	**L-M**	**A-G**	**K-E**	**L-M**	**A-G**			
Capture rate	[%]	90.12	89.76	92.40	89.94	89.55	92.12			
Rich loading		0.4936	0.4925	0.4994	0.4931	0.4919	0.4986			
Ttop	[°C]	46.43	46.38	48.25	46.41	46.34	48.22			
Tmax	[°C]	50.59	50.52	52.55	50.58	50.49	52.52			
Tbtm	[°C]	26.73	26.80	26.35	26.76	26.83	26.37			

Figure 4.63 illustrates the temperature profile of the Scenario H14 simulated with all five E_M-profiles in three different amine-packages. Table 4.48 provides the key results from simulation.

4.7.2 Comparison of amine packages for scenario 2B5

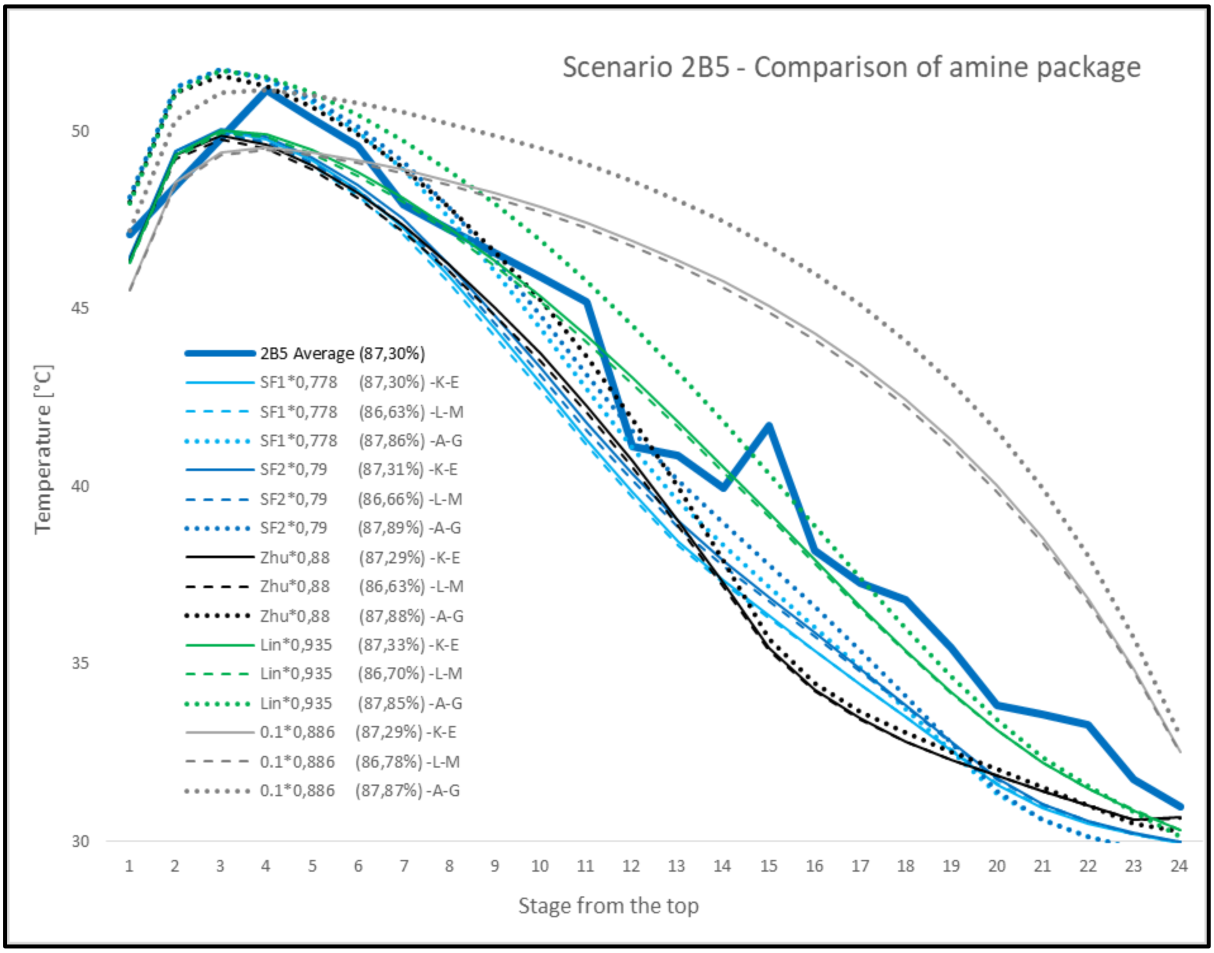


Figure 4.64: Comparison of Amine fluid packages for Scenario 2B5

Table 4.49: Comparison of key results from simulation with different amine packages for scenario 2B5

Comparison of amine Packages in Aspen HYSYS for scenario 2B5										
		Zhu*0.88			**Lin*0.935**			**0.1*0,886**		
		K-E	**L-M**	**A-G**	**K-E**	**L-M**	**A-G**	**K-E**	**L-M**	**A-G**
Capture rate	[%]	87.29	86.63	87.88	87.32	86.70	87.85	87.29	86.78	87.87
Rich loading		0.4634	0.4615	0.4643	0.4635	0.4616	0.4644	0.4634	0.4618	0.4643
Ttop	[°C]	46.36	46.31	48.02	46.31	46.27	47.96	45.55	45.50	47.20
Tmax	[°C]	49.88	49.78	51.56	50.02	49.95	51.69	49.53	49.46	51.16
Tbtm	[°C]	30.67	30.66	30.27	30.32	30.32	30.15	32.51	32.48	32.93
		SF1*0,778			**SF1*0,79**					
		K-E	**L-M**	**A-G**	**K-E**	**L-M**	**A-G**			
Capture rate	[%]	87.30	86.63	87.86	87.31	86.66	87.89			
Rich loading		0.4635	0.4615	0.4643	0.4635	0.4615	0.4644			
Ttop	[°C]	46.44	46.39	48.13	46.45	46.39	48.14			
Tmax	[°C]	50.02	49.93	51.74	50.05	49.94	51.76			
Tbtm	[°C]	29.96	29.97	29.60	29.97	29.97	29.60			

Figure 4.64 illustrates the temperature profile of the Scenario 2B5 simulated with all five E_M-profiles in three different amine-packages. Table 4.49 provides the key results from simulation.

4.7.3 Comparison of amine packages for scenario 6w

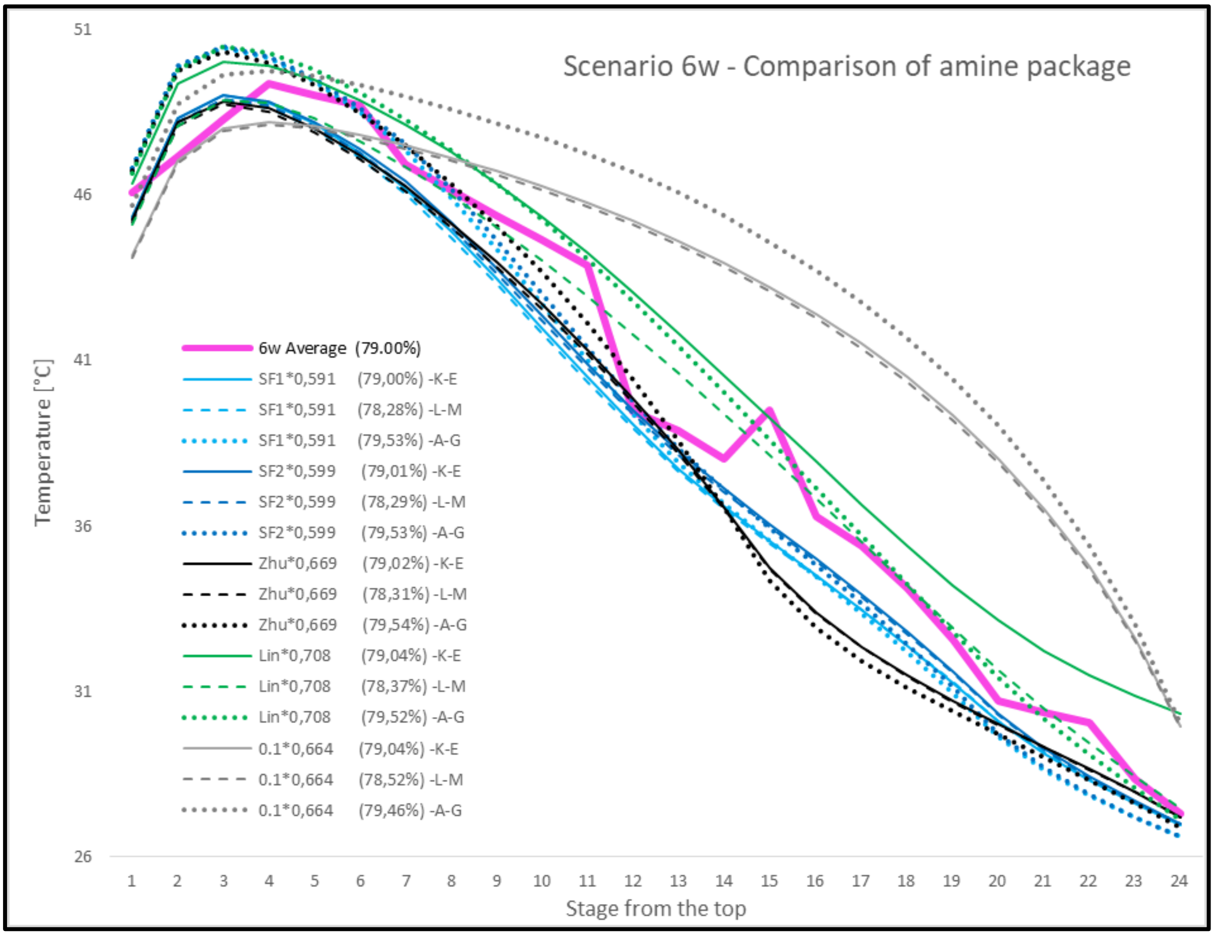


Figure 4.65: Comparison of Amine fluid packages for Scenario 6w

Table 4.50: Comparison of key results from simulation with different amine packages for scenario 6w

Comparison of amine Packages in Aspen HYSYS for scenario 6w										
		Zhu*0.669			**Lin*0.708**			**0.1*0,664**		
		K-E	**L-M**	**A-G**	**K-E**	**L-M**	**A-G**	**K-E**	**L-M**	**A-G**
Capture rate	[%]	79.02	78.31	79.54	79.04	78.37	79.52	79.04	78.52	79.46
Rich loading		0.4426	0.4407	0.4433	0.4427	0.4408	0.4433	0.4426	0.4412	0.4431
Ttop	[°C]	45.26	45.19	46.72	46.31	45.09	46.65	44.16	44.10	45.66
Tmax	[°C]	48.82	48.71	50.30	50.01	48.84	50.45	48.18	48.11	49.74
Tbtm	[°C]	27.21	27.20	26.89	30.32	27.44	27.11	29.91	29.88	30.03
		SF1*0,591			**SF1*0,599**					
		K-E	**L-M**	**A-G**	**K-E**	**L-M**	**A-G**			
Capture rate	[%]	79.00	78.28	79.53	79.01	78.29	79.53			
Rich loading		0.4426	0.4406	0.4433	0.4426	0.4406	0.4433			
Ttop	[°C]	45.34	46.39	48.13	45.33	46.39	46.80			
Tmax	[°C]	48.99	49.93	51.74	48.99	48.88	50.45			
Tbtm	[°C]	26.98	29.97	29.60	27.01	27.01	26.63			

Figure 4.65 illustrates the temperature profile of the Scenario 6w simulated with all five E_M-profiles in three different amine-packages. Table 4.50 provides the key results from simulation.

4.7.4 Comparison of amine packages for scenario Goal1

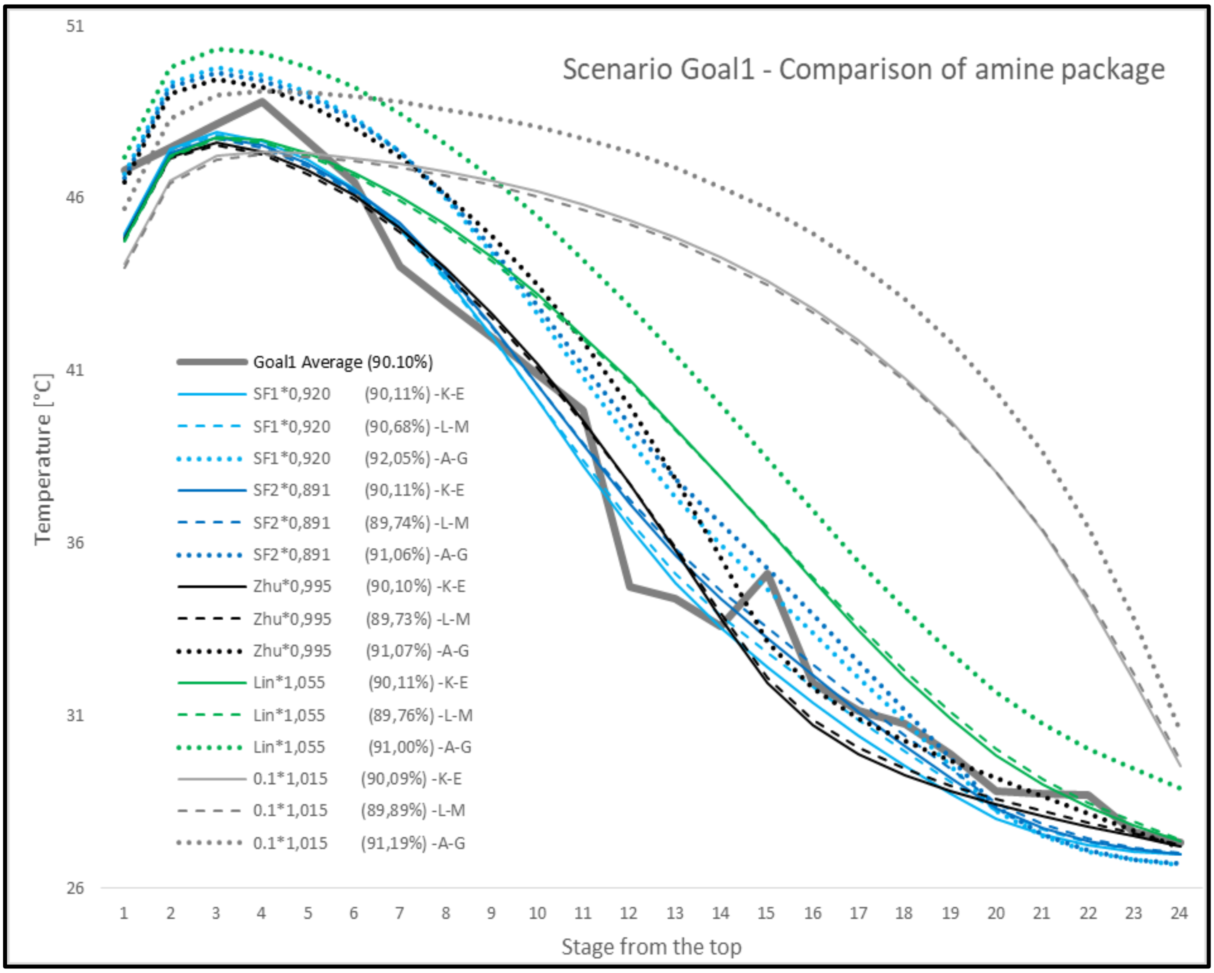


Figure 4.66: Comparison of Amine fluid packages for Scenario Goal1

Table 4.51: Comparison of key results from simulation with different amine packages for scenario Goal1

Comparison of amine Packages in Aspen HYSYS for scenario Goal1										
		Zhu*0.995			Lin*1.055			0.1*0.01015		
		K-E	L-M	A-G	K-E	L-M	A-G	K-E	L-M	A-G
Capture rate	[%]	90.10	89.73	91.07	90.11	89.76	91.00	90.09	89.89	91.19
Rich loading		0.4873	0.4861	0.4896	0.4875	0.4862	0.4894	0.4872	0.4865	0.4900
Ttop	[°C]	44.82	44.77	46.47	44.78	44.73	47.19	44.07	44.00	45.70
Tmax	[°C]	47.62	47.54	49.45	47.78	47.71	50.33	47.36	47.12	49.11
Tbtm	[°C]	27.20	27.24	27.14	27.34	27.39	28.90	29.51	29.68	30.53
		SF1*0.920			SF2*0.891					
		K-E	L-M	A-G	K-E	L-M	A-G			
Capture rate	[%]	90.10	90.68	92.05	90.11	89.74	91.06			
Rich loading		0.4904	0.4893	0.4929	0.4874	0.4861	0.4896			
Ttop	[°C]	44.98	44.94	46.69	44.88	44.85	46.60			
Tmax	[°C]	47.90	47.83	49.78	47.75	47.71	49.64			
Tbtm	[°C]	26.95	26.98	26.68	26.98	26.99	26.69			

Figure 4.66 illustrates the temperature profile of the Scenario Goal1 simulated with all five E_M-profiles in three different amine-packages. Table 4.51 provides the key results from simulation.

4.7.5 Comparison of amine packages for scenario F17

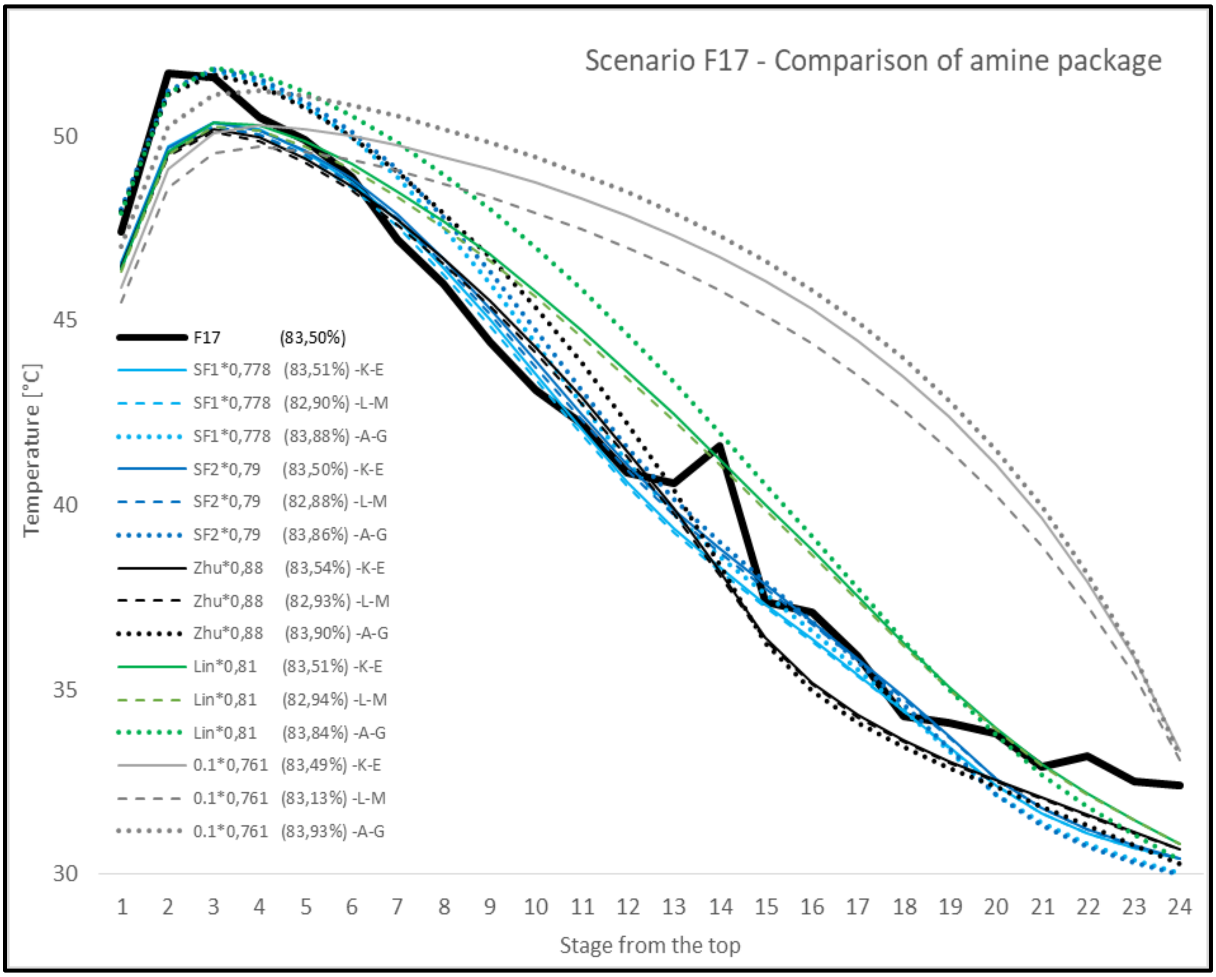


Figure 4.67: Comparison of Amine fluid packages for Scenario F17

Table 4.52: Comparison of key results from simulation with different amine packages for scenario F17

Comparison of amine Packages in Aspen HYSYS for scenario F17										
		Zhu*0,88			Lin*0,81			0.1*0,761		
		K-E	L-M	A-G	K-E	L-M	A-G	K-E	L-M	A-G
Capture rate	[%]	83.54	82.93	83.90	83.51	82.94	83.84	83.49	83.13	83.93
Rich loading		0.4254	0.4337	0.4357	0.4353	0.4337	0.4355	0.4353	0.4342	0.4357
Ttop	[°C]	46.46	46.40	47.94	46.41	46.34	47.90	45.88	45.49	47.01
Tmax	[°C]	50.20	50.11	51.67	50.36	50.25	51.83	50.29	49.70	52.22
Tbtm	[°C]	30.67	30.66	30.27	30.82	30.81	30.39	33.33	33.08	33.21
		SF1*0,778			SF2*0,79					
		K-E	L-M	A-G	K-E	L-M	A-G			
Capture rate	[%]	83.51	82.90	83.88	83.50	82.88	83.86			
Rich loading		0.4354	0.4336	0.4356	0.4353	0.4336	0.4355			
Ttop	[°C]	46.56	46.49	47.99	46.54	46.48	48.03			
Tmax	[°C]	50.17	50.04	51.48	50.35	50.26	51.82			
Tbtm	[°C]	30.42	30.42	30.04	30.44	30.44	29.98			

Figure 4.67 illustrates the temperature profile of the Scenario F17 simulated with all five E_M-profiles in three different amine-packages. Table 4.52 provides the key results from simulation.

5 Suggested method for estimating E_M-factor

From the simulations in sub-chapter 4.3, there is an interest for studying the connections between E_M-factor and performance data, with the interest of finding a method of estimating the E_M-factor for any given scenario.

Table 5.1: Comparison of key performance data from each scenario

Scenario	E_M - Factor for SF1 (E_M)	Lean Amine flow [kg/h]	Gas inlet flow [Sm3/h]	Ratio [Sm^3/ kg]	Amine inlet temp [˚C]	Gas inlet temp [˚C]	Lean loading	Rich loading	Max temp [˚C]	Removal grade (RG%) [%]
H14	1.000	54900	46970	0.86	36.5	25.0	0.2300	0.4800	51.2	90.00
Goal1	0.920	44391	46864	1.06	36.5	25.0	0.2000	0.5000	48.8	90.10
2B5	0.778	49485	46981	0.95	36.8	28.2	0.2000	0.5000	51.1	87.30
F17	0.671	57434	59430	1.03	37.0	29.8	0.2000	0.4800	51.7	83.50
6w	0.591	54915	46602	0.85	36.9	25.0	0.2500	0.4600	49.4	79.00

Based on the data in table 5.1, it becomes clear that the E_M-factor decreases almost linearly with the removal grade, with some exceptions. Equation 5.1 was used to create a line with linear interpolation between E_M-factor for E_M=SF1 and removal grade for scenario H14 and 6w. This was done to investigate the nonlinearities, since these two scenarios contains similar experimental data. E_M=SF1 is illustrated by the filled blue rectangles in Figure 5.1.

$$E_M - factor = E_{M[0]} + \left(RG\% - RG\%_{[0]}\right)\frac{E_{M[1]} - E_{M[0]}}{RG\%_{[1]} - RG\%_{[0]}} \tag{5.1}$$

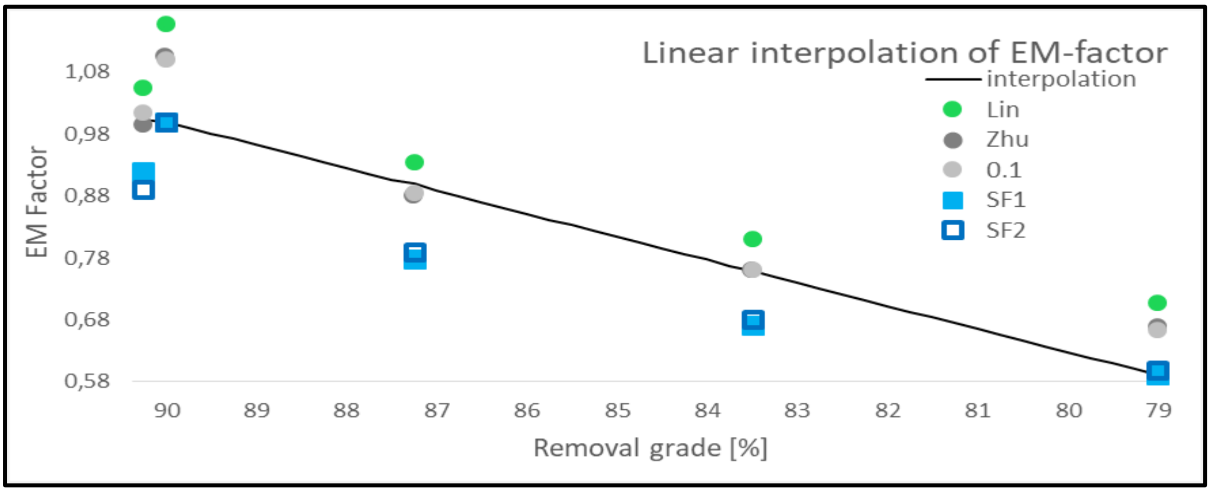


Figure 5.1: Linear interpolation between E_M-factors

The deviation from the line is calculated for scenario Goal1 (-0.08), 2B5 (-0.12) and F17 (-0.09). From these results one can assume that the ratio of amine and gas impacts the choice of E_M-factor. It is therefore assumed that if the experimental performance data were closer to the data for scenario H14 and 6w, the E_M-factor could be calculated for any removal grade from equation 5.1.

If the key data is deviating from the data in scenario H14 and 6w, the suggested method could be combined with an estimating method e.g. you could calculate the E_M-factor with equation 5.1 and simulate with the calculated E_M-factor. If the simulated removal grade is higher than performance removal grade, you could guess a lower value for E_M-factor and continue with e.g the bisection method until an E_M-factor which predicts the correct removal grade is found. In the same way you would guess a higher value for E_M-factor if the simulated removal grade is lower than performance data.

It is assumed that this method will converge to the correct E_M-factor quicker than the try and fail method suggested in sub-chapter 3.2.2.

6 Discussion

In this chapter, the verification simulations in Aspen HYSYS and Aspen Plus are evaluated. The simulations with estimated E_M-profiles in Aspen HYSYS and estimated E_M-profiles and interfacial area factor in Aspen Plus are evaluated. The comparison between estimated simulations in Equilibrium-based and rate-based model are evaluated. The simulations with default E_M-profiles compared with estimated E_M=SF1 in Aspen HYSYS are evaluated. The comparison of simulation with different amine packages in Aspen HYSYS are evaluated. And at last, a comparison of results from this work and results from earlier work is discussed, before some further work is suggested.

6.1 Evaluation of verification simulation in Aspen HYSYS

6.1.1 Evaluation of scenario H14 verification in Aspen HYSYS

The verification of scenario H14 for Zhu, Sætre and Røsvik was not producing identical temperature profile with any of their results, but a similar temperature profile for both scenario H14 with $E_M = 0.1$ and E_M = Zhu. The removal grade for E_M=0.1 was lower than performance data (-1.58%), lower than Zhu (-0.98%), higher than Sætre (+1.42%) and lower than Røsvik (-0.88%). While the rich loading was higher than performance data (+0.0085), higher than Zhu (+0.0015) and lower than Sætre (-0.0035). The removal grade for E_M=Zhu was lower than performance data (-1.43%), lower than Zhu (-0.82%), higher than Sætre (+1.67%) and lower than Røsvik (-0.73%). While the rich loading was higher than performance data (+0.0090), higher than Zhu (+0.0010) and lower than Sætre (-0.0020).

Zhu got a higher removal grade and a lower rich loading while Sætre got a lower removal grade and higher rich loading for botm E_M=0.1 and E_M=Zhu. The reason for this deviation is assumed to be because Zhu used a lower input flue gas flow than given by Hamborg et al., (2014) [7] for scenario H14. This assumption gets supported when the results are compared to Sætre's verification in his master thesis from 2016 [28], where he verified Zhu with the same input flue gas flow as Zhu and got a removal grade and rich loading almost identical with Zhu.

6.1.2 Evaluation of scenario 2B5 verification in Aspen HYSYS

The verification of Sætre's simulation of 2B5 results in a non-identical but slightly similar temperature profile for both E_M=0.1 and E_M=Zhu. The removal grade for E_M=0.1 was slightly higher than Sætre (+3.07%) and performance data (+2.77%) while the rich loading was lower than Sætre (-0.0200) and performance data (-0.0300). The removal grade for E_M =Zhu was also slightly higher than Sætre (+3.00%) and performance data (+3%) while the rich loading was lower than Sætre (-0.0200) and performance data (-0.0300).

The reason for these deviations might be caused by uncertainties in measurements, variations in different versions of simulation programs or unknown differences in process input variables to simulation.

6.1.3 Evaluation of scenario 6w verification in Aspen HYSYS

The verification on Sætre's work on scenario 6w also produces a temperature profile similar but not identical to Sætre, for both E_M =0.1 and E_M =Zhu. The removal grade for E_M =0.1 were higher than for Sætre (+2.72%) and performance data (+10.72%) while the rich loading was lower than Sætre (-0.0200) but higher than performance data (+0.0100). The removal grade of E_M =Zhu was also slightly higher than Sætre (+2.70%) and performance data (+10.60%) while rich loading was lower than for Sætre (-0.0200) and higher than for performance data (+0.0100).

6.1.4 Evaluation of scenario Goal1 verification in Aspen HYSYS

The verification on Sætre's work on scenario Goal1 produces a curve fairly similar to sætre for both E_M=0.1 and E_M=Zhu. The removal grade for E_M =0.1 were higher than for Sætre (+0.94%) but lower than performance data (-3.06%), while the rich loading was a little bit lower than both (-0.0070). For E_M =Zhu the removal grade was also higher than Sætre (+1.22%) and lower than performance data (-2.68%), while the rich loading was lower than both (-0.0060).

6.1.5 Evaluation of scenario F17 verification in Aspen HYSYS

The verification of Røsvik's simulation of scenario F17, with E_M=0.1, produced a temperature profile similar to Røsvik, but with slightly higher main temperature. The removal grade deviated from both Røsvik (+5.28%) and performance data (+8.18%). The verification of Røsvik's simulation of scenario F17, with E_M=Zhu, produced results that deviated a lot from Røsvik, but fitted the temperature profile for the performance data better than Røsvik's simulation. The removal grade on the other hand deviated from both Røsvik (+2.67%) and performance data (+6.87%). The verification of Røsviks simulation of scenario F17 with E_M=Lin, produced a slightly higher temperature profile, the removal grade had some deviations from Røsvik (+3.60%) and the performance data (+5.50%). The simulated rich loading was slightly lower than the rich loading from performance data for all E_M-profiles, E_M=0.1 (-0.1200), E_M=Zhu (-0.0200), E_M=Lin (-0.0300).

The reason for the deviations is assumed to be for the reason that Røsvik used a much lower input pressure than given in Faramarzi et al., (2017) [32] for scenario F17. In addition, the E_M-profiles used in this verification will give a removal grade higher than performance data because they have a too high overall efficiency to be able to fit this scenario well, this we can also see in scenario 6w which also have a lower removal grade.

6.2 Evaluation of verification simulation in Aspen Plus

6.2.1 Evaluation of scenario H14 verification in Aspen Plus

The verification of scenario H14 for Sætre and Røsvik's equilibrium-based Aspen Plus simulation, produced close to identical results for temperature profile for both E_M=0.1 and E_M=Zhu. The removal grade for E_M=0.1 was lower than performance data (-1.60%), higher than Sætre (+1.20%) and equal to Røsvik. While the rich loading was higher than performance data (+0.0080), lower than Sætre (-0.0030). The removal grade for E_M=Zhu was lower than performance data (-1.61%), higher than Sætre (+1.49%) and lower than Røsvik (-0.61%). While the rich loading was higher than performance data (+0.008) and lower than Sætre (-0.0020).

The rate-based verification of scenario H14 for Sætre and Røsvik, produced close to identical temperature profiles for Sætre, when IAF was set to 0.55, and Røsvik when IAF was set to 0.65. The removal grade for IAF=0.55 was lower than performance data (-1.62%) and lower than Sætre (-0.12%) while the rich loading was higher than performance data (+0.0091) and higher than Sætre (+0.0001). The removal grade for IAF=0.65 was lower than performance data (-1.28%) and lower than Røsvik (-0.38%).

6.2.2 Evaluation of scenario 2B5 verification in Aspen Plus

The verification of scenario 2B5 for Sætre's equilibrium-based Aspen Plus simulation, produced close to identical results for temperature profile for E_M=0.1, while E_M=Zhu had some deviations. The removal grade for E_M=0.1 was lower than performance data (-0.10%) and equal to Sætre. The rich loading was lower than performance data (-0.0113) and lower than Sætre (-0.0013). The removal grade for E_M=Zhu was higher than performance data (+1.09%), and higher than Sætre (+0.99%). The rich loading was lower than performance data (-0.0120) and lower than Sætre (-0.0020).

The rate-based verification of scenario 2B5 for Sætre, produced close to identical temperature profiles when IAF was set to 0.55. The removal grade for IAF=0.55 was lower than performance data (-1.28%) and higher than Sætre (+0.02%) while the rich loading was higher than performance data (+0.0146) and lower than Sætre (-0.0046).

6.2.3 Evaluation of scenario 6w verification in Aspen Plus

The verification of scenario 6w for Sætre's equilibrium-based Aspen Plus simulation, produced close to identical results for temperature profile for E_M=0.1, while E_M=Zhu deviated more.. The removal grade for E_M=0.1 was higher than performance data (+10.49%) and higher than Sætre (+2.29%). The rich loading was higher than performance data (-0.0107) and lower than Sætre (-0.0203). The removal grade for E_M=Zhu was higher than performance data (+10.68%), and higher than Sætre (+2.78%). The rich loading was higher than performance data (+0.0102) and lower than Sætre (-0.0198).

The rate-based verification of scenario 6w for Sætre, produced temperature profiles with similar curves as Sætre but higher temperatures, both when IAF was set to 0.55

and 0.65. The removal grade for IAF=0.55 was higher than performance data (-14.53%) and higher than Sætre (+7.43%) while the rich loading was higher than performance data (+0.0219) and lower than Sætre (-0.0061). The removal grade for IAF=0.65 was higher than performance data (-16.19%) and higher than Sætre (+9.09%) while the rich loading was higher than performance data (+0.0265) and lower than Sætre (-0.0015).

The removal grade was closer to Sætre for IAF=0.55, while the rich loading was closer for IAF=0.65, none of them gave a god fit to temperature profile. It is assumed that Sætre used a lower interfacial area factor.

6.2.4 Evaluation of scenario Goal1 verification in Aspen Plus

The verification of scenario Goal1 for Sætre's equilibrium-based Aspen Plus simulation, produced temperature profiles with similar curves as Sætre for both E_M=0.1, and E_M=Zhu. The removal grade for E_M=0.1 was lower than performance data (-0.47%) and higher than Sætre (+6.93%). The rich loading was lower than both performance data and Sætre (-0.0146). The removal grade for E_M=Zhu was lower than performance data (-0.28%), and higher than Sætre (+7.12%). The rich loading was lower than both performance data and Sætre (-0.0140).

The rate-based verification of scenario Goal1 for Sætre, produced temperature profiles with similar curves as Sætre, but higher temperatures. The removal grade for IAF=0.55 was higher than performance data (+0.11%) and higher than Sætre (+11.31%) while the rich loading was lower than performance data (-0.0123) and lower than Sætre (-0.0020). The removal grade for IAF=0.65 was higher than performance data (+0.30%) and higher than Sætre (+11.50%) while the rich loading was lower than performance data (-0.0120) and lower than Sætre (-0.0020).

The removal grade was closer to Sætre for IAF=0.55, while the rich loading was closer for IAF=0.65, none of them gave a god fit to temperature profile.

6.2.5 Evaluation of scenario F17 verification in Aspen Plus

The verification of scenario F17 for Røsvik's equilibrium-based Aspen Plus simulation, produced similar results for temperature profile for E_M=0.1, while E_M=Zhu had some deviations. The temperature profile for E_M=Lin is close to identical with Røsvik. The removal grade for E_M=0.1 was higher than performance data (+4.90%) and higher than Sætre (+1.75%). The rich loading was higher than performance data (+0.0080). The removal grade for E_M=Zhu was higher than performance data (+4.89%), and higher than Sætre (+1.19%). The rich loading was higher than performance data (+0.0080). The removal grade for E_M=Lin was higher than performance data (+2.74%), and lower than Sætre (-0.06%). The rich loading was higher than performance data (+0.0129).

The rate-based verification of scenario F17 for Røsvik, produced close to identical temperature profiles when IAF was set to 0.55. The removal grade for IAF=0.55 was higher than performance data (+0.26%) and lower than Sætre (-0.04%) while the rich loading was higher than performance data (+0.0450).

6.3 Evaluation of simulation with estimated E_M in Aspen HYSYS

6.3.1 Evaluation of scenario H14 with estimated E_M in Aspen HYSYS

For scenario H14 it was estimated two new E_M-profiles, E_M=SF1 and E_M=SF2. These two profiles are based on the idea of higher CO_2 removal efficiency at the top of each packing section in the absorber column, and were created by equation 3.7 in sub-chapter 3.2.1. The simulation in figure 4.28 indicates that both these E_M's fit the performance data well. It looks as E_M=SF1 have the best fit for temperature profile, while E_M=SF2 have the removal grade closest to performance data. The deviations are small for both E_M=SF1 and E_M=SF2. Compared with E_M=Zhu, it looks as though the new sets might have an even better fit for both temperature and removal grade for scenario H14.

6.3.2 Evaluation of scenario 2B5 with estimated E_M in Aspen HYSYS

For scenario 2B5, the E_M-profiles created for scenario H14 were scaled and fitted to the performance removal grade for scenario 2B5. 2B5 is a scenario with four different sets of temperature measurements, and a given average removal grade. In figure 4.30 the simulation is compared with a blue line of average temperature as well as the measured temperatures. The simulated results of the new developed E_M-profiles, E_M=SF1 and E_M=SF2, did not fit well for the average temperature profile based on the average removal grade, but had a sufficient fit to the temperature profile of plant data C and D. For this scenario the E_M-profile with the best fit to the average temperature profile was E_M=Lin*0.935.

One can see that the measurement in plant data A is slightly higher than for C and D, while B is in between. The independent removal grade for each data set can be assumed to vary a lot, as the temperature varies a lot. It is assumed that E_M=SF1 and E_M=SF2 would fit the average line best if plant data A was neglected.

6.3.3 Evaluation of scenario 6w with estimated E_M in Aspen HYSYS

For scenario 6w, the E_M-profiles created for scenario H14 were scaled and fitted to the performance removal grade for scenario 6w just like for scenario 2B5, 6w is also a scenario with four different sets of temperature measurements, and a given average removal grade. In figure 4.32 the simulation is compared with a purple line of average temperature as well as the measured temperatures. The simulated results of the new developed E_M-profiles based on the average removal grade did fit the average temperature profile better than for scenario 2B5, but was a little too low. Just like for scenario SB5, E_M=SF1 and E_M=SF2 had a sufficient fit to the temperature profile of plant data C and D, but also for B.

If plant data A was removed from the average line the temperature profile would fit better. Like for scenario 2B5, the independent removal grade for each data set for scenario 6w can be assumed to vary a lot for these four data sets, as the temperature varies a lot.

6.3.4 Evaluation of scenario Goal1 with estimated E_M in Aspen HYSYS

For scenario Goal1, the E_M-profiles created for scenario H14 were scaled to fit the performance removal grade for scenario Goal1, just like for scenario 2B5 and 6w. Goal1 is also a scenario with four different sets of temperature measurements, and a given average removal grade. In figure 4.34 the simulation is compared with a gray line of average temperature as well as the measured temperatures. The simulated results for the new developed E_M-profiles based on the average removal grade, did give a sufficient fit to the average performance data. Just like for scenario SB5, E_M=SF1 and E_M=SF2 had a sufficient fit to the temperature profile of plant data B, C and D, while A deviated a lot.

If plant data A was removed from the average line the temperature profile would fit even better. The independent removal grade for each data set for scenario Goal1 can be assumed to vary a lot for these four data sets, as the temperature varies a lot.

6.3.5 Evaluation of scenario F17 with estimated E_M in Aspen HYSYS

For scenario F17 the E_M-profiles created for scenario H14 were used. They were scaled down and fitted to the removal grade given in the performance data by equation 3.8 in sub-chapter 3.2.2. As were E_M=Zhu and E_M=Lin. The simulation in figure 4.36 indicates that the best fit in both temperature profile and removal grade was E_M=SF2, but E_M=SF1 and E_M=Zhu.

By the results from these simulation it looks like the estimation method of E_M-profile by equation 3.7 and 3.8 gives satisfactory results. E_M=Zhu have proven to give a good fit to several scenarios in earlier master theses, but these results provides better results for E_M=SF1 and E_M=SF2. The main difference between Zhu and SF1 & SF2, is that Zhu has constant low efficiency from stage 13 and down. While SF1 & SF2 have constant low efficiency from stage 20 and down. The fact that SF1 & SF2 fit better than Zhu might deciphering that the bottom packing have a higher removal efficiency than suggested in earlier theses.

6.4 Evaluation of simulation with estimated E_M and IAF in Aspen Plus

6.4.1 Evaluation of scenario H14 with estimated E_M and IAF in Aspen Plus

For the equilibrium-based model, the E_M-profiles used for simulation of scenario H14 in Aspen HYSYS were scaled to fit the removal grade for scenario H14 in Aspen Plus by adjusting the E_M-factor. From figure 4.38 it is visible that this gave similar temperature profiles as in Aspen HYSYS with god fit to the performance temperature for E_M=Zhu*1.12, E_M=SF1*0.995 and E_M=SF2*1.005, while E_M=Lin*1.17 and E_M=0.1*1.1 deviated from the performance data. All E_M-profiles were easy to fit with removal grade by adjusting the E_M-factor.

For the rate-based model, the IAF was adjusted up to give the best fit to removal grade. For scenario H14 the IAF was not able to fit the removal grade to 90%. The highest achieved removal grade was for IAF=1, which gave a removal grade of 88.82%. The temperature profile deviated from performance data and simulations with equilibrium-based model.

6.4.2 Evaluation of scenario 2B5 with estimated E_M and IAF in Aspen Plus

For the equilibrium-based model, the E_M-profiles were scaled to fit the removal grade for scenario 2B5 in Aspen Plus by adjusting the E_M-factor. From figure 4.40 it is visible that this gave similar temperature profiles as in Aspen HYSYS. With the best fit to average-temperature profile for E_M=Lin*1.005.

For the rate-based model, the IAF was adjusted up to give the best fit to removal grade. For scenario 2B5 the IAF was not able to fit the removal grade to 87.20%. The highest achieved removal grade was for IAF=1, which gave a removal grade of 86.14%. The temperature profile deviated from performance data and simulations with equilibrium-based model. The temperature profile is very similar to the rate-based temperature in scenario H14.

6.4.3 Evaluation of scenario 6w with estimated E_M and IAF in Aspen Plus

For the equilibrium-based model, the E_M-profiles were scaled to fit the removal grade for scenario 6w in Aspen Plus by adjusting the E_M-factor. From figure 4.42 it is visible that this gave similar temperature profiles as in Aspen HYSYS. With the best fit to average-temperature profile for E_M=SF1*0.603 and E_M=SF2*0.612. E_M=Lin*0.722 fit the performance temperature better in Aspen Plus than in Aspen HYSYS.

For the rate-based model, the IAF was adjusted up to give the best fit to removal grade. For scenario 6w the best result was achieved with IAF=0.29, which gave a removal grade of 79.04%, performance data is 79.00%. The temperature profile deviated from performance data and simulations with equilibrium-based model, but have a better fit to the performance temperatures than rate-based for scenario H14 and 2B5.

6.4.4 Evaluation of scenario Goal1 with estimated E_M and IAF in Aspen Plus

For the equilibrium-based model, the E_M-profiles were scaled to fit the removal grade for scenario Goal1 in Aspen Plus by adjusting the E_M-factor. From figure 4.44 it is visible that this gave similar temperature profiles as in Aspen HYSYS. Overall the temperature profiles fit the performance temperature better in HYSYS. The best fit to average-temperature profile was for E_M=Zhu*1.015.

For the rate-based model, the IAF was adjusted to give the best fit to removal grade. For scenario Goal1 the best result was achieved with IAF=0.51, which gave a removal grade of 90.11%, performance data is 90.10%. The temperature profile deviated from performance data, but had a similar profile as E_M=Lin*1.074.

6.4.5 Evaluation of scenario F17 with estimated E_M and IAF in Aspen Plus

For the equilibrium-based model, the E_M-profiles were scaled to fit the removal grade for scenario F17 in Aspen Plus by adjusting the E_M-factor. From figure 4.46 it is visible that this gave similar temperature profiles as in Aspen HYSYS, but in Aspen HYSYS the best fit was for E_M=SF2, E_M=SF1 and E_M=Zhu. In Aspen Plus the best fit to performance temperature was for E_M=Lin*0.863. Overall the temperature profiles fit the performance temperature better in HYSYS.

For the rate-based model, the IAF was adjusted up to give the best fit to removal grade. For scenario F17 the best result was achieved with IAF=0.51, which gave a removal grade of 83.48%, performance data is 83.50%. The temperature profile had a similar profile as E_M=Lin*0.863, and had an ok fit to the performance temperature.

The results from these simulation indicates that there is small deviations between the equilibrium-based model in Aspen Plus and Aspen HYSYS. The E_M-profiles can easily be scaled with the E_M-factor to fit the removal grade of any scenario, in both Aspen plus and Aspen HYSYS, but the E_M-profile must be adjusted for the simulation tool.

The rate-based method proved to be able to adjust to removal grade for some scenarios, while other scenario was less adjustable, this is assumed to be because the simulation reaches equilibrium. For the scenarios where the rate-based simulation was able to predict the requested removal grade the temperature profile fit the performance data better, but never as good as the E_M-fitted profiles. Typically the temperature profile lays between the fitted E_M-profiles and the E_M-profile with constant Murphree efficiency of 0.1.

6.5 Evaluation of Comparison between Aspen Plus and HYSYS

6.5.1 Evaluation of Comparison for scenario H14

For equilibrium-based simulation in Aspen Plus and Aspen HYSYS the results were very similar. The average temperature for each E_M-profile was higher for the simulations in Aspen Plus than the simulations in Aspen HYSYS. For scenario H14 the average temperature for E_M=SF1 and E_M=SF2 was 1.3°C higher in Aspen Plus. The temperature were 2.4°C, 2.6°C and 2.9°C for E_M=Zhu, E_M=Lin and E_M=0.1 respectively. The rich loading is almost exactly the same for Aspen Plus and Aspen HYSYS, the small deviations are assumed to be because the removal grade is calculated with E_M-factor of three decimals. If the removal grade was calculated to an accurate 90% for all E_M-profiles the deviations between rich loading in Aspen Plus and Aspen HYSYS is assumed to be 0.0004, because this is the deviation between E_M=Zhu (HYSYS) and E_M=Lin (Plus) which both have an accurate removal grade of 90.00%.

Scenario H14 is one of the scenarios where rate-based couldn't predict accurate removal grade. With highest predicted removal grade =88.82%, the rate-based model predicted rich loading of 0.4894, which is closer to performance data than equilibrium-based model, by 0.0030. The temperature on the other hand, deviates a lot from performance temperature.

For scenario H14 the best fit for temperature profile was E_M=SF1 and E_M=SF2 in HYSYS.

6.5.2 Evaluation of Comparison for scenario 2B5

For scenario 2B5 the temperature deviation between Aspen Plus and Aspen HYSYS less visible than for Scenario H14. For scenario 2B5 the average temperature for E_M=SF1 was 0.07 °C higher in Aspen Plus. The temperature were 0,05°C, 0.2°C, 0.4°C and 1.1°C for E_M=SF2, E_M=Zhu, E_M=Lin and E_M=0.1 respectively. The rich loading is higher in Aspen Plus than in Aspen HYSYS. If the removal grade was calculated to an accurate 87.30% for all E_M-profiles the deviations between rich loading in Aspen Plus and Aspen HYSYS is assumed to be 0.0250, because this is the deviation between E_M =SF1 (HYSYS) and E_M =0.1 (Plus) which both have an accurate removal grade of 87.30%.

Scenario 2B5 is the other scenario where rate-based couldn't predict accurate removal grade. With the highest predicted removal grade =86.14%, the rate-based model predicted rich loading of 0.4857, which is between equilibrium-based model in Aspen HYSYS and Aspen Plus, where Aspen Plus is closest to performance data (0.5000). The temperature profile deviates a lot from performance temperature.

For scenario 2B5 the best fit for temperature profile was E_M=Lin in Plus and HYSYS.

6.5.3 Evaluation of Comparison for scenario 6w

For scenario 6w the average temperature for E_M=SF1, E_M=SF2 and E_M=Zhu was 0.06 °C higher in Aspen Plus. The temperature were 1.1°C higher in Aspen Plus for E_M=0.1 and 0.06 °C lower in Aspen Plus for E_M=Lin. If the removal grade had been calculated to an accurate 79.00% for all E_M-profiles the deviations between rich loading in Aspen Plus and Aspen HYSYS is assumed to be 0.0007, because this is the deviation between E_M=SF2 & E_M =Lin (Plus) and E_M =Lin & E_M =0.1 (HYSYS) which have an removal grade of 79.04 and 79.03%.

For Scenario 6w the rate-based model was able to estimate removal grade to 79.04% and rich loading to be 0.4870. From performance data the rich loading is 0.4600 which is between equilibrium-based (0.4418) and rate-based (0.4870), where Aspen HYSYS is closest to performance data. The temperature profile lays between the fitted E_M-profiles and E_M=0.1

For scenario 6w the best fit for temperature profile was E_M=SF2 and E_M=Lin in Plus.

6.5.4 Evaluation of Comparison for scenario Goal1

For scenario Goal1 the average temperature for E_M=SF1, E_M=SF2 and E_M=Zhu was 1.9 °C higher in Aspen Plus. The temperature were 2.0°C and 2.1°C for E_M=Lin and E_M=0.1 respectively. If the removal grade had been calculated to an accurate 90.10% for all E_M-profiles the deviations between rich loading in Aspen Plus and Aspen HYSYS is assumed to be 0.0004, because this is the deviation between E_M =Lin in Plus and HYSYS.

For Scenario Goal1 the rate-based model was able to estimate removal grade to 90.11% and rich loading to be 0.4870. From performance data the rich loading is 0.5000, all models have very similar values for rich loading but Aspen HYSYS is closest to performance data, followed by equilibrium-based in Aspen Plus, and rate-based last. The rate-base temperature profile lays is very close to E_M=Lin (Plus).

For scenario Goal1 the best fit for temperature profile was E_M=SF1, E_M=SF2 and E_M=Zhu in HYSYS.

6.5.5 Evaluation of Comparison for scenario F17

For scenario F17 the average temperature for each E_M-profile was higher for the simulations in Aspen HYSYS than the simulations in Aspen Plus. The average temperature for E_M=SF1 and E_M=SF2 was 0.6°C higher in Aspen HYSYS. The temperature were 0.5°C, 0.4°C and 0.3°C for E_M=Zhu, E_M=Lin and E_M=0.1 respectively. If the removal grade had been calculated to an accurate 83.50% for all E_M-profiles the deviations between rich loading in Aspen Plus and Aspen HYSYS is assumed to be 0.0500, because this is the deviation between E_M=SF2 (HYSYS) and E_M=0.1 (Plus) which both have an accurate removal grade of 83.50%.

For Scenario F17 the rate-based model was able to estimate removal grade to 83.48% and rich loading to be 0.4836. From performance data the rich loading is 0.4800. For this scenario Aspen Plus rate-based and equilibrium-based model is very similar and closest to performance data, while equilibrium-based in HYSYS is off by 0.0400. The rate-base temperature profile lays is very close to E_M=Lin (HYSYS).

For scenario F17 the best fit for temperature profile was E_M=SF1 and E_M=SF2 in HYSYS.

By the results from these simulation it looks like there is very small deviations between the equilibrium-based model in Aspen Plus and Aspen HYSYS. The temperature profiles seem to have higher average temperatures in Aspen Plus, even though this is not accurate for all E_M-profiles in all scenarios.

The overall best fit for temperature profile have been for equilibrium-based model in Aspen HYSYS, with E_M-profiles E_M=SF1, E_M=SF2 and E_M=Lin. Lin have had the best fit for scenario 2B5 and 6w, but like mentioned earlier, these scenarios have four sets of measurements. And if data set A had been removed the average line is assumed to fit E_M=SF1 and E_M=SF2.

The overall best fit for rich loading have been alternately equally good for equilibrium-based model in Aspen HYSYS and Aspen Plus.

When all factors are added up the best predictions for all parameters where achieved by equilibrium-based model in Aspen HYSYS.

6.6 Evaluation of simulation with default Murphree efficiencies in Aspen HYSYS

The default E_M-profiles predicted by Aspen HYSYS was compared to the estimated E_M-profile, E_M=SF1, for all scenarios. Since the only adjustable variable in these simulations was the number of stages, it was harder to achieve the exact removal grade, compared with estimating the E_M-profile by calculation where the results can be just as accurate as requested depending on the amount of decimals used for the E_M-factor.

6.6.1 Evaluation of scenario H14 with default Murphree efficiencies

For scenario H14 the removal grade from both the default simulation (89.64%) and E_M=SF1 (90.12%) was close to performance data (90.00%). The rich loading was higher for both default (0.0120) and SF1 (0.0130). The best fit for the temperature profile was for E_M=SF1. The only stages where the default is close to performance data is stage 1, 6 and 24.

6.6.2 Evaluation of scenario 2B5 with default Murphree efficiencies

For scenario 2B5 the removal grade from both the default simulation (86.80%) and E_M=SF1 (87.30%) was close to performance data (87.30%). The rich loading was lower for both default (-0.0380) and SF1 (-0.0370). The best fit for the temperature profile was for E_M=SF1. The only stages the default is close to performance data is 6, 7 and 8.

6.6.3 Evaluation of scenario 6w with default Murphree efficiencies

For scenario 6w the removal grade from both the default simulation (79.80%) and E_M=SF1 (79.00%) was close to performance data (79.00%). The rich loading was lower for both default (-0.0150) and SF1 (-0.0170). The best fit for the temperature profile was for E_M=SF1. The only stages the default is near performance data is 8, 9 and 10.

6.6.4 Evaluation of scenario Goal1 with default Murphree efficiencies

For scenario Goal1 the removal grade from both the default simulation (90.39%) and E_M=SF1 (90.10%) was close to performance data (90.10%). The rich loading was lower for both default (-0.0120) and SF1 (-0.0090). The best fit for the temperature profile was for E_M=SF1. The only stages the default is near performance data is 6 and 24.

6.6.5 Evaluation of scenario F17 with default Murphree efficiencies

For scenario F17 the removal grade from both the default simulation (82.80%) and E_M=SF1 (83.51%) was close to performance data (83.50%). The rich loading was lower for both default (-0.0470) and SF1 (-0.0450). The best fit for the temperature profile was for E_M=SF1. The only stages the default is near performance data is 7 and 8.

The trend for the simulation of all scenarios is that the simulated temperature profile with default E_M-profile provides a bad fit to the temperature profile for performance data. The rich loading is very similar for default and estimated efficiency, and the removal grade is easier to adjust correctly with estimated efficiency.

When the default E_M-profile is compared with the estimated E_M-profile, one can see that the estimated profile decreases linearly with varying slope for the different sections in the packed column. While the default efficiency decreases with a polynomial profile for all stages.

The amount of stages required to achieve the requested removal grade seem to increase with the E_M-factor. This is presented below in table 6.1.

Table 6.1: Correolation between E_M-factor and amount of stages

Scenario	**H14**	**Goal1**	**2B5**	**F17**	**6w**
E_M-Factor for SF1	1.000	0.920	0.778	0.671	0.591
stages	14	13	10	8	8

6.7 Evaluation of comparison of different amine packages

The results from the simulations of all scenarios shows that the amine package named Li-Mather always will give a lower removal grade than Kent-Eisenberg, and Acid Gas always will give a higher removal grade than Kent-Eisenberg.

6.7.1 Evaluation of scenario H14 with different amine packages

For scenario H14, L-M gives an average removal grade 0.45% lower than K-E for all simulated E_M's, while A-G gives an average removal grade 1.92% higher than K-E.

For scenario H14, L-M have an average rich loading 0.0013 lower than K-E for all simulated E_M's, while A-G gives an average rich loading 0.0045 higher than K-E.

6.7.2 Evaluation of scenario 2B5 with different amine packages

For scenario 2B5, L-M gives an average removal grade 0.62% lower than K-E for all simulated E_M's, while A-G gives a removal grade 0.59% higher than K-E.

For scenario 2B5, L-M have an average rich loading 0.0019 lower than K-E for all simulated E_M's, while A-G gives an average rich loading 0.0009 higher than K-E.

6.7.3 Evaluation of scenario 6w with different amine packages

For scenario 6w L-M gives an average removal grade 0.39% lower than K-E for all simulated E_M's, while A-G gives an average removal grade 0.49% higher than K-E.

For scenario 6w, L-M have an average rich loading 0.0018 lower than K-E for all simulated E_M's, while A-G gives an average rich loading 0.0006 higher than K-E.

6.7.4 Evaluation of scenario Goal1 with different amine packages

For scenario goal1 L-M gives an average removal grade 0.32% lower than K-E for all simulated E_M's, while A-G gives an average removal grade 1.19% higher than K-E.

For scenario goal1, L-M have an average rich loading 0.0012 lower than K-E for all simulated E_M's, while A-G gives an average rich loading 0.0002 higher than K-E.

6.7.5 Evaluation of scenario F17 with different amine packages

For scenario F17, L-M gives a removal grade 0.59% lower than K-E, while A-G gives a removal grade 0.34% higher than K-E.

For scenario F17, L-M have an average rich loading 0.0016 lower than K-E for all simulated E_M's, while A-G gives an average rich loading 0.0003 higher than K-E.

Overall the average removal grade for Li-Mather is 0.47% lower than Kent-Eisenberg, and Acid-Gas is 0.91% higher than Kent-Eisenberg.

The overall average rich loading is also lowest for Li-Mather, which is 0.0016 lower than Kent-Eisenberg, while Acid-Gas is 0.0013 higher than Kent-Eisenberg.

It is also visible from the graphs in figure 4.63-4.67 that the temperature profiles of Kent-Eisenberg and Li-Mather are very similar while Acid-Gas keeps a temperature of about 2 °C higher than K-E and L-M, but the deviation decreases for the lowest stages where all the amine packages finishes with about the same temperature.

6.8 Comparison between results from this work and results from earlier work

Scenario H14, 2B5, 6w and Goal1 was used in the paper by Øi, Sætre and Hamborg (2018) [34]. From this paper it was found that an equilibrium-based model with E_M=Zhu gave good predictions to Scenario H14 and Goal1, but not for scenario 2B5 and 6w. They found scenario 2B5 and 6w to be well predicted with a linear decreasing E_M-profile with $E_M=0.192$ at top stage and $E_M=0.008$ at bottom stage.

These results are consistent with the results from this report, except that we have a different performance removal grade for scenario H14 and 6w. Øi, Sætre and Hamborg used performance removal grades of 88.50% for both Scenario H14 and 6w. I found the removal grade for scenario H14 to be about 90.00% from Hamborg et al., (2014) [7] and from appendix D in Sætre (2016) [28] I found removal grade for scenario 6w to be 79.00%.

It is naturally that Scenario H14 and Goal1 would fit the same E_M-profile as they have almost the same removal grade of 90.00% and 90.10% respectively. This is consistent with the results from the simulations in this report where the E_M-factor used for the E_M-profiles in scenario Goal1 was close to 1 e.g. small scaling factor, and very similar E_M-profiles for Scenario H14 and Goal1. It is also naturally that 2B5 and 6w would get good predictions with the same E_M-profile if the removal grades for Scenario 2B5 and 6w was 87.30% and 88.50% as these removal grades are fairly close to each other. But this was not the case in this report where the removal grades used for scenario 2B5 and 6w was 87.30% and 79.00%.

From figure 2 in Øi, Sætre and Hamborg, for scenario H14, they got a god temperature profile with the equilibrium-based model in Aspen HYSYS, and an ok temperature profile with the equilibrium-based model in Aspen Plus. The temperature profile achieved with the rate-based model in Aspen Plus deviated from the performance data but the deviation was less than 6 °C. Compared with the results for scenario H14 in this theses, the temperature profiles from the equilibrium-based model in Aspen Plus and Aspen HYSYS was consistent with their results. But the temperature profile from the rate-based model in Aspen Plus did not fit the performance data, and deviated with as much as 11.2 °C. The rate-based simulation in this thesis achieved removal grade closer to performance data than Øi, Sætre and Hamborg, but it reached equilibrium and was not able to achieve performance removal grade

From figure 3 in Øi, Sætre and Hamborg, for scenario 6w, they got a god temperature profile for all simulations. For rate based simulation they used IAF=0.55 to achieve a removal grade of 86.10%. In this thesis the rate-based simulation used IAF=0.29 to achieve a removal grade of 79.00%. When the results are compared the temperature profile for their rate-based model had a better fit to performance data, but not to the removal grade if the correct removal grade is 79.00%.

From figure 4 in Øi, Sætre and Hamborg, for scenario 2B5, they got a god temperature profile for all simulations, and a good fit to removal grade for equilibrium-based simulations in Aspen Plus and Aspen HYSYS. The results from this thesis achieved equally as good temperature profile and removal grade for the equilibrium-based simulations, but the temperature profile for the rate-based simulation deviated from the performance data. The rate-based simulation in this thesis achieved removal grade closer to performance data than Øi, Sætre and Hamborg, but it reached equilibrium and was not able to achieve performance removal grade.

From figure 5 in Øi, Sætre and Hamborg, for scenario Goal1, they got an ok temperature profile for all simulations, but none of them achieved a removal grade close to performance data. For the rate-based simulation Øi et al., used IAF=0.55, and in this thesis the IAF=0.51. In this thesis all of the simulation tools were able to achieve the requested removal grade. The temperature profile from equilibrium-based model in Aspen HYSYS fit well for the performance data. The temperature profile from equilibrium-based model in Aspen Plus was a little too high but had an ok fit, and temperature profile from rate-based model in Aspen Plus was even higher.

With all these results in mind one can conclude that the E_M-factor have been a necessary tool to easily achieve the right removal grade, and might even be easier to estimate than the IAF used in rate-based simulation. The E_M-factor will always increase linearly with the removal grade, but this does not always seem to be the case with the interfacial area factor.

Øi, Sætre and Hamborg concluded that the equilibrium-based and rate-based model perform equally well in both fitting performance data and in predicting performance at changed conditions. With the new developed E_M-factor the equilibrium-based model can predict reliable performance data at changed conditions. From the simulations in this report the equilibrium-based model, with estimated Murphree efficiency and E_M-factor, predicts more reliable performance data than the rate-based model with estimated interfacial area factor. The reason why the equilibrium-based model with estimated E_M-profiles gives a better prediction than rate-based model, is that many parameters can be fitted.

6.9 Further work

The estimated E_M-profiles SF1 and SF2 gave a god fit to the performance data, but there is room for improvement. Several fittings of E_M profiles should be made, based on the method in sub-chapter 3.2.1, to get an even better fit for temperature profile. The new estimated E_M-sets should be tested on several scenarios with different removal grades, with the new developed E_M-factor in sub-chapter 3.2.2.

It would also be interesting to test the calculation for estimating E_M-factor in equation 5.1, on different scenarios, and see if there is connections with experimental data and E_M-factor based on linearity of removal grade.

Another interesting topic might be to use the methods developed in this thesis to estimate a Murphree efficiency profile with another amine package. In this thesis, the removal grade have always been estimated to fit with Kent Eisenberg as amine package. It might be interesting to try to fit the removal grade with the amine packages Li Mather or Acid Gas in Aspen HYSYS, or the equilibrium-based model Electrolyte-NRTL in Aspen Plus, and see if this gives an even better fit with the temperature profile.

It would also be interesting to compare an equilibrium-based model and a rate-based model. Results from this work reveals that there is definitely possibilities to fit parameters in equilibrium-based model. In this work the only parameter that was varied in the rate-based model was the interfacial area factor. In the rate-based tool in Aspen Plus, there are several parameters that may be adjusted. In principle any rate-based parameters could be used as variables to fit performance data, but this may lead to a model with doubtful predictability. One possibility is to divide the absorption column into 2 or 3 sections with different IAF in each section.

The fact that the best fit of E_M-profiles are the ones with decreasing Murphree efficiency from the top stage to the bottom stage indicates that the simulation is approaching equilibrium. The temperature profile flattens out on the lowest stages, and the E_M-profile produces a temperature profile that fits the performance data better, when the Murphree efficiencies are close to zero on the lowest stages. It would be interesting to do the simulations with an 18 m packing height and see if the results is consistent with the results from the simulation with 24 m.

It would also be interesting to simulate the entire process with both the absorption and the desorption column.

7 Conclusion

The CO_2 capture from exhaust gas is an important topic to limit man-made greenhouse gas emissions. One mature method to capture CO_2 is to absorb it in an aqueous amine solution. An important step in the research to improve the technology is to create simulation tools that is able to predict the performance of the absorber. There have been developed many calculation models for process simulation, Aspen HYSYS and Aspen Plus are common tools for simulating the capture of CO_2 in to amine solutions.

In this thesis the amine based CO_2 capture process at TCM where CO_2 from flue gas is absorbed into 30wt% MEA solution, have been simulated in Aspen HYSYS and Aspen Plus. The main purpose of the simulation have been to fit the removal grade, temperature profile and rich loading to the performance data. The performance data used in this paper is five different scenarios obtained from test-campaigns at TCM in 2013 and 2015. These scenarios have been simulated in earlier master theses from USN, and some of the results are verified in this thesis.

The rate-based model in Aspen Plus and the equilibrium-based model in Aspen Plus and Aspen HYSYS have been compared. The conclusion is that the equilibrium-based model is easier to adjust to fit the requested parameters. The equilibrium-based model predicts sufficient results in both Aspen HYSYS and Aspen Plus, but the results from this thesis proved that the most reliable predictions was achieved in Aspen HYSYS. The result might have been the opposite if the E_M-profile was created for the equilibrium-based model in Aspen Plus, and scaled with an E_M-factor to fit the removal grade in Aspen HYSYS.

An E_M-factor was developed in this thesis, this factor made it possible to achieve the requested removal grade, with an accuracy depending on the amount of decimals used in the E_M-factor. Two methods of estimating the E_M-factor have been proposed. The first is a try and fail method that can be combined with e.g. the bisection-method to converge towards the right answer. The second method is to estimate the E_M-factor based on experimental data. Assuming there is some linearity between the gas/amine-ratio and the deviation from the linearity of E_M-factor and removal grade. By the linear interpolation equations in chapter 5 the required E_M-factor to achieve the requested removal grade can be calculated. With the interfacial area factor, used to estimate the removal grade in the rate-based model, the calibration is less predictable, because the factor does not always seem to be linear with the result.

Some earlier papers have stated that the equilibrium-based model and the rate-based model perform equally well in fitting performance data and in predicting performance at changed conditions. Some state that the rate-based model is more reliable than the equilibrium-based model. From the results in this thesis the equilibrium-based model have proven to predict reliable results, and can easily be adjusted to predict reliable results even when the conditions are changed.

The results from this study show that it is possible to fit a rate-based model by adjusting the interfacial area factor, and to fit an equilibrium-based model by adjusting the Murphree efficiency for each stage. In this work the equilibrium and rate-based models both predicts reliable results for removal grade and rich loading, but the equilibrium-based model provides more reliable results than the rate-based model in predicting temperature profile. Which is natural as many parameters have been estimated. In addition, with the new developed E_M-factor the equilibrium-based model is able to predict reliable performance at changed conditions.

References

[1] **Contribution of Working Group III to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change.** *AR5 Climate Change 2014: Mitigation of Climate Change.* s.l. : IPCC, 2014.

[2] **NOAA.** NASA Global Climate Change. [Online] April 29, 2019. [Cited: April 30, 2019.] https://climate.nasa.gov/vital-signs/carbon-dioxide/.

[3] **Metz B, Davidson O, de Coninck H. C., Loos M, and Meyer L. A.** *IPCC Special Report on Carbon Dioxide Capture and Storage.* s.l. : Intergovernal Panel on Climate Change, 2005.

[4] **CCSA.** What is CCS? [Online] Carbon Capture & Storage Assosiation, 01 25, 2019. http://www.ccsassociation.org/what-is-ccs/capture/.

[5] **Leung Dennis Y.C., Caramanna Giorgio , M. Mercedes Maroto-Valer.** *An overview of current status of carbon dioxide capture and storage technologies.* s.l. : Renewable and Sustainable Energy Reviews, V39:426-443, 2014.

[6] **Global CCS Institute.** *Fact sheet: Transporting CO2.* 2015.

[7] **Hamborg E.S, V Smith, T Cents, N Brigman, O Falk-Pedersen, T De Cazenove, Milan Chhaganlal, Jane K. Feste, Øyvind Ullestad, Helge Ulvatn, Oddvar Gorset, Inga Askestad, L. K. Gram, B. F. Fostås, M. I. Shah, A. Maxson, D. Thimsen.** *Results from MEA testing at the CO2 Technology Centre Mongstad, Part II: Verification of baseline results.* s.l. : Energy Procedia 63:5994 – 6011, 2014.

[8] **Thimsen, D.Maxson, A. Smith,V. Cents,T. Falk-Pedersen,O. Gorset,O. HamborgE.S.** *Results from MEA testing at the CO2 Technology.* s.l. : Energy Procedia;, 2014.

[9] **Øi, Lars Erik.** *Removal of CO2 from exhaust gas.* Porsgrunn : Faculty of Technology, Telemark University College, PhD, 2012.

[10] **Desvignes, Coarlie.** *Simulation of Post-combustion CO2 capture process with amines at CO2 Technology Centre Mongstad.* s.l. : Lyon CPE, Master Thesis, 2015.

[11] **Luis, Petricia.** *Use of monoethanolamine (MEA) for CO2 capture in a global scenario.* s.l. : Desalination 380:93–99, 2016.

[12] **Øi, Lars Erik.** *Aspen HYSYS Simulation of CO2 Removal by Amine Absorption from Gas Based Power Plant.* Gøteborg : SIMS2007 Conference, 2007.

[13] **Tobiesen, Finn A. Svendsen, Hallvard F. Juliussen, Olav.** *Experimental validation of a rigorous absorber model for CO2 postcombustion capture.* s.l. : AIChE Journal, Vol 53(4) pp. 846-865, 2007.

[14] **Kvamsdal, Hanne M. Rochelle, Gary T.** *Effects of the Temperature Bulge in CO2 Absorption from Flue Gas by Aqueous Monoethanolamine.* s.l. : Industrial & Engineering Chemistry Research, Vol 47(3), pp 867-875, 2008.

[15] **Luo, X, J.N. Knudsen, D. de Montigny, Sanpasertparnich T. , R. Idem, D. Gelowitz, R. Notz, S. Hoch, H. Hasse, E. Lemaire, P. Alix, F.A. Tobiesen, O. Juliussen, M. Köpcke, H.F. Svendsen.** *Comparison and validation of simulation codes against sixteen sets.* s.l. : Energy Procedia Vol 1, pp. 1249-1256, 2009.

[16] **Hansen, Espen.** *Comparison of Process simulation programs for CO2 removal.* Porsgrunn : Faculty of Technology, Telemark University College, Master Thesis, 2011.

[17] **Bergstrøm, Jostein Tvete.** *Equilibrium based and rate-based simulation of CO2 absorption in monoethanolamine.* Porsgrunn : Faculty of Technology, Telemark University College, Master Thesis, 2012.

[18] **Øi, Lars Erik.** *Comparison of Aspen HYSYS and Aspen Plus simulation of CO2 absorption into MEA from Atmospheric Gas.* s.l. : Energy Procedia, Vol 23, pp. 360-369, 2012.

[19] **Ying Zhang, Chau-Chyun Chen.** *Modeling CO2 absorption and desorption by aqueous monoethanolamine solution with Aspen rate-based model.* s.l. : Energy Procedia, Vol 37, pp. 1584-1596, 2013.

[20] **Kvam, S. H. P.** *Vapor recompression in absorption and desorption process for CO2 capture.* Porsgrunn : Faculty of Technology, Telemark University College, Master Thesis, 2013.

[21] **Birkelund, Even Solnes.** *CO2 Absorption and Desorption Simulation with Aspen HYSYS.* Tromsø : Faculty of Science and Technology Department of Engineering and Safety, University of Tromsø, Masters Thesis, 2013.

[22] **Øi, L.E. Bråthen,T. Berg,C. Brekne,S.K. Flatin,M. Johansen,R. Moen,I.G. Thomassen,E.** *Optimization of configurations for amine based CO2 absorption.* s.l. : Energy Procedia, Vol 51, pp. 224-233, 2014.

[23] **Øi, L.E. Kvam, S.H.P.** *Comparison of energy consumption for different CO2 absorption.* s.l. : Energy Procedia, vol 63, pp. 1186-1195, 2014.

[24] **Larsen, Inga M. Strømmen.** *Simulation and validation of CO2 mass transfer processes in aqueous MES solution with Aspen Plus at CO2 Technology Centre Mongstad.* Porsgrunn : Faculty of Technology, Telemark University College, Masters Thesis, 2014.

[25] **Hamborg E. S., I. M. S. Larsen, M. Shah, T. D. Cazenove, N. Brigman, T. Cents, et al.,.** *Simulations and Validations of CO2 mass transfer processes in aqueous monoethanolamine solutions with Aspen Plus at CO2 Technology Centre Mongstad.* Canada : Presented at the 3rd Post Combustion Capture Conference (PCCC3), 2015.

[26] **Aromada, Solomon Aforkoghene. Øi, Lars Erik.** *Simulation of Improved Absorption Configurations for CO2.* s.l. : Linköping University Electronic Press, Linköpings universitet, 2015.

[27] **Zhu, Ye.** *Simulation of CO2 capture at Mongstad using Aspen HYSYS.* Porsgrunn : Faculty of Technology, Telemark University College, Masters Thesis, 2015.

[28] **Sætre, Kai Arne.** *Evaluation of process simulation tools at TCM.* Porsgrunn : Faculty of Technology, University College of Southeastern Norway, Master Thesis, 2016.

[29] **Pouladi, B. Hassankiadeh, M.N. Behroozshad, F.** *Dynamic simulation and optimization of an industrial-scale absorption tower for CO2 capturing from ethane gas.* s.l. : Energy Reports, Vol 2, pp. 54-61, 2015.

[30] **Garcia, M. Knuutila, H.K. Gu, S.** *ASPEN PLUS simulation model for CO2 removal with MEA: Validation of desorption model with experimental data.* s.l. : Journal of Environmental Chemical Engineering, Vol 5, pp. 4693-4701, 2017.

[31] **Rehan, M. Rahmanian,N. Hyatt,X. Peletiri, S.P. Nizami, A-S.** *Energy Savings in CO2 Capture System through intercooling Mechanism.* s.l. : Energy Procedia, Vol 142, pp. 3683-3688, 2017.

[32] **Faramarzi, L. Thimsen,D. Hume,S. Maxon,A. Wattson,G. Pedersen,S. Gjernes,E. Fostås,B.F. Lombardo,G. Cents,T. Morken,A.K. Shah,M.I. T.de Cazenove, Hamborg,E.S.** *Results from MEA testing at the CO2 Technology Centre Mongstad: Verification of baseline results in 2015.* s.l. : Energy Procedia 114:1128 – 1145, 2017.

[33] **Røsvik, Ole.** *Process simulation of CO2 capture at Mongstad.* Porsgrunn : Faculty of Technology, University College of Southeastern Norway, Master Thesis, 2018.

[34] **Øi, L.E. Sætre,K.A. Hamborg,E.S.** *Comparison of Simulation Tools to Fit and Predict Performance Data of CO2 Absorption into Monoethanol Amine at.* Oslo : Proceedings of The 59th Conference on Simulation and Modelling (SIMS 59), 2018.

[35] **Tomcej, R.A. Otto,F.D. Ranwala,H.A. Morrell,B.R.** *Tray design for selective absorption.* Norman, Oklahoma : Gas Conditioning Conference, 1987.

[36] **Rangwala, H.A. Morrell,B.R. Mather,A.E. Otto,F.D.** *Absorption of CO2 into Aqueous Tertiary Amine/MEA Solutions.* s.l. : The Canadian Journal of Chemical Engineering, Vol 70, pp. 482-490, 1992.

[37] **Murphree, E. V.** *Rectifying Column Calculations – With Particular Reference to N Component Mixtures.* s.l. : Industrial & Engineering Chemistry, Vol 17, pp. 747-750, 1925.

[38] **NOAA.** Trends in Atmospheric Carbon Dioxide. [Online] December 2018. [Cited: January 25, 2019.] https://www.esrl.noaa.gov/gmd/ccgg/trends/full.html.

List of tables and figures

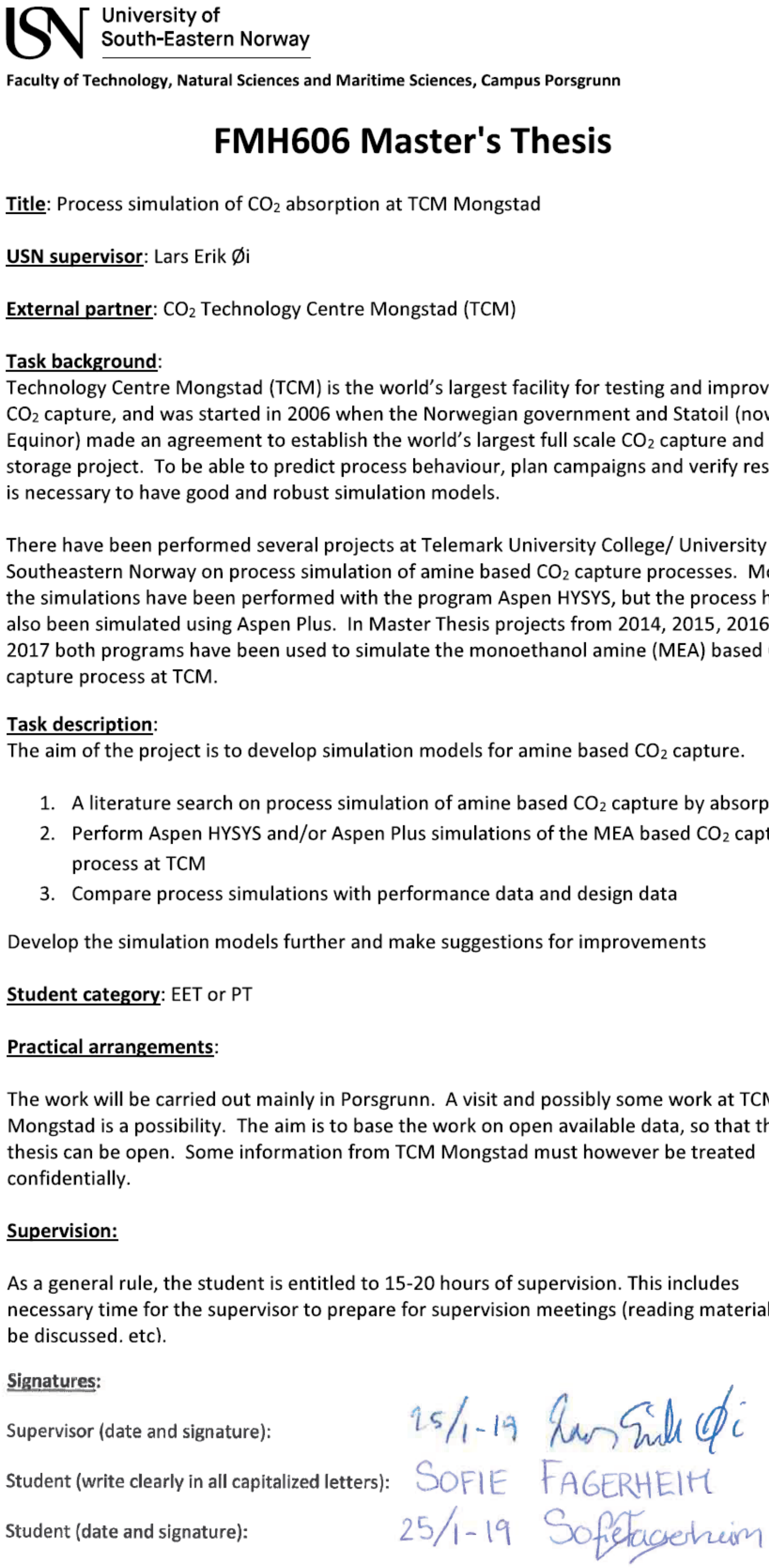
Figure Index:

Table Index:

Appendices

Appendix A – Task description
Appendix B – TCM data for scenario H14
Appendix C – TCM data for scenario 2B5
Appendix D – TCM data for scenario 6w
Appendix E – TCM data for scenario Goal1
Appendix F – TCM data for scenario F17
Appendix G – Data from verification (HYSYS)
Appendix H – Data from verification (Plus)
Appendix I – Data from simulation with estimated E_M (HYSYS)
Appendix J – Data from simulation with estimated E_M (Plus)
Appendix K – Data from comparison of Aspen HYSYS and Aspen Plus
Appendix L – Data from simulation with default E_M (HYSYS)
Appendix M – Data from simulation with different Amine Packages (HYSYS)

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 at TCM Mongstad

USN supervisor: Lars Erik Øi

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 was 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, plan campaigns and verify results it is necessary to have good and robust simulation models.

There have been performed several projects at Telemark University College/ University of Southeastern 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 Master Thesis projects from 2014, 2015, 2016 and 2017 both programs have been used to simulate the monoethanol amine (MEA) based CO_2 capture process at TCM.

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 amine based CO_2 capture by absorption
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

Develop the simulation models further and make suggestions for improvements

Student category: EET or PT

Practical arrangements:

The work will be carried out mainly in Porsgrunn. A visit and possibly some work at TCM Mongstad is a possibility. The aim is to base the work on open available data, so that the thesis can be open. Some information from TCM Mongstad 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).

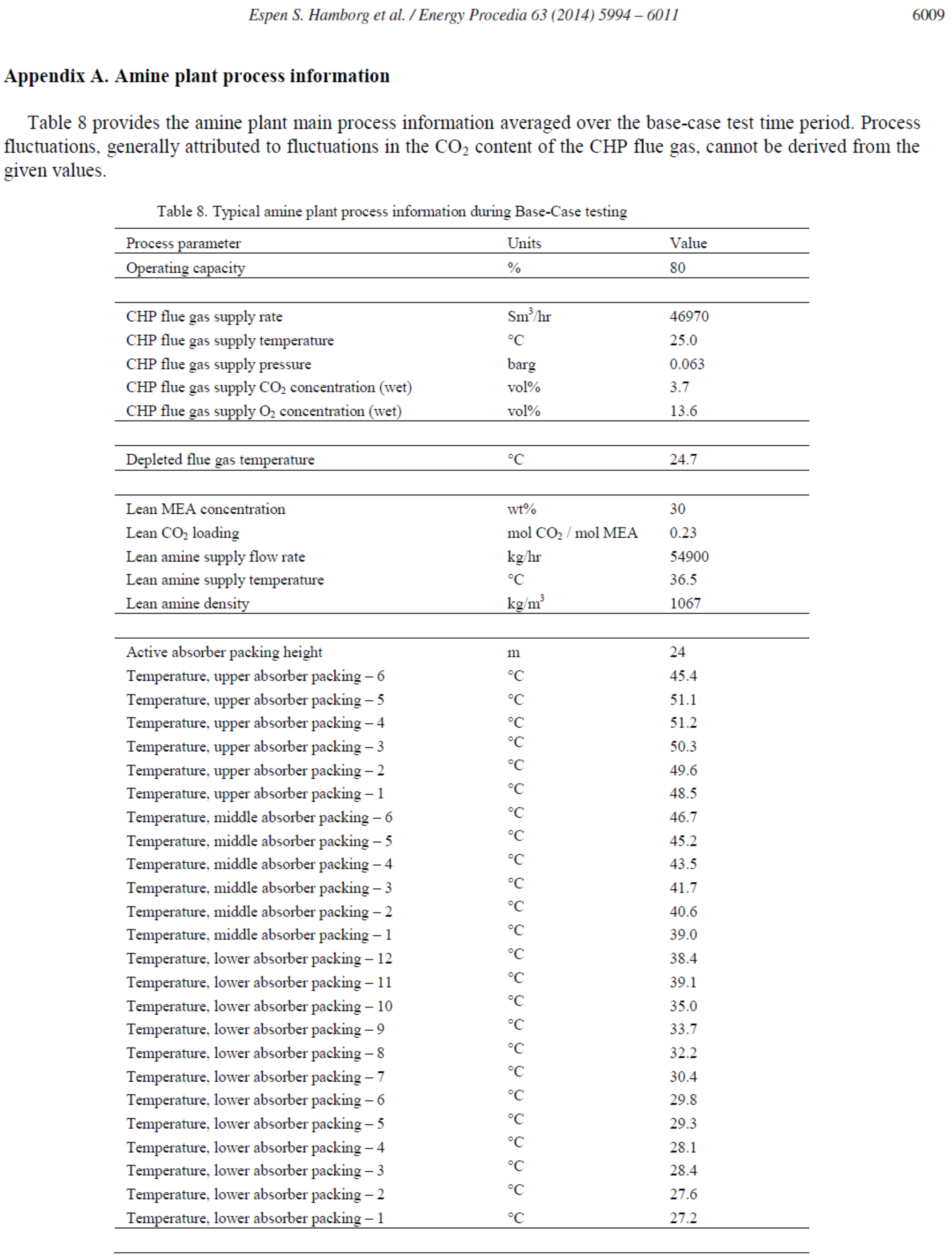
Signatures:

Supervisor (date and signature): 25/1-19 Lars Erik Øi

Student (write clearly in all capitalized letters): SOFIE FAGERHEIM

Student (date and signature): 25/1-19 Sofie Fagerheim

Appendix B – TCM data for scenario H14



Appendix A. Amine plant process information

Table 8 provides the amine plant main process information averaged over the base-case test time period. Process fluctuations, generally attributed to fluctuations in the CO_2 content of the CHP flue gas, cannot be derived from the given values.

Table 8. Typical amine plant process information during Base-Case testing

Process parameter	Units	Value
Operating capacity	%	80
CHP flue gas supply rate	Sm^3/hr	46970
CHP flue gas supply temperature	°C	25.0
CHP flue gas supply pressure	barg	0.063
CHP flue gas supply CO_2 concentration (wet)	vol%	3.7
CHP flue gas supply O_2 concentration (wet)	vol%	13.6
Depleted flue gas temperature	°C	24.7
Lean MEA concentration	wt%	30
Lean CO_2 loading	mol CO_2 / mol MEA	0.23
Lean amine supply flow rate	kg/hr	54900
Lean amine supply temperature	°C	36.5
Lean amine density	kg/m^3	1067
Active absorber packing height	m	24
Temperature, upper absorber packing – 6	°C	45.4
Temperature, upper absorber packing – 5	°C	51.1
Temperature, upper absorber packing – 4	°C	51.2
Temperature, upper absorber packing – 3	°C	50.3
Temperature, upper absorber packing – 2	°C	49.6
Temperature, upper absorber packing – 1	°C	48.5
Temperature, middle absorber packing – 6	°C	46.7
Temperature, middle absorber packing – 5	°C	45.2
Temperature, middle absorber packing – 4	°C	43.5
Temperature, middle absorber packing – 3	°C	41.7
Temperature, middle absorber packing – 2	°C	40.6
Temperature, middle absorber packing – 1	°C	39.0
Temperature, lower absorber packing – 12	°C	38.4
Temperature, lower absorber packing – 11	°C	39.1
Temperature, lower absorber packing – 10	°C	35.0
Temperature, lower absorber packing – 9	°C	33.7
Temperature, lower absorber packing – 8	°C	32.2
Temperature, lower absorber packing – 7	°C	30.4
Temperature, lower absorber packing – 6	°C	29.8
Temperature, lower absorber packing – 5	°C	29.3
Temperature, lower absorber packing – 4	°C	28.1
Temperature, lower absorber packing – 3	°C	28.4
Temperature, lower absorber packing – 2	°C	27.6
Temperature, lower absorber packing – 1	°C	27.2

Rich solution return temperature	°C	27.7

Temperature above upper absorber packing	°C	38.1
Wash water 1 supply flow rate	kg/hr	55000
Wash water 1 inlet temperature	°C	28.4
Wash water 1 withdrawal temperature	°C	43.9

Temperature above Wash Water 1	°C	36.2
Wash water 2 supply flow rate	kg/hr	62000
Wash water 2 inlet temperature	°C	23.5
Wash water 2 withdrawal temperature	°C	35.0
Temperature above Wash Water 2	°C	24.7

Rich CO_2 loading	mol CO_2 / mol MEA	0.48
Rich solution supply flow rate	kg/hr	57200
Rich solution supply temperature	°C	108.6
Lean solution return temperature	°C	119.1
Rich amine density	kg/m^3	1114

Reboiler steam flow rate	kg/hr	4800
Reboiler steam temperature	°C	169
Reboiler steam pressure	barg	4.42
Reboiler condensate temperature	°C	118.8
Reboiler condensate pressure	barg	4.11

Stripper overhead pressure	barg	0.90
Stripper overhead temperature	°C	99.8

Stripper overhead reflux flow rate	kg/hr	1370
Stripper overhead reflux temperature	°C	23.3

Stripper sump temperature	°C	119.3
Reboiler solution temperature	°C	122.3

Lean vapour compressor system	-	off

Product CO_2 flow rate	kg/hr	2670
Product CO_2 discharge temperature	°C	17.7
Product CO_2 discharge pressure	barg	0.023

Appendix C – TCM data for scenario 2B5

This data is provided to USN from TCM for scenario 2B5, the data table below is collected from appendix J in Sætre, 2016 [28].

TCM DATA for Scenario 2B5

Unit

Flue gas composition / absorber inlet	CO2	mol%	0,0357
	H2O	mol%	0,0370
	O2	mol%	0,1460
	N2	mol%	0,7720
	Ar	mol%	0,0090
Flue gas inlet flow	Sm3/h		46981,61
	mol/h		1986,40
Flue gas inlet temperature	°C		28,20
Flue gas inlet pressure	kPa		106,30
Lean solvent flowrate	kg/h		49485,00
Lean solvent loading	mol/mol		0,20
Lean solven temperature	°C		36,80
MEA wt% (lean, CO2 free)	wt%		31,60
Rich solvent flowrate	kg/h		52064,00
Rich solvent loading	mol/mol		0,50
Rich solvent temperature	°C		32,20
CO2 recovery	%		**87,20**

Loading profile

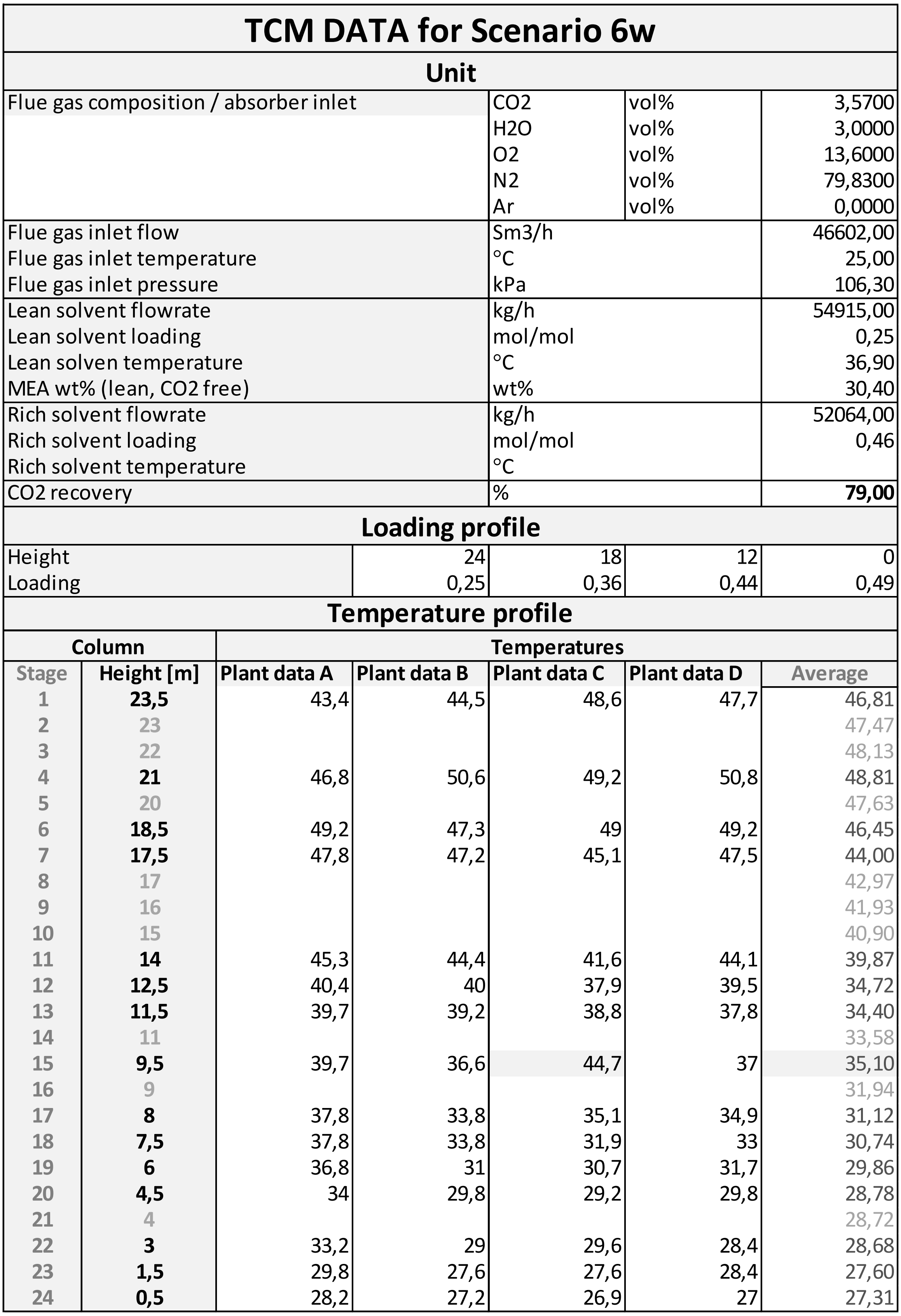
Height	24	18	12	0
Loading	0,2			0,5

Temperature profile

Column		Temperatures				
Stage	Height [m]	Plant data A	Plant data B	Plant data C	Plant data D	Average
1	**23,5**	44,93	45,71	49,28	48,47	47,10
2	23					48,44
3	22					49,79
4	**21**	0,00	51,44	50,16	51,81	51,14
5	20					50,36
6	**18,5**	49,90	48,28	49,89	50,28	49,59
7	**17,5**	48,74	48,51	45,81	48,62	47,92
8	17					47,24
9	16					46,56
10	15					45,88
11	**14**	46,48	45,94	42,80	45,58	45,20
12	**12,5**	42,15	41,68	39,51	41,18	41,13
13	**11,5**	42,41	41,80	40,54	38,68	40,86
14	11					39,94
15	**9,5**	43,10	39,04	47,11	37,56	41,70
16	9					38,20
17	**8**	41,54	35,96	35,64	35,98	37,28
18	**7,5**	41,55	37,47	33,93	34,21	36,79
19	**6**	40,53	34,40	33,41	33,38	35,43
20	**4,5**	37,74	33,37	31,82	32,45	33,84
21	4					33,56
22	**3**	37,06	32,49	32,04	31,49	33,27
23	**1,5**	33,39	31,12	31,03	31,37	31,73
24	**0,5**	31,84	30,92	30,56	30,65	30,99

Appendix D – TCM data for scenario 6w

This data is provided to USN from TCM for scenario 6w, the data table below is collected from appendix D in Sætre, 2016 [28].



TCM DATA for Scenario 6w

Unit

Flue gas composition / absorber inlet	CO2	vol%	3,5700
	H2O	vol%	3,0000
	O2	vol%	13,6000
	N2	vol%	79,8300
	Ar	vol%	0,0000
Flue gas inlet flow	Sm3/h		46602,00
Flue gas inlet temperature	°C		25,00
Flue gas inlet pressure	kPa		106,30
Lean solvent flowrate	kg/h		54915,00
Lean solvent loading	mol/mol		0,25
Lean solven temperature	°C		36,90
MEA wt% (lean, CO2 free)	wt%		30,40
Rich solvent flowrate	kg/h		52064,00
Rich solvent loading	mol/mol		0,46
Rich solvent temperature	°C		
CO2 recovery	%		**79,00**

Loading profile

Height	24	18	12	0
Loading	0,25	0,36	0,44	0,49

Temperature profile

Column		Temperatures				
Stage	Height [m]	Plant data A	Plant data B	Plant data C	Plant data D	Average
1	**23,5**	43,4	44,5	48,6	47,7	46,81
2	23					47,47
3	22					48,13
4	**21**	46,8	50,6	49,2	50,8	48,81
5	20					47,63
6	**18,5**	49,2	47,3	49	49,2	46,45
7	**17,5**	47,8	47,2	45,1	47,5	44,00
8	17					42,97
9	16					41,93
10	15					40,90
11	**14**	45,3	44,4	41,6	44,1	39,87
12	**12,5**	40,4	40	37,9	39,5	34,72
13	**11,5**	39,7	39,2	38,8	37,8	34,40
14	11					33,58
15	**9,5**	39,7	36,6	44,7	37	35,10
16	9					31,94
17	**8**	37,8	33,8	35,1	34,9	31,12
18	**7,5**	37,8	33,8	31,9	33	30,74
19	**6**	36,8	31	30,7	31,7	29,86
20	**4,5**	34	29,8	29,2	29,8	28,78
21	4					28,72
22	**3**	33,2	29	29,6	28,4	28,68
23	**1,5**	29,8	27,6	27,6	28,4	27,60
24	**0,5**	28,2	27,2	26,9	27	27,31

Appendix E – TCM data for scenario Goal1

This data is provided to USN from TCM for scenario Goal1, the data table below is collected from appendix K in Sætre, 2016 [28].

TCM DATA for Scenario Goal1

Unit

Flue gas composition / absorber inlet	CO2	mol%	0,0362
	H2O	mol%	0,0310
	O2	mol%	0,1430
	N2	mol%	0,7810
	Ar	mol%	0,0090
Flue gas inlet flow	Sm3/h		46868,00
Flue gas inlet temperature	°C		25,00
Flue gas inlet pressure	kPa		106,30
Lean solvent flowrate	kg/h		44391,00
Lean solvent loading	mol/mol		0,20
Lean solven temperature	°C		36,50
MEA wt% (lean, CO2 free)	wt%		32,40
Rich solvent flowrate	kg/h		47502,00
Rich solvent loading	mol/mol		0,50
Rich solvent temperature	°C		28,60
CO2 recovery	%		**90,10**

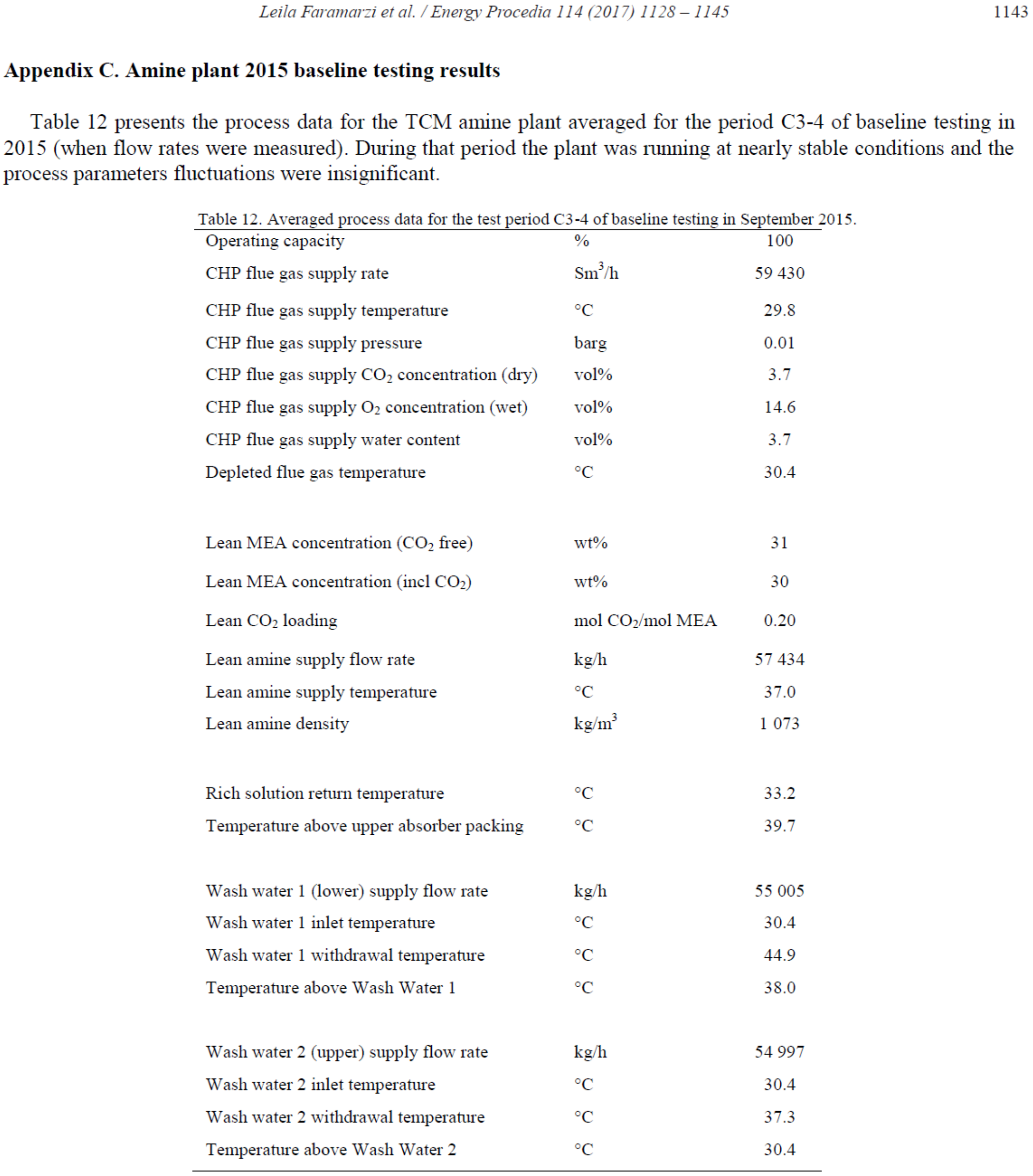
Loading profile

Height	24	18	12	0
Loading	0,2			0,5

Temperature profile

Column		Temperatures				
Stage	Height [m]	Plant data A	Plant data B	Plant data C	Plant data D	Average
1	**23,5**	45,66	46,50	47,79	47,28	46,81
2	23					47,47
3	22					48,13
4	**21**	0,00	49,46	47,20	49,77	48,81
5	20					47,63
6	**18,5**	47,01	44,30	47,01	47,50	46,45
7	**17,5**	45,12	44,93	40,81	45,15	44,00
8	17					42,97
9	16					41,93
10	15					40,90
11	**14**	41,49	40,85	36,49	40,63	39,87
12	**12,5**	35,63	35,26	33,06	34,94	34,72
13	**11,5**	35,28	35,02	34,36	32,94	34,40
14	11					33,58
15	**9,5**	35,58	32,62	40,42	31,79	35,10
16	9					31,94
17	**8**	33,97	30,13	30,06	30,34	31,12
18	**7,5**	34,11	30,89	28,86	29,11	30,74
19	**6**	33,52	28,96	28,42	28,54	29,86
20	**4,5**	31,31	28,37	27,58	27,88	28,78
21	4					28,72
22	**3**	30,80	0,00	27,78	27,46	28,68
23	**1,5**	28,58	27,19	27,24	27,39	27,60
24	**0,5**	28,02	27,23	26,94	27,03	27,31

Appendix F – TCM data for scenario F17



Leila Faramarzi et al. / Energy Procedia 114 (2017) 1128 – 1145 1143

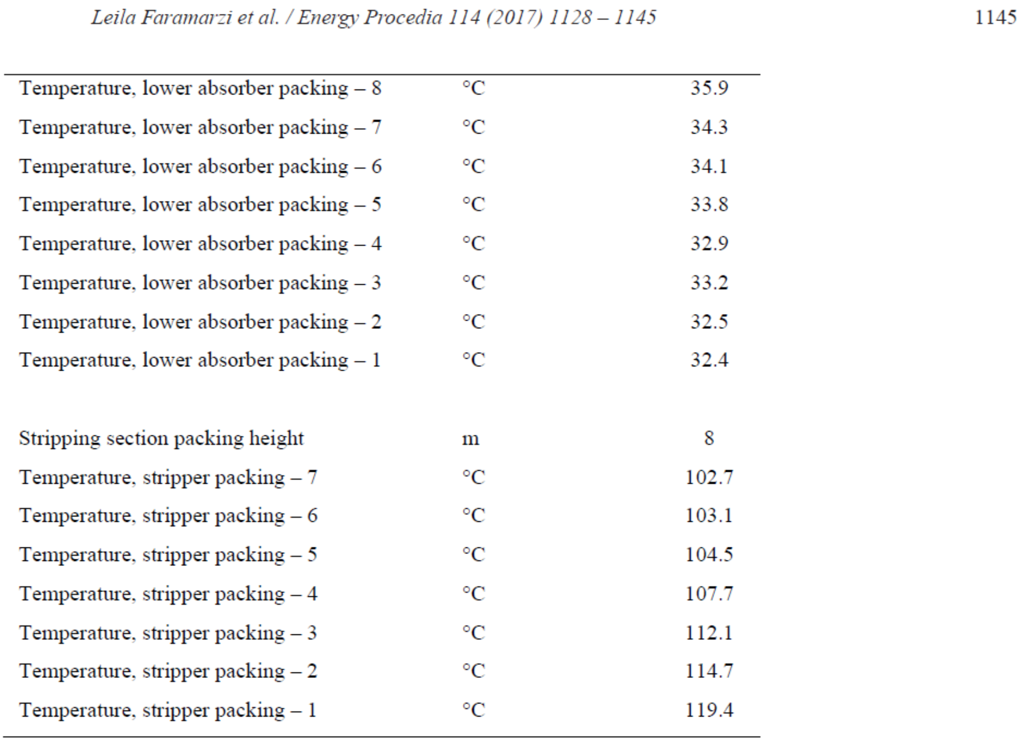
Appendix C. Amine plant 2015 baseline testing results

Table 12 presents the process data for the TCM amine plant averaged for the period C3-4 of baseline testing in 2015 (when flow rates were measured). During that period the plant was running at nearly stable conditions and the process parameters fluctuations were insignificant.

Table 12. Averaged process data for the test period C3-4 of baseline testing in September 2015.

Operating capacity	%	100
CHP flue gas supply rate	Sm^3/h	59 430
CHP flue gas supply temperature	°C	29.8
CHP flue gas supply pressure	barg	0.01
CHP flue gas supply CO_2 concentration (dry)	vol%	3.7
CHP flue gas supply O_2 concentration (wet)	vol%	14.6
CHP flue gas supply water content	vol%	3.7
Depleted flue gas temperature	°C	30.4
Lean MEA concentration (CO_2 free)	wt%	31
Lean MEA concentration (incl CO_2)	wt%	30
Lean CO_2 loading	mol CO_2/mol MEA	0.20
Lean amine supply flow rate	kg/h	57 434
Lean amine supply temperature	°C	37.0
Lean amine density	kg/m^3	1 073
Rich solution return temperature	°C	33.2
Temperature above upper absorber packing	°C	39.7
Wash water 1 (lower) supply flow rate	kg/h	55 005
Wash water 1 inlet temperature	°C	30.4
Wash water 1 withdrawal temperature	°C	44.9
Temperature above Wash Water 1	°C	38.0
Wash water 2 (upper) supply flow rate	kg/h	54 997
Wash water 2 inlet temperature	°C	30.4
Wash water 2 withdrawal temperature	°C	37.3
Temperature above Wash Water 2	°C	30.4

Rich CO_2 loading	mol CO_2/mol MEA	0.48
Rich solution supply flow rate	kg/h	60 775
Rich solution supply temperature	°C	110.7
Lean solution return temperature	°C	121.3
Rich amine density	kg/m^3	1 125
Reboiler steam flow rate	kg/h	5 398
Reboiler steam temperature	°C	156
Reboiler steam pressure	barg	2.04
Reboiler condensate temperature	°C	132.8
Reboiler condensate pressure	barg	1.96
Stripper overhead pressure	barg	0.91
Stripper overhead temperature	°C	96.1
Stripper overhead reflux flow rate	kg/h	1 227
Stripper overhead reflux temperature	°C	17.64
Stripper sump temperature	°C	121.0
Reboiler solution temperature	°C	125.1
Lean vapour compressor system	-	off
Product CO_2 flow rate	kg/h	3 325
Product CO_2 discharge temperature	°C	17.9
Product CO_2 discharge pressure	barg	0.017
Product CO_2 water content	vol%	1.3
Active absorber packing height	m	24
Temperature, upper absorber packing – 6	°C	47.4
Temperature, upper absorber packing – 5	°C	51.7
Temperature, upper absorber packing – 4	°C	51.6
Temperature, upper absorber packing – 3	°C	50.5
Temperature, upper absorber packing – 2	°C	49.9
Temperature, upper absorber packing – 1	°C	48.9
Temperature, middle absorber packing – 6	°C	47.2
Temperature, middle absorber packing – 5	°C	46.0
Temperature, middle absorber packing – 4	°C	44.4
Temperature, middle absorber packing – 3	°C	43.1
Temperature, middle absorber packing – 2	°C	42.2
Temperature, middle absorber packing – 1	°C	40.9
Temperature, lower absorber packing – 12	°C	40.6
Temperature, lower absorber packing – 11	°C	41.6
Temperature, lower absorber packing – 10	°C	37.4
Temperature, lower absorber packing – 9	°C	37.1



Leila Faramarzi et al. / Energy Procedia 114 (2017) 1128 – 1145 1145

Temperature, lower absorber packing – 8	°C	35.9
Temperature, lower absorber packing – 7	°C	34.3
Temperature, lower absorber packing – 6	°C	34.1
Temperature, lower absorber packing – 5	°C	33.8
Temperature, lower absorber packing – 4	°C	32.9
Temperature, lower absorber packing – 3	°C	33.2
Temperature, lower absorber packing – 2	°C	32.5
Temperature, lower absorber packing – 1	°C	32.4
Stripping section packing height	m	8
Temperature, stripper packing – 7	°C	102.7
Temperature, stripper packing – 6	°C	103.1
Temperature, stripper packing – 5	°C	104.5
Temperature, stripper packing – 4	°C	107.7
Temperature, stripper packing – 3	°C	112.1
Temperature, stripper packing – 2	°C	114.7
Temperature, stripper packing – 1	°C	119.4

Appendix G – Data from verification (HYSYS)

Scenario H14

Stage	EM	Temperature				
		Scenario H14	Zhu (2015)	Sætre (2016)	Røsvik (2018)	Fagerheim (2019)
Removal grade		90%	89.4%	89.3%	89.3%	88.42%
Rich loading		0.48	0.487	0.478	-	0.4885
1	0.100	45,4	44,29	46,6	44,52	45,20
2	0.100	51,1	47,45	50	47,72	48,50
3	0.100	51,2	48,58	51	48,82	49,56
4	0.100	50,3	48,92	51,2	49,1	49,79
5	0.100	49,6	48,93	51,1	49,07	49,70
6	0.100	48,5	48,81	50,9	48,89	49,48
7	0.100	46,7	48,62	50,6	48,64	49,19
8	0.100	45,2	48,38	50,3	48,32	48,85
9	0.100	43,5	48,09	49,9	48	48,46
10	0.100	41,7	47,75	49,5	47,68	48,03
11	0.100	40,6	47,37	49	47,31	47,54
12	0.100	39	46,92	48,5	46,86	46,98
13	0.100	38,4	46,42	47,9	46,3	46,36
14	0.100	39,1	45,84	47,3	45,6	45,65
15	0.100	35	45,19	46,5	44,81	44,84
16	0.100	33,7	44,41	45,6	43,94	43,93
17	0.100	32,2	43,5	44,6	42,77	42,88
18	0.100	30,4	42,44	43,5	41,47	41,69
19	0.100	29,8	41,21	42,1	40,13	40,32
20	0.100	29,3	39,79	40,5	38,73	38,71
21	0.100	28,1	38,06	38,6	37,1	36,86
22	0.100	28,4	35,97	36,4	35,13	34,71
23	0.100	27,6	33,41	33,7	32,72	32,26
24	0.100	27,2	30,26	30,4	29,84	29,48

Table G.1: Temperature profiles for Scenario H14 with $E_M = 0.1$

Stage	EM	Temperature				
		Scenario H14	Zhu (2015)	Sætre (2016)	Røsvik (2018)	Fagerheim (2019)
Removal grade		90%	89.39%	89.4%	89.3%	88.57%
Rich loading		0.48	0.4789	0.4784	-	0.4890
1	0.2300	45,4	45,48	47,7	45,66	46,14
2	0.2192	51,1	48,7	51,1	49,02	49,41
3	0.2085	51,2	49,56	51,8	49,94	50,16
4	0.1977	50,3	49,5	51,6	49,89	49,95
5	0.1869	49,6	49,03	50,9	49,44	49,34
6	0.1800	48,5	48,32	50,1	48,77	48,49
7	0.1762	46,7	47,41	49,1	47,94	47,44
8	0.1546	45,2	46,29	48	46,98	46,16
9	0.1438	43,5	45,04	46,6	45,88	44,74
10	0.1331	41,7	43,66	45	44,64	43,18
11	0.1223	40,6	42,18	43,2	43,25	41,45
12	0.1115	39	40,53	41,2	41,72	39,61
13	0.1007	38,4	38,77	39,1	39,99	37,73
14	0.0900	39,1	36,91	36,9	38,12	35,87
15	0.0100	35	34,98	34,7	36,17	34,09
16	0.0100	33,7	33,59	33,3	34,23	32,80
17	0.0100	32,2	32,51	32,2	32,85	31,79
18	0.0100	30,4	31,64	31,4	31,82	30,96
19	0.0100	29,8	30,91	30,7	30,99	30,23
20	0.0100	29,3	30,22	30	30,3	29,56
21	0.0100	28,1	29,56	29,3	29,65	28,93
22	0.0100	28,4	28,85	28,7	28,99	28,31
23	0.0100	27,6	28,08	28	28,26	27,67
24	0.0100	27,2	27,22	27,3	27,38	27,00

Table G.2: Temperature profiles for Scenario H14 with E_M = Zhu

Scenario 2B5

Stage	EM	Temperature		
		Scenario H14	Sætre (2016)	Fagerheim (2019)
Removal grade		87,2%	86.9%	89,97%
Rich loading		0.5	0,4893	0.4715
1	0.100	47,10	45,8	45,80
2	0.100	48,44	48,8	48,86
3	0.100	49,79	49,6	49,74
4	0.100	51,14	49,7	49,89
5	0.100	50,36	49,6	49,79
6	0.100	49,59	49,3	49,58
7	0.100	47,92	49	49,33
8	0.100	47,24	48,6	49,04
9	0.100	46,56	48,2	48,70
10	0.100	45,88	47,7	48,33
11	0.100	45,20	47,2	47,91
12	0.100	41,13	46,6	47,43
13	0.100	40,86	45,9	46,90
14	0.100	39,94	45,2	46,30
15	0.100	41,70	44,3	45,62
16	0.100	38,20	43,4	44,84
17	0.100	37,28	42,3	43,95
18	0.100	36,79	41,1	42,93
19	0.100	35,43	39,8	41,76
20	0.100	33,84	38,2	40,42
21	0.100	33,56	36,6	38,88
22	0.100	33,27	34,9	37,06
23	0.100	31,73	33,3	34,95
24	0.100	30,99	31,8	32,51

Table G.3: T-profiles for scenario 2B5 with $E_M = 0.1$

Stage	EM	Temperature		
		Scenario H14	Sætre (2016)	Fagerheim (2019)
Removal grade		87,2%	87,2%	90,2%
Rich loading		0.5	0.4901	0,4722
1	0.2300	47,10	46,20	46,63
2	0.2192	48,44	49,10	49,67
3	0.2085	49,79	49,60	50,29
4	0.1977	51,14	49,20	50,08
5	0.1869	50,36	48,50	49,54
6	0.1800	49,59	47,50	48,80
7	0.1762	47,92	46,40	47,89
8	0.1546	47,24	45,00	46,78
9	0.1438	46,56	43,50	45,55
10	0.1331	45,88	41,70	44,18
11	0.1223	45,20	39,90	42,67
12	0.1115	41,13	38,10	41,04
13	0.1007	40,86	36,40	39,26
14	0.0900	39,94	34,90	37,41
15	0.0100	41,70	33,70	35,55
16	0.0100	38,20	32,90	34,34
17	0.0100	37,28	32,30	33,50
18	0.0100	36,79	31,90	32,86
19	0.0100	35,43	31,60	32,33
20	0.0100	33,84	31,30	31,86
21	0.0100	33,56	31,10	31,43
22	0.0100	33,27	30,90	31,02
23	0.0100	31,73	30,70	30,62
24	0.0100	30,99	30,50	30,21

Table G.4: T- profiles for scenario 2B5 with E_M = Zhu

Scenario 6w

Stage	EM	Temperature		
		Scenario H14	Sætre (2016)	Fagerheim (2019)
Removal grade		79,0%	87,0%	89,72%
Rich loading		0,46	0,4920	0.4721
1	0.100	46,05	45,00	45,04
2	0.100	47,15	48,10	48,21
3	0.100	48,25	49,10	49,27
4	0.100	49,35	49,30	49,52
5	0.100	49,01	49,20	49,46
6	0.100	48,68	48,90	49,27
7	0.100	46,90	48,60	49,02
8	0.100	46,14	48,30	48,72
9	0.100	45,38	47,90	48,38
10	0.100	44,61	47,40	48,00
11	0.100	43,85	46,90	47,56
12	0.100	39,45	46,30	47,07
13	0.100	38,88	45,60	46,52
14	0.100	38,00	44,90	45,89
15	0.100	39,50	44,00	45,17
16	0.100	36,27	43,00	44,36
17	0.100	35,40	42,00	43,43
18	0.100	34,13	40,70	42,35
19	0.100	32,55	39,30	41,11
20	0.100	30,70	37,60	39,67
21	0.100	30,38	35,80	37,98
22	0.100	30,05	33,70	35,91
23	0.100	28,35	31,50	33,41
24	0.100	27,33	29,10	30,33

Table G.5: T-profiles for scenario 6w with $E_M = 0.1$

Stage	EM	Temperature		
		Scenario H14	Sætre (2016)	Fagerheim (2019)
Removal grade		79,0%	86,9%	89,6%
Rich loading		0,46	0.4910	0,4721
1	0.2300	46,05	45,80	46,24
2	0.2192	47,15	48,80	49,48
3	0.2085	48,25	49,50	50,29
4	0.1977	49,35	49,30	50,17
5	0.1869	49,01	48,60	49,67
6	0.1800	48,68	47,70	48,95
7	0.1762	46,90	46,60	48,05
8	0.1546	46,14	45,20	46,95
9	0.1438	45,38	43,80	45,71
10	0.1331	44,61	42,10	44,34
11	0.1223	43,85	40,30	42,82
12	0.1115	39,45	38,50	41,16
13	0.1007	38,88	36,60	39,33
14	0.0900	38,00	34,90	37,39
15	0.0100	39,50	33,40	35,37
16	0.0100	36,27	32,20	33,93
17	0.0100	35,40	31,30	32,81
18	0.0100	34,13	30,60	31,89
19	0.0100	32,55	29,90	31,08
20	0.0100	30,70	29,30	30,32
21	0.0100	30,38	28,70	29,59
22	0.0100	30,05	28,20	28,86
23	0.0100	28,35	27,60	28,11
24	0.0100	27,33	27,00	27,30

Table G.6: T- profiles for scenario 6w with E_M = Zhu

Scenario Goal1

Stage	EM	Temperature		
		Scenario H14	Sætre (2016)	Fagerheim (2019)
Removal grade		90,1%	86,1%	89,82%
Rich loading		0.5	0.5	0.4863
1	0.100	46,81	45,1	44,03
2	0.100	47,47	47,9	46,46
3	0.100	48,13	48,6	47,16
4	0.100	48,81	48,7	47,30
5	0.100	47,63	48,5	47,24
6	0.100	46,45	48,2	47,10
7	0.100	44,00	47,8	46,92
8	0.100	42,97	47,4	46,69
9	0.100	41,93	46,9	46,42
10	0.100	40,90	46,4	46,10
11	0.100	39,87	45,8	45,73
12	0.100	34,72	45,1	45,29
13	0.100	34,40	44,3	44,78
14	0.100	33,58	43,4	44,19
15	0.100	35,10	42,5	43,51
16	0.100	31,94	41,4	42,72
17	0.100	31,12	40,1	41,80
18	0.100	30,74	38,7	40,72
19	0.100	29,86	37,1	39,48
20	0.100	28,78	35,3	38,04
21	0.100	28,72	33,5	36,33
22	0.100	28,68	31,7	34,35
23	0.100	27,60	30,1	32,07
24	0.100	27,31	28,5	29,55

Table G.7: T- profiles for scenario Goal1 with $E_M = 0.1$

Stage	EM	Temperature		
		Scenario H14	Sætre (2016)	Fagerheim (2019)
Removal grade		90,1%	86,2%	90,20%
Rich loading		0.5	0.5	0.4876
1	0.2300	46,81	45,50	44,83
2	0.2192	47,47	48,10	47,22
3	0.2085	48,13	48,50	47,64
4	0.1977	48,81	48,00	47,38
5	0.1869	47,63	47,10	46,83
6	0.1800	46,45	45,90	46,09
7	0.1762	44,00	44,60	45,16
8	0.1546	42,97	43,00	44,00
9	0.1438	41,93	41,20	42,68
10	0.1331	40,90	39,20	41,20
11	0.1223	39,87	37,10	39,56
12	0.1115	34,72	35,10	37,74
13	0.1007	34,40	33,40	35,80
14	0.0900	33,58	32,00	33,82
15	0.0100	35,10	30,80	31,91
16	0.0100	31,94	30,00	30,70
17	0.0100	31,12	29,40	29,86
18	0.0100	30,74	29,00	29,26
19	0.0100	29,86	28,60	28,79
20	0.0100	28,78	28,30	28,41
21	0.0100	28,72	28,00	28,07
22	0.0100	28,68	27,80	27,77
23	0.0100	27,60	27,50	27,48
24	0.0100	27,31	27,30	27,20

Table G.8: T-profiles for scenario Goal1 with E_M = Zhu

Scenario F17

Stage	EM	Temperature		
		Scenario H14	Røsvik (2018)	Fagerheim (2019)
Removal grade		83.5%	86.6%	91.88%
Rich loading		0.48	-	0.3554
1	0.100	47,40	45,84	45,72
2	0.100	51,70	48,57	48,82
3	0.100	51,60	49,26	49,77
4	0.100	50,50	49,31	49,96
5	0.100	49,90	49,14	49,88
6	0.100	48,90	48,88	49,70
7	0.100	47,20	48,58	49,47
8	0.100	46,00	48,24	49,19
9	0.100	44,40	47,85	48,89
10	0.100	43,10	47,42	48,54
11	0.100	42,20	46,95	48,14
12	0.100	40,90	46,42	47,70
13	0.100	40,60	45,84	47,20
14	0.100	41,60	45,20	46,63
15	0.100	37,40	44,51	45,98
16	0.100	37,10	43,77	45,24
17	0.100	35,90	42,92	44,39
18	0.100	34,30	41,89	43,43
19	0.100	34,10	40,41	42,32
20	0.100	33,80	38,92	41,03
21	0.100	32,90	37,22	39,53
22	0.100	33,20	35,01	37,76
23	0.100	32,50	32,80	35,62
24	0.100	32,40	30,98	33,00

Table G.9: T-profiles for scenario F17 with $E_M = 0.1$

Stage	EM	Temperature		
		Scenario H14	Røsvik (2018)	Fagerheim (2019)
Removal grade		83.5%	87.90%	90.57%
Rich loading		0.48	-	0.4552
1	0.2300	47,40	46,04	47,09
2	0.2192	51,70	48,40	50,39
3	0.2085	51,60	48,63	51,16
4	0.1977	50,50	48,14	51,03
5	0.1869	49,90	47,34	50,56
6	0.1800	48,90	46,30	49,88
7	0.1762	47,20	45,02	49,04
8	0.1546	46,00	43,46	48,01
9	0.1438	44,40	41,52	46,86
10	0.1331	43,10	39,20	45,57
11	0.1223	42,20	36,55	44,14
12	0.1115	40,90	33,81	42,56
13	0.1007	40,60	31,24	40,85
14	0.0900	41,60	29,05	38,98
15	0.0100	37,40	27,48	36,99
16	0.0100	37,10	26,70	35,69
17	0.0100	35,90	26,53	34,75
18	0.0100	34,30	26,71	34,01
19	0.0100	34,10	27,09	33,39
20	0.0100	33,80	27,59	32,83
21	0.0100	32,90	28,11	32,31
22	0.0100	33,20	28,63	31,79
23	0.0100	32,50	29,13	31,28
24	0.0100	32,40	29,59	30,75

Table G.10: T-profiles for scenario F17 with E_M = Zhu

Stage	EM	Temperature		
		Scenario H14	Røsvik (2018)	Fagerheim (2019)
Removal grade		83.5%	85.6%	89.2%
Rich loading		0.48	-	0.4514
1	0,17	47,40	45,6	46,92
2	0,17	51,70	47,83	50,24
3	0,17	51,60	48,19	51,09
4	0,17	50,50	47,89	51,07
5	0,17	49,90	47,3	50,70
6	0,16	48,90	46,5	50,15
7	0,15	47,20	45,55	49,48
8	0,14	46,00	44,45	48,70
9	0,13	44,40	43,2	47,82
10	0,12	43,10	41,83	46,85
11	0,11	42,20	40,35	45,78
12	0,1	40,90	38,75	44,63
13	0,09	40,60	37,11	43,41
14	0,08	41,60	35,54	42,13
15	0,07	37,40	34,19	40,82
16	0,06	37,10	33,17	39,49
17	0,05	35,90	32,52	38,11
18	0,04	34,30	32,14	36,77
19	0,03	34,10	31,91	35,48
20	0,02	33,80	31,76	34,29
21	0,01	32,90	31,59	33,23
22	0,01	33,20	31,37	32,36
23	0,01	32,50	31,05	31,60
24	0,01	32,40	30,64	30,88

Table G.11: Temperature profiles for scenario F17 with E_M = Lin

Appendix H – Data from verification (Plus)

Scenario H14

Stage	EM	Temperature			
		Scenario H14	Sætre (2016)	Røsvik (2018)	Fagerheim (2019)
Removal grade		90%	88.43%	88.4%	88.40%
Rich loading		0.48	0,488	-	0.4880
1	0.100	45,4	46,6	46,65	46,60
2	0.100	51,1	50	50,12	50,05
3	0.100	51,2	51	51,12	51,03
4	0.100	50,3	51,2	51,28	51,19
5	0.100	49,6	51,1	51,17	51,08
6	0.100	48,5	50,9	50,95	50,86
7	0.100	46,7	50,6	50,67	50,58
8	0.100	45,2	50,3	50,35	50,26
9	0.100	43,5	49,9	49,99	49,90
10	0.100	41,7	49,5	49,59	49,50
11	0.100	40,6	49	49,13	49,04
12	0.100	39	48,5	48,61	48,52
13	0.100	38,4	47,9	48,02	47,93
14	0.100	39,1	47,3	47,35	47,26
15	0.100	35	46,5	46,59	46,50
16	0.100	33,7	45,6	45,71	45,63
17	0.100	32,2	44,6	44,71	44,62
18	0.100	30,4	43,5	43,54	43,45
19	0.100	29,8	42,1	42,17	42,08
20	0.100	29,3	40,5	40,57	40,48
21	0.100	28,1	38,6	38,67	38,58
22	0.100	28,4	36,4	36,41	36,33
23	0.100	27,6	33,7	33,72	33,64
24	0.100	27,2	30,4	30,5	30,43

Table H.1: Temperature profiles for Scenario H14 with $E_M = 0.1$

Stage	EM	Temperature			
		Scenario H14	Sætre (2016)	Røsvik (2018)	Fagerheim (2019)
Removal grade		90%	88.43	89.0%	88.39%
Rich loading		0.48	0.4880	-	0.4880
1	0.2300	45,4	47,7	47,83	47,69
2	0.2192	51,1	51,1	51,31	51,11
3	0.2085	51,2	51,8	52,03	51,79
4	0.1977	50,3	51,6	51,82	51,54
5	0.1869	49,6	50,9	51,27	50,94
6	0.1800	48,5	50,1	50,51	50,12
7	0.1762	46,7	49,1	49,58	49,11
8	0.1546	45,2	48	48,48	47,93
9	0.1438	43,5	46,6	47,21	46,54
10	0.1331	41,7	45	45,74	44,95
11	0.1223	40,6	43,2	44,09	43,14
12	0.1115	39	41,2	42,26	41,15
13	0.1007	38,4	39,1	40,28	39,01
14	0.0900	39,1	36,9	38,22	36,82
15	0.0100	35	34,7	36,16	34,68
16	0.0100	33,7	33,3	34,13	33,27
17	0.0100	32,2	32,2	32,74	32,22
18	0.0100	30,4	31,4	31,71	31,39
19	0.0100	29,8	30,7	30,85	30,66
20	0.0100	29,3	30	30,11	29,98
21	0.0100	28,1	29,3	29,42	29,33
22	0.0100	28,4	28,7	28,74	28,68
23	0.0100	27,6	28	28,05	28,00
24	0.0100	27,2	27,3	27,33	27,28

Table H.2: Temperature profiles for Scenario H14 with E_M = Zhu

Sætre (2016)	Røsvik (2018)	Fagerheim (2019)[0.55]	Fagerheim (2019)[0.65]
88.50%	88.70%	88.38%	88.73%
0.4883	-	0.4881	0.4891
47,30	47,73	48,82	50,46
51,30	53,39	51,93	52,45
52,10	51,41	52,21	52,34
52,00	51,45	52,11	52,17
51,80	50,63	51,95	51,97
51,70	49,93	51,78	51,75
51,50	48,99	51,59	51,51
51,20	47,92	51,38	51,25
51,00	46,66	51,16	50,96
50,70	45,20	50,92	50,65
50,40	43,56	50,65	50,30
50,10	41,73	50,37	49,93
49,80	39,75	50,07	49,52
49,50	37,68	49,74	49,07
49,10	35,61	49,39	48,59
48,70	33,63	49,01	48,07
48,20	31,86	48,60	47,51
47,80	30,36	48,17	46,91
47,30	29,16	47,70	46,26
46,70	28,23	47,21	45,58
46,20	27,50	46,69	44,85
45,60	26,94	46,14	44,07
44,90	26,50	45,55	43,26
44,30	26,07	44,93	42,40
43,60		44,28	41,51
42,90		43,60	40,58
42,11		42,88	39,63
41,30		42,14	38,65
40,50		41,36	37,66
39,70		40,57	36,67
38,80		39,74	35,69
38,00		38,90	34,73
37,10		38,04	33,81
36,20		37,17	32,93
35,30		36,29	32,10
34,50		35,42	31,34
33,60		34,56	30,64
32,80		33,72	30,00
32,00		32,89	29,43
31,30		32,10	28,93
30,60		31,35	28,47
29,90		30,63	28,07
29,30		29,96	27,71
28,80		29,33	27,39
28,20		28,75	27,11
27,70		28,21	26,85
27,30		27,71	26,62
26,80		27,24	26,42
26,30		26,82	26,24
25,70		26,43	26,09

Table H.3: Temperature profiles for scenario H14 with Rate-base model

Scenario 2B5

Stage	EM	Temperature		
		Scenario H14	Sætre (2016)	Fagerheim (2019)
Removal grade		87,2%	87.2%	87.2%
Rich loading		0.5	0.4900	0.4887
1	0.100	47,10	47,20	47,19
2	0.100	48,44	50,30	50,33
3	0.100	49,79	51,10	51,10
4	0.100	51,14	51,20	51,17
5	0.100	50,36	51,00	51,01
6	0.100	49,59	50,80	50,76
7	0.100	47,92	50,50	50,47
8	0.100	47,24	50,10	50,13
9	0.100	46,56	49,80	49,75
10	0.100	45,88	49,30	49,33
11	0.100	45,20	48,90	48,85
12	0.100	41,13	48,30	48,31
13	0.100	40,86	47,70	47,70
14	0.100	39,94	47,00	47,01
15	0.100	41,70	46,20	46,22
16	0.100	38,20	45,20	45,33
17	0.100	37,28	44,30	44,30
18	0.100	36,79	43,10	43,12
19	0.100	35,43	41,70	41,77
20	0.100	33,84	40,20	40,22
21	0.100	33,56	38,40	38,47
22	0.100	33,27	36,50	36,54
23	0.100	31,73	34,50	34,50
24	0.100	30,99	32,40	32,41

Table H.4: Temperature profiles for Scenario 2B5 with $E_M = 0.1$

Stage	EM	Temperature		
		Scenario H14	Sætre (2016)	Fagerheim (2019)
Removal grade		87,3%	0,87	88.39%
Rich loading		0.5	0.4901	0.4880
1	0.2300	47,10	47,80	47,69
2	0.2192	48,44	50,80	51,11
3	0.2085	49,79	51,20	51,79
4	0.1977	51,14	50,90	51,54
5	0.1869	50,36	50,20	50,94
6	0.1800	49,59	49,30	50,12
7	0.1762	47,92	48,20	49,11
8	0.1546	47,24	46,90	47,93
9	0.1438	46,56	45,50	46,54
10	0.1331	45,88	43,80	44,95
11	0.1223	45,20	41,90	43,14
12	0.1115	41,13	40,00	41,15
13	0.1007	40,86	38,00	39,01
14	0.0900	39,94	36,20	36,82
15	0.0100	41,70	34,60	34,68
16	0.0100	38,20	33,70	33,27
17	0.0100	37,28	33,00	32,22
18	0.0100	36,79	32,50	31,39
19	0.0100	35,43	32,20	30,66
20	0.0100	33,84	31,80	29,98
21	0.0100	33,56	31,50	29,33
22	0.0100	33,27	31,20	28,68
23	0.0100	31,73	30,90	28,00
24	0.0100	30,99	30,70	27,28

Table H.5: Temperature profiles for Scenario 2B5 with E_M = Zhu

Sætre (2016)	Fagerheim (2019)[0.5	Fagerheim (2019)[0.6
86.00%	86.02%	86.12%
0.4900	0.4854	0.4856
48,35	49,35	50,75
51,20	51,54	51,72
51,40	51,54	51,49
51,30	51,37	51,26
51,00	51,17	51,01
50,86	50,96	50,74
50,60	50,73	50,44
50,30	50,47	50,11
50,00	50,20	49,75
49,75	49,91	49,36
49,40	49,59	48,93
49,00	49,25	48,47
48,66	48,89	47,97
48,25	48,50	47,44
47,80	48,08	46,86
47,33	47,63	46,24
46,83	47,16	45,58
46,30	46,65	44,88
45,70	46,12	44,13
45,13	45,56	43,35
44,50	44,96	42,53
43,85	44,34	41,68
43,20	43,69	40,79
42,44	43,01	39,89
41,70	42,30	38,97
40,94	41,57	38,04
40,16	40,82	37,12
39,36	40,05	36,22
38,56	39,27	35,35
37,76	38,48	34,54
36,96	37,69	33,78
36,18	36,91	33,10
35,43	36,14	32,50
34,71	35,40	31,99
34,00	34,69	31,55
33,40	34,02	31,19
32,84	33,40	30,90
32,30	32,84	30,66
31,88	32,34	30,47
31,50	31,90	30,32
31,17	31,51	30,20
30,89	31,18	30,11
30,66	30,90	30,04
30,47	30,67	29,99
30,30	30,47	29,94
30,16	30,31	29,91
30,03	30,18	29,89
29,89	30,08	29,88
29,70	30,00	29,87
29,45	29,94	29,88

Table H.6: Temperature profiles for scenario 2B5 with Rate-base model

Scenario 6w

Stage	EM	Temperature		
		Scenario H14	Sætre (2016)	Fagerheim (2019)
Removal grade		79,0%	87.20%	89.49%
Rich loading		0,46	0,4910	0.4707
1	0.100	46,05	46,50	46,31
2	0.100	47,15	49,80	49,63
3	0.100	48,25	50,70	50,62
4	0.100	49,35	50,90	50,80
5	0.100	49,01	50,70	50,72
6	0.100	48,68	50,50	50,53
7	0.100	46,90	50,20	50,28
8	0.100	46,14	49,90	49,99
9	0.100	45,38	49,50	49,67
10	0.100	44,61	49,10	49,30
11	0.100	43,85	48,60	48,89
12	0.100	39,45	48,00	48,42
13	0.100	38,88	47,40	47,89
14	0.100	38,00	46,70	47,29
15	0.100	39,50	45,90	46,60
16	0.100	36,27	45,00	45,81
17	0.100	35,40	43,90	44,90
18	0.100	34,13	42,70	43,84
19	0.100	32,55	41,30	42,61
20	0.100	30,70	39,70	41,15
21	0.100	30,38	37,80	39,40
22	0.100	30,05	35,60	37,28
23	0.100	28,35	33,10	34,64
24	0.100	27,33	30,20	31,27

Table H.7: Temperature profiles for Scenario 6w with $E_M = 0.1$

Stage	EM	Temperature		
		Scenario H14	Sætre (2016)	Fagerheim (2019)
Removal grade		79,0%	86.90%	89.68%
Rich loading		0,46	0.4900	0,4702
1	0.2300	46,05	47,40	47,62
2	0.2192	47,15	50,60	51,00
3	0.2085	48,25	51,20	51,73
4	0.1977	49,35	51,00	51,57
5	0.1869	49,01	50,30	51,06
6	0.1800	48,68	49,40	50,36
7	0.1762	46,90	48,30	49,49
8	0.1546	46,14	47,10	48,46
9	0.1438	45,38	45,60	47,26
10	0.1331	44,61	43,90	45,87
11	0.1223	43,85	42,10	44,28
12	0.1115	39,45	40,10	42,46
13	0.1007	38,88	38,00	40,41
14	0.0900	38,00	36,00	38,15
15	0.0100	39,50	34,20	35,76
16	0.0100	36,27	32,90	34,21
17	0.0100	35,40	31,90	33,08
18	0.0100	34,13	31,20	32,17
19	0.0100	32,55	30,50	31,38
20	0.0100	30,70	29,90	30,65
21	0.0100	30,38	29,30	29,94
22	0.0100	30,05	28,70	29,21
23	0.0100	28,35	28,10	28,45
24	0.0100	27,33	27,50	27,64

Table H.8: Temperature profiles for Scenario 6w with E_M = Zhu

Sætre (2016)	Fagerheim (2019)[0.5	Fagerheim (2019)[0.6
86.10%	93.53%	95.19%
0.4880	0.4819	0.4865
47,57	48,92	50,86
50,90	52,02	52,86
51,40	52,38	52,85
51,33	52,35	52,78
51,15	52,27	52,71
50,94	52,18	52,63
50,70	52,08	52,54
50,40	51,97	52,44
50,20	51,85	52,32
49,90	51,72	52,20
49,62	51,58	52,06
49,29	51,43	51,91
48,94	51,26	51,74
48,60	51,08	51,56
48,20	50,88	51,35
47,70	50,67	51,13
47,30	50,43	50,88
46,80	50,18	50,61
46,30	49,91	50,31
45,70	49,62	49,99
45,12	49,31	49,63
44,51	48,97	49,25
43,86	48,60	48,83
43,19	48,21	48,38
42,49	47,79	47,89
41,76	47,35	47,36
41,00	46,87	46,79
40,22	46,36	46,18
39,40	45,82	45,53
38,60	45,25	44,84
37,78	44,64	44,10
36,90	44,00	43,32
36,12	43,32	42,50
35,29	42,61	41,63
34,48	41,86	40,73
33,70	41,08	39,79
32,90	40,26	38,82
32,20	39,41	37,83
31,50	38,52	36,81
30,80	37,61	35,79
30,20	36,67	34,77
29,70	35,70	33,75
29,13	34,72	32,76
28,64	33,72	31,80
28,19	32,71	30,87
27,77	31,69	29,98
27,37	30,67	29,14
26,99	29,65	28,36
26,60	28,63	27,62
26,17	27,63	26,94

Table H.9: Temperature profiles for scenario 6w with Rate-base model

Scenario Goal1

Stage	EM	Temperature		
		Scenario H14	Sætre (2016)	Fagerheim (2019)
Removal grade		90,1%	82.7%	89,63%
Rich loading		0.5	0.5000	0.4854
1	0.100	46,81	46,30	47,22
2	0.100	47,47	49,00	49,99
3	0.100	48,13	49,60	50,37
4	0.100	48,81	49,50	50,03
5	0.100	47,63	49,20	49,41
6	0.100	46,45	48,80	48,62
7	0.100	44,00	48,30	47,65
8	0.100	42,97	47,80	46,45
9	0.100	41,93	47,30	45,10
10	0.100	40,90	46,60	43,57
11	0.100	39,87	45,90	41,84
12	0.100	34,72	45,00	39,91
13	0.100	34,40	44,10	37,80
14	0.100	33,58	42,90	35,59
15	0.100	35,10	41,70	33,36
16	0.100	31,94	40,20	32,03
17	0.100	31,12	38,60	31,15
18	0.100	30,74	36,80	30,48
19	0.100	29,86	35,00	29,93
20	0.100	28,78	33,30	29,43
21	0.100	28,72	31,70	28,95
22	0.100	28,68	30,30	28,48
23	0.100	27,60	29,20	28,00
24	0.100	27,31	28,10	27,52

Table H.10: Temperature profiles for Scenario Goal1 with $E_M = 0.1$

Stage	EM	Temperature		
		Scenario H14	Sætre (2016)	Fagerheim (2019)
Removal grade		90,1%	82.7%	89.82%
Rich loading		0.5	0.5000	0,4860
1	0.2300	46,81	45,50	46,39
2	0.2192	47,47	49,00	49,23
3	0.2085	48,13	49,00	49,90
4	0.1977	48,81	48,20	49,93
5	0.1869	47,63	47,00	49,78
6	0.1800	46,45	45,50	49,56
7	0.1762	44,00	43,80	49,29
8	0.1546	42,97	41,70	48,98
9	0.1438	41,93	39,40	48,64
10	0.1331	40,90	37,00	48,25
11	0.1223	39,87	35,00	47,82
12	0.1115	34,72	33,20	47,33
13	0.1007	34,40	31,80	46,77
14	0.0900	33,58	30,70	46,13
15	0.0100	35,10	29,80	45,41
16	0.0100	31,94	29,20	44,58
17	0.0100	31,12	28,80	43,62
18	0.0100	30,74	28,50	42,52
19	0.0100	29,86	28,30	41,22
20	0.0100	28,78	28,00	39,71
21	0.0100	28,72	27,90	37,91
22	0.0100	28,68	27,70	35,77
23	0.0100	27,60	27,50	33,23
24	0.0100	27,31	27,40	30,29

Table H.11: Temperature profiles for Scenario Goal1 with E_M = Zhu

Sætre (2016)	Fagerheim (2019)[0.5	Fagerheim (2019)[0.6
78.90%	90.21%	90.40%
0.4900	0.4877	0.4880
46,70	49,51	50,90
49,00	51,05	51,11
49,00	50,96	50,93
48,70	50,82	50,75
48,30	50,66	50,56
47,90	50,49	50,34
47,50	50,30	50,09
47,10	50,10	49,82
46,60	49,88	49,52
46,10	49,63	49,20
45,60	49,37	48,83
45,00	49,08	48,43
44,40	48,77	48,00
43,80	48,43	47,52
43,10	48,06	47,00
42,40	47,67	46,44
41,70	47,24	45,83
40,90	46,79	45,17
40,10	46,30	44,47
39,20	45,78	43,72
38,40	45,22	42,91
37,50	44,63	42,06
36,60	44,01	41,16
35,70	43,35	40,22
34,80	42,65	39,24
33,90	41,92	38,22
33,00	41,15	37,17
32,20	40,35	36,11
31,40	39,52	35,04
30,70	38,67	33,98
30,00	37,79	32,94
29,40	36,89	31,96
28,90	35,98	31,04
28,40	35,06	30,21
28,10	34,15	29,48
27,80	33,26	28,86
27,50	32,39	28,34
27,30	31,57	27,92
27,20	30,79	27,58
27,00	30,08	27,32
26,90	29,44	27,12
26,80	28,87	26,96
26,80	28,39	26,84
26,70	27,97	26,75
26,70	27,63	26,69
26,60	27,34	26,64
26,60	27,11	26,60
26,50	26,93	26,58
26,40	26,78	26,56
26,20	26,68	26,57

Table H.12: Temperature profiles for scenario Goal1 with Rate-base model

Scenario F17

Stage	EM	Temperature		
		Scenario H14	Røsvik (2018)	Fagerheim (2019)
Removal grade		83.5%	86.65%	88.40%
Rich loading		0.48	-	0.4880
1	0.100	47,40	47,34	46,60
2	0.100	51,70	50,12	50,05
3	0.100	51,60	50,69	51,03
4	0.100	50,50	50,66	51,19
5	0.100	49,90	50,45	51,08
6	0.100	48,90	50,17	50,86
7	0.100	47,20	49,85	50,58
8	0.100	46,00	49,48	50,26
9	0.100	44,40	49,06	49,90
10	0.100	43,10	48,60	49,50
11	0.100	42,20	48,07	49,04
12	0.100	40,90	47,47	48,52
13	0.100	40,60	46,79	47,93
14	0.100	41,60	46,02	47,26
15	0.100	37,40	45,14	46,50
16	0.100	37,10	44,14	45,63
17	0.100	35,90	42,98	44,62
18	0.100	34,30	41,66	43,45
19	0.100	34,10	40,15	42,08
20	0.100	33,80	38,47	40,48
21	0.100	32,90	36,66	38,58
22	0.100	33,20	34,86	36,33
23	0.100	32,50	33,20	33,64
24	0.100	32,40	31,74	30,43

Table H.13: Temperature profiles for Scenario F17 with E_M = 0.1

Stage	EM	Temperature		
		Scenario H14	Røsvik (2018)	Fagerheim (2019)
Removal grade		83.5%	87,20%	88.39%
Rich loading		0.48	-	0.4880
1	0.2300	47,40	47,72	47,69
2	0.2192	51,70	50,32	51,11
3	0.2085	51,60	50,55	51,79
4	0.1977	50,50	50,07	51,54
5	0.1869	49,90	49,28	50,94
6	0.1800	48,90	48,29	50,12
7	0.1762	47,20	47,09	49,11
8	0.1546	46,00	45,67	47,93
9	0.1438	44,40	44,01	46,54
10	0.1331	43,10	42,13	44,95
11	0.1223	42,20	40,10	43,14
12	0.1115	40,90	38,06	41,15
13	0.1007	40,60	36,22	39,01
14	0.0900	41,60	34,70	36,82
15	0.0100	37,40	33,48	34,68
16	0.0100	37,10	32,53	33,27
17	0.0100	35,90	31,98	32,22
18	0.0100	34,30	31,63	31,39
19	0.0100	34,10	31,38	30,66
20	0.0100	33,80	31,18	29,98
21	0.0100	32,90	31,02	29,33
22	0.0100	33,20	30,88	28,68
23	0.0100	32,50	30,75	28,00
24	0.0100	32,40	30,63	27,28

Table H.14: Temperature profiles for Scenario F17 with E_M = Zhu

Stage	EM	Temperature		
		Scenario H14	Røsvik (2018)	Fagerheim (2019)
Removal grade		83.5%	86.30%	86.24%
Rich loading		0.48	-	0.4929
1	0,17	47,40	47,58	47,974
2	0,17	51,70	50,26	50,7865
3	0,17	51,60	50,63	51,1983
4	0,17	50,50	50,33	50,9067
5	0,17	49,90	49,77	50,3442
6	0,16	48,90	49,03	49,5992
7	0,15	47,20	48,16	48,7174
8	0,14	46,00	47,15	47,7061
9	0,13	44,40	46,02	46,5651
10	0,12	43,10	44,76	45,2953
11	0,11	42,20	43,38	43,9039
12	0,1	40,90	41,89	42,4088
13	0,09	40,60	40,34	40,844
14	0,08	41,60	38,77	39,2638
15	0,07	37,40	37,25	37,7384
16	0,06	37,10	35,86	36,3364
17	0,05	35,90	34,64	35,1054
18	0,04	34,30	33,61	34,0635
19	0,03	34,10	32,76	33,2072
20	0,02	33,80	32,09	32,5233
21	0,01	32,90	31,58	31,9987
22	0,01	33,20	31,22	31,6305
23	0,01	32,50	30,94	31,3458
24	0,01	32,40	30,71	31,105

Table H.15: Temperature profiles for Scenario F17 with E_M = Lin

Røsvik (2018)	Fagerheim (2019)[0.5	Fagerheim (2019)[0.6
88.50%	83.76%	83.94%
0.4883	0.4846	0.4852
47,13	49,38	50,75
51,27	51,23	51,37
49,74	51,18	51,14
49,63	51,00	50,91
48,97	50,81	50,67
48,38	50,60	50,40
47,66	50,37	50,11
46,87	50,13	49,80
45,98	49,86	49,46
44,99	49,59	49,10
43,91	49,29	48,71
42,73	48,97	48,29
41,46	48,64	47,84
40,12	48,28	47,36
38,72	47,90	46,85
37,30	47,50	46,30
35,89	47,08	45,73
34,55	46,63	45,12
33,32	46,16	44,49
32,27	45,67	43,82
31,43	45,16	43,12
30,81	44,62	42,39
30,37	44,06	41,64
30,08	43,48	40,86
	42,87	40,07
	42,25	39,26
	41,60	38,44
	40,95	37,62
	40,27	36,81
	39,58	36,02
	38,89	35,25
	38,19	34,52
	37,49	33,84
	36,79	33,22
	36,11	32,67
	35,45	32,19
	34,80	31,78
	34,19	31,44
	33,62	31,16
	33,09	30,95
	32,61	30,78
	32,18	30,65
	31,80	30,55
	31,48	30,48
	31,21	30,42
	30,98	30,38
	30,79	30,36
	30,64	30,34
	30,52	30,33
	30,42	30,33

Table H.16: Temperature profiles for scenario F17 with Rate-base model

Appendix I – Data from simulation with estimated Murphree efficiency (HYSYS)

Scenario H14

Scenario H14		SF1 (90,12%)		SF2 (89,94%)		Zhu *1.106 (90.00%)			Lin *1.159 (90,00%)			0.1 *1.101 (90.01%)		
		Removal grade	90,12	Removal grad	89,94	Removal grade		90	Removal grade		90	Removal grade		90,01
		Rich loading	0,4936	Rich loading	0,4931	Rich loading		0,4933	Rich loading		0,4885	Rich loading		0,4427
Height (m)	Step	EM	T	EM	T	EM	EM	T	EM	EM	T	EM	EM	T
24	1	0,245	46,43423	0,24	46,411369	0,23	0,25	46,15531546	0,17	0,19703	45,19928	0,1	0,1101	46,31302
23	2	0,2425	49,80819	0,235	49,783948	0,2192	0,24	49,4357382	0,17	0,19703	48,50233	0,1	0,1101	49,33061
22	3	0,24	50,59425	0,23	50,581542	0,2085	0,23	50,1848433	0,17	0,19703	49,56453	0,1	0,1101	50,01751
21	4	0,2375	50,3917	0,225	50,407563	0,1977	0,22	49,98058266	0,17	0,19703	49,78902	0,1	0,1101	49,90349
20	5	0,235	49,72219	0,22	49,792754	0,1869	0,21	49,36624789	0,17	0,19703	49,69899	0,1	0,1101	49,47054
19	6	0,2325	48,7175	0,215	48,885781	0,18	0,20	48,5158092	0,16	0,18544	49,47788	0,1	0,1101	48,85475
18	7	0,23	47,37409	0,23	47,704211	0,1762	0,19	47,46149473	0,15	0,17385	49,18967	0,1	0,1101	48,11853
17	8	0,2	45,64572	0,2	46,103334	0,1546	0,17	46,18145711	0,14	0,16226	48,85018	0,1	0,1101	47,28099
16	9	0,17	43,69197	0,17	44,254003	0,1438	0,16	44,76568279	0,13	0,15067	48,46368	0,1	0,1101	46,34905
15	10	0,14	41,60845	0,14	42,262455	0,1331	0,15	43,21078415	0,12	0,13908	48,02784	0,1	0,1101	45,32775
14	11	0,11	39,57541	0,11	40,275671	0,1223	0,14	41,49319485	0,11	0,12749	47,53463	0,1	0,1101	44,22469
13	12	0,08	37,7206	0,08	38,424106	0,1115	0,12	39,66731114	0,1	0,1159	46,98238	0,1	0,1101	43,04981
12	13	0,05	36,11771	0,055	36,799821	0,1007	0,11	37,78956234	0,09	0,10431	46,35338	0,1	0,1101	41,81853
11	14	0,0475	34,79678	0,0525	35,427972	0,09	0,10	35,93070121	0,08	0,09272	45,64306	0,1	0,1101	40,54881
10	15	0,045	33,64282	0,05	34,202939	0,01	0,01	34,15152262	0,07	0,08113	44,83812	0,1	0,1101	39,26551
9	16	0,0425	32,5978	0,0475	33,079114	0,01	0,01	32,85558966	0,06	0,06954	43,92198	0,1	0,1101	37,93476
8	17	0,04	31,63047	0,045	32,030922	0,01	0,01	31,84359623	0,05	0,05795	42,87751	0,1	0,1101	36,63035
7	18	0,0375	30,71945	0,0425	31,045598	0,01	0,01	31,00376577	0,04	0,04636	41,68521	0,1	0,1101	35,37716
6	19	0,035	29,85226	0,04	30,106005	0,01	0,01	30,26902753	0,03	0,03477	40,32256	0,1	0,1101	34,2037
5	20	0,0001	29,01557	0,0001	29,199105	0,01	0,01	29,59664412	0,02	0,02318	38,71654	0,1	0,1101	33,14101
4	21	0,0001	28,32445	0,0001	28,455056	0,01	0,01	28,95771203	0,01	0,01159	36,85763	0,1	0,1101	32,22497
3	22	0,0001	27,72883	0,0001	27,819038	0,01	0,01	28,33151258	0,01	0,01159	34,71193	0,1	0,1101	31,49707
2	23	0,0001	27,20374	0,0001	27,259634	0,01	0,01	27,68963246	0,01	0,01159	32,25969	0,1	0,1101	30,87855
1	24	0,0001	26,72995	0,0001	26,756237	0,01	0,01	27,01435771	0,01	0,01159	29,48468	0,1	0,1101	30,31713
Calculated efficiency		94,83380484 %		94,56295847 %		92,4054	94,5707405 %		90,95945	94,5822 %		92,02336	94,59836 %	
simulated efficiency		90,12 %		89,94 %		90	90 %		90	90 %		90,01	90,01 %	
difference		4,713804836		4,62295847	0	2,40538	4,57074049	0	0,959447	4,582202	0	2,013356	4,588361	

Table I.1: Data from simulation of scenario H14 in Aspen HYSYS (Kent-Eisenberg)

Scenario 2B5

Scenario 2B5		SF1*0,778 (87,30%)			SF2*0,79 (87,31%)			Zhu*0,88 (87,29%)			Lin*0,935 (87,32%)			0.1*0,886 (87,29%)		
		Removal grade		87,3	Removal grade		87,31	Removal grade		87,29	Removal grade		87,32	Removal grade		87,29
		Rich loading		0,4635	Rich loading		0,4635	Rich loading		0,4634	Rich loading		0,4635	Rich loading		0,4634
Height (m)	Step	EM (H14)	EM*0,778	T	EM(H14)	EM*0,79	T	EM(H14)	EM*0,88	T	EM	EM*0,935	T	EM	EM*0,886	T
24	1	0,245	0,1906	46,44101	0,24	0,1896	46,45285	0,23	0,20263	46,36482	0,17	0,1590	46,31302	0,1	0,0886	45,55251
23	2	0,2425	0,1887	49,4237	0,235	0,1857	49,4429	0,2192	0,193115	49,30871	0,17	0,1590	49,33061	0,1	0,0886	48,54922
22	3	0,24	0,1867	50,01988	0,23	0,1817	50,05084	0,2085	0,183689	49,88009	0,17	0,1590	50,01751	0,1	0,0886	49,40882
21	4	0,2375	0,1848	49,77749	0,225	0,1778	49,83095	0,1977	0,174174	49,6286	0,17	0,1590	49,90349	0,1	0,0886	49,53891
20	5	0,235	0,1828	49,17348	0,22	0,1738	49,26648	0,1869	0,164659	49,04514	0,17	0,1590	49,47054	0,1	0,0886	49,4152
19	6	0,2325	0,1809	48,33231	0,215	0,1699	48,49098	0,18	0,15858	48,27815	0,16	0,1496	48,85475	0,1	0,0886	49,19119
18	7	0,23	0,1789	47,26312	0,23	0,1817	47,52709	0,1762	0,155232	47,35258	0,15	0,1403	48,11853	0,1	0,0886	48,91454
17	8	0,2	0,1556	45,93161	0,2	0,1580	46,26198	0,1546	0,136203	46,24646	0,14	0,1309	47,28099	0,1	0,0886	48,5983
16	9	0,17	0,1323	44,44316	0,17	0,1343	44,82589	0,1438	0,126688	45,03704	0,13	0,1216	46,34905	0,1	0,0886	48,24397
15	10	0,14	0,1089	42,87605	0,14	0,1106	43,30419	0,1331	0,117261	43,70836	0,12	0,1122	45,32775	0,1	0,0886	47,84895
14	11	0,11	0,0856	41,30946	0,11	0,0869	41,77883	0,1223	0,107746	42,26122	0,11	0,1029	44,22469	0,1	0,0886	47,40872
13	12	0,08	0,0622	39,82779	0,08	0,0632	40,3344	0,1115	0,098232	40,70858	0,1	0,0935	43,04981	0,1	0,0886	46,91777
12	13	0,05	0,0389	38,46205	0,055	0,0435	39,01699	0,1007	0,088717	39,03163	0,09	0,0841	41,81853	0,1	0,0886	46,36922
11	14	0,0475	0,0370	37,3481	0,0525	0,0415	37,90777	0,09	0,07929	37,27153	0,08	0,0748	40,54881	0,1	0,0886	45,75536
10	15	0,045	0,0350	36,3421	0,05	0,0395	36,87716	0,01	0,00881	35,45702	0,07	0,0655	39,26551	0,1	0,0886	45,06664
9	16	0,0425	0,0331	35,37985	0,0475	0,0375	35,86871	0,01	0,00881	34,28323	0,06	0,0561	37,93476	0,1	0,0886	44,29154
8	17	0,04	0,0311	34,43302	0,045	0,0356	34,85999	0,01	0,00881	33,45555	0,05	0,0468	36,63035	0,1	0,0886	43,41663
7	18	0,0375	0,0292	33,48937	0,0425	0,0336	33,84153	0,01	0,00881	32,82256	0,04	0,0374	35,37716	0,1	0,0886	42,42652
6	19	0,035	0,0272	32,54433	0,04	0,0316	32,81053	0,01	0,00881	32,30053	0,03	0,0281	34,2037	0,1	0,0886	41,30311
5	20	0,0001	0,0001	31,59555	0,0001	0,0001	31,76481	0,01	0,00881	31,84156	0,02	0,0187	33,14101	0,1	0,0886	40,02391
4	21	0,0001	0,0001	30,9512	0,0001	0,0001	31,05818	0,01	0,00881	31,41722	0,01	0,0094	32,22497	0,1	0,0886	38,56275
3	22	0,0001	0,0001	30,50387	0,0001	0,0001	30,56884	0,01	0,00881	31,01064	0,01	0,0094	31,49707	0,1	0,0886	36,84885
2	23	0,0001	0,0001	30,18842	0,0001	0,0001	30,22393	0,01	0,00881	30,60989	0,01	0,0094	30,87855	0,1	0,0886	34,85052
1	24	0,0001	0,0001	29,95775	0,0001	0,0001	29,97253	0,01	0,00881	30,6743	0,01	0,0094	30,31713	0,1	0,0886	32,50742

Calculated efficiency		94,8338	89,4175		94,5630	89,4306		92,4054	89,4033		90,9594	89,3142		92,0234	89,2101	
simulated efficiency		90,12	87,3		89,94	87,31		88,28	87,29		88,91	87,32		89,97	87,29	
difference		4,713805	2,117526		4,622958	2,120555		4,125385	2,113253		2,049447	1,9941963		2,053356	1,920121	

Table I.2: Data from simulation of scenario 2B5 in Aspen HYSYS (Kent-Eisenberg)

Scenario 6w

Scenario 6w		SF1*0,591 (79,00%)			SF2*0,599 (79,01%)			Zhu*0,669 (79,02%)			Lin*0,708 (79,04%)			0.1*0,664 (79,04%)		
		Removal grade		79	Removal grade		79,01	Removal grade		79,02	Removal grade		79,04	Removal grade		79,04
		Rich loading		0,4426	Rich loading		0,4426	Rich loading		0,4426	Rich loading		0,4427	Rich loading		0,4426
Height (m)	Step	EM (H14)	EM*0,778	T	EM(H14)	EM*0,79	T	EM(H14)	EM*0,88	T	EM	EM*0,935	T	EM	EM*0,886	T
24	1	0,245	0,1906	46,44101	0,24	0,1896	46,45285	0,23	0,20263	46,36482	0,17	0,1590	46,31302	0,1	0,0886	45,55251
23	2	0,2425	0,1887	49,4237	0,235	0,1857	49,4429	0,2192	0,193115	49,30871	0,17	0,1590	49,33061	0,1	0,0886	48,54922
22	3	0,24	0,1867	50,01988	0,23	0,1817	50,05084	0,2085	0,183689	49,88009	0,17	0,1590	50,01751	0,1	0,0886	49,40882
21	4	0,2375	0,1848	49,77749	0,225	0,1778	49,83095	0,1977	0,174174	49,6286	0,17	0,1590	49,90349	0,1	0,0886	49,53891
20	5	0,235	0,1828	49,17348	0,22	0,1738	49,26648	0,1869	0,164659	49,04514	0,17	0,1590	49,47054	0,1	0,0886	49,4152
19	6	0,2325	0,1809	48,33231	0,215	0,1699	48,49098	0,18	0,15858	48,27815	0,16	0,1496	48,85475	0,1	0,0886	49,19119
18	7	0,23	0,1789	47,26312	0,23	0,1817	47,52709	0,1762	0,155232	47,35258	0,15	0,1403	48,11853	0,1	0,0886	48,91454
17	8	0,2	0,1556	45,93161	0,2	0,1580	46,26198	0,1546	0,136203	46,24646	0,14	0,1309	47,28099	0,1	0,0886	48,5983
16	9	0,17	0,1323	44,44316	0,17	0,1343	44,82589	0,1438	0,126688	45,03704	0,13	0,1216	46,34905	0,1	0,0886	48,24397
15	10	0,14	0,1089	42,87605	0,14	0,1106	43,30419	0,1331	0,117261	43,70836	0,12	0,1122	45,32775	0,1	0,0886	47,84895
14	11	0,11	0,0856	41,30946	0,11	0,0869	41,77883	0,1223	0,107746	42,26122	0,11	0,1029	44,22469	0,1	0,0886	47,40872
13	12	0,08	0,0622	39,82779	0,08	0,0632	40,3344	0,1115	0,098232	40,70858	0,1	0,0935	43,04981	0,1	0,0886	46,91777
12	13	0,05	0,0389	38,46205	0,055	0,0435	39,01699	0,1007	0,088717	39,03163	0,09	0,0841	41,81853	0,1	0,0886	46,36922
11	14	0,0475	0,0370	37,3481	0,0525	0,0415	37,90777	0,09	0,07929	37,27153	0,08	0,0748	40,54881	0,1	0,0886	45,75536
10	15	0,045	0,0350	36,3421	0,05	0,0395	36,87716	0,01	0,00881	35,45702	0,07	0,0655	39,26551	0,1	0,0886	45,06664
9	16	0,0425	0,0331	35,37985	0,0475	0,0375	35,86871	0,01	0,00881	34,28323	0,06	0,0561	37,93476	0,1	0,0886	44,29154
8	17	0,04	0,0311	34,43302	0,045	0,0356	34,85999	0,01	0,00881	33,45555	0,05	0,0468	36,63035	0,1	0,0886	43,41663
7	18	0,0375	0,0292	33,48937	0,0425	0,0336	33,84153	0,01	0,00881	32,82256	0,04	0,0374	35,37716	0,1	0,0886	42,42652
6	19	0,035	0,0272	32,54433	0,04	0,0316	32,81053	0,01	0,00881	32,30053	0,03	0,0281	34,2037	0,1	0,0886	41,30311
5	20	0,0001	0,0001	31,59555	0,0001	0,0001	31,76481	0,01	0,00881	31,84156	0,02	0,0187	33,14101	0,1	0,0886	40,02391
4	21	0,0001	0,0001	30,9512	0,0001	0,0001	31,05818	0,01	0,00881	31,41722	0,01	0,0094	32,22497	0,1	0,0886	38,56275
3	22	0,0001	0,0001	30,50387	0,0001	0,0001	30,56884	0,01	0,00881	31,01064	0,01	0,0094	31,49707	0,1	0,0886	36,84885
2	23	0,0001	0,0001	30,18842	0,0001	0,0001	30,22393	0,01	0,00881	30,60989	0,01	0,0094	30,87855	0,1	0,0886	34,85052
1	24	0,0001	0,0001	29,95775	0,0001	0,0001	29,97253	0,01	0,00881	30,6743	0,01	0,0094	30,31713	0,1	0,0886	32,50742
Calculated efficiency		94,8338	81,1911		94,5630	81,1672		92,4054	81,1847		90,9594	81,0858		92,0234	80,7753	
simulated efficiency		90,02	79,00		89,88	79,01		89,60	79,02		88,91	79,04		89,72	79,04	
difference		4,813805	2,191092		4,682958	2,1572		2,805385	2,16466		2,049447	2,045797		2,303356	1,735271	

Table I.3: Data from simulation of scenario 6w in Aspen HYSYS (Kent-Eisenberg)

Scenario Goal1

Scenario Goal1		SF1*0,854 (90,11%)			SF2*0,886 (90,09%)			Zhu*0,966 (90,09%)			Lin*1,029 (90,10%)			0.1*0,974 (90,09%)		
		Removal grade		90,11	Removal grade		90,09	Removal grade		90,09	Removal grade		90,1	Removal grade		90,09
		Rich loading		0,4207	Rich loading		0,4207	Rich loading		0,4207	Rich loading		0,4207	Rich loading		0,4207
Height (m)	Step	EM (H14)	EM*0,778	T	EM(H14)	EM*0,79	T	EM(H14)	EM*0,88	T	EM	EM*0,935	T	EM	EM*0,886	T
24	1	0,245	0,1906	46,44101	0,24	0,1896	46,45285	0,23	0,20263	46,36482	0,17	0,1590	46,31302	0,1	0,0886	45,55251
23	2	0,2425	0,1887	49,4237	0,235	0,1857	49,4429	0,2192	0,193115	49,30871	0,17	0,1590	49,33061	0,1	0,0886	48,54922
22	3	0,24	0,1867	50,01988	0,23	0,1817	50,05084	0,2085	0,183689	49,88009	0,17	0,1590	50,01751	0,1	0,0886	49,40882
21	4	0,2375	0,1848	49,77749	0,225	0,1778	49,83095	0,1977	0,174174	49,6286	0,17	0,1590	49,90349	0,1	0,0886	49,53891
20	5	0,235	0,1828	49,17348	0,22	0,1738	49,26648	0,1869	0,164659	49,04514	0,17	0,1590	49,47054	0,1	0,0886	49,4152
19	6	0,2325	0,1809	48,33231	0,215	0,1699	48,49098	0,18	0,15858	48,27815	0,16	0,1496	48,85475	0,1	0,0886	49,19119
18	7	0,23	0,1789	47,26312	0,23	0,1817	47,52709	0,1762	0,155232	47,35258	0,15	0,1403	48,11853	0,1	0,0886	48,91454
17	8	0,2	0,1556	45,93161	0,2	0,1580	46,26198	0,1546	0,136203	46,24646	0,14	0,1309	47,28099	0,1	0,0886	48,5983
16	9	0,17	0,1323	44,44316	0,17	0,1343	44,82589	0,1438	0,126688	45,03704	0,13	0,1216	46,34905	0,1	0,0886	48,24397
15	10	0,14	0,1089	42,87605	0,14	0,1106	43,30419	0,1331	0,117261	43,70836	0,12	0,1122	45,32775	0,1	0,0886	47,84895
14	11	0,11	0,0856	41,30946	0,11	0,0869	41,77883	0,1223	0,107746	42,26122	0,11	0,1029	44,22469	0,1	0,0886	47,40872
13	12	0,08	0,0622	39,82779	0,08	0,0632	40,3344	0,1115	0,098232	40,70858	0,1	0,0935	43,04981	0,1	0,0886	46,91777
12	13	0,05	0,0389	38,46205	0,055	0,0435	39,01699	0,1007	0,088717	39,03163	0,09	0,0841	41,81853	0,1	0,0886	46,36922
11	14	0,0475	0,0370	37,3481	0,0525	0,0415	37,90777	0,09	0,07929	37,27153	0,08	0,0748	40,54881	0,1	0,0886	45,75536
10	15	0,045	0,0350	36,3421	0,05	0,0395	36,87716	0,01	0,00881	35,45702	0,07	0,0655	39,26551	0,1	0,0886	45,06664
9	16	0,0425	0,0331	35,37985	0,0475	0,0375	35,86871	0,01	0,00881	34,28323	0,06	0,0561	37,93476	0,1	0,0886	44,29154
8	17	0,04	0,0311	34,43302	0,045	0,0356	34,85999	0,01	0,00881	33,45555	0,05	0,0468	36,63035	0,1	0,0886	43,41663
7	18	0,0375	0,0292	33,48937	0,0425	0,0336	33,84153	0,01	0,00881	32,82256	0,04	0,0374	35,37716	0,1	0,0886	42,42652
6	19	0,035	0,0272	32,54433	0,04	0,0316	32,81053	0,01	0,00881	32,30053	0,03	0,0281	34,2037	0,1	0,0886	41,30311
5	20	0,0001	0,0001	31,59555	0,0001	0,0001	31,76481	0,01	0,00881	31,84156	0,02	0,0187	33,14101	0,1	0,0886	40,02391
4	21	0,0001	0,0001	30,9512	0,0001	0,0001	31,05818	0,01	0,00881	31,41722	0,01	0,0094	32,22497	0,1	0,0886	38,56275
3	22	0,0001	0,0001	30,50387	0,0001	0,0001	30,56884	0,01	0,00881	31,01064	0,01	0,0094	31,49707	0,1	0,0886	36,84885
2	23	0,0001	0,0001	30,18842	0,0001	0,0001	30,22393	0,01	0,00881	30,60989	0,01	0,0094	30,87855	0,1	0,0886	34,85052
1	24	0,0001	0,0001	29,95775	0,0001	0,0001	29,97253	0,01	0,00881	30,6743	0,01	0,0094	30,31713	0,1	0,0886	32,50742
Calculated efficiency		94,8338	0,0000	#	94,5630	91,6593		92,4054	94,1292		90,9594	91,6139		92,0234	94,0620	
simulated efficiency		90,3	90,11	#	90,02	90,09		90,2	90,09		89,91	90,1		89,97	90,09	
difference		4,533805	-90,11	#	4,542958	1,569294		2,205385	4,03917		1,049447	1,513906		2,053356	3,971972	

Table I.4: Data from simulation of scenario Goal1 in Aspen HYSYS (Kent-Eisenberg)

Scenario F17

Scenario F17		SF1*0,671 (83,51%)			SF2*0,68 (83,50%)			Zhu*0,76 (83,54%)			Lin*0,81 (83,51%)			0.1*0,761 (83,49%)		
		Removal grade		83,51	Removal grade		83,5	Removal grade		83,54	Removal grade		83,51	Removal grade		83,49
		Rich loading		0,4354	Rich loading		0,4353	Rich loading		0,4354	Rich loading		0,4353	Rich loading		0,4353
Height (m)	Step	EM (H14)	EM*0,671	T	EM(H14)	EM*0,68	T	EM(H14)	EM*0,76	T	EM	EM*0,81	T	EM	EM*0,761	T
24	1	0,245	0,1644	46,56386	0,24	0,1632	46,535464	0,23	0,1748	46,455015	0,17	0,13685	46,412	0,1	0,0761	45,88199
23	2	0,2425	0,1627	49,69863	0,235	0,1598	49,664709	0,2192	0,166592	49,541338	0,17	0,13685	49,58039	0,1	0,0761	49,10222
22	3	0,24	0,1610	50,38244	0,23	0,1564	50,354819	0,2085	0,15846	50,19734	0,17	0,13685	50,35815	0,1	0,0761	50,09258
21	4	0,2375	0,1594	50,17242	0,225	0,1530	50,162358	0,1977	0,150252	49,977286	0,17	0,13685	50,27677	0,1	0,0761	50,28837
20	5	0,235	0,1577	49,58039	0,22	0,1496	49,604363	0,1869	0,142044	49,404879	0,17	0,13685	49,85083	0,1	0,0761	50,19976
19	6	0,2325	0,1560	48,75399	0,215	0,1462	48,836643	0,18	0,1368	48,649504	0,16	0,1288	49,23669	0,1	0,0761	49,99853
18	7	0,23	0,1543	47,71706	0,23	0,1564	47,895007	0,1762	0,133912	47,748128	0,15	0,12075	48,50725	0,1	0,0761	49,74036
17	8	0,2	0,1342	46,44547	0,2	0,1360	46,684662	0,1546	0,117496	46,686465	0,14	0,1127	47,68652	0,1	0,0761	49,44154
16	9	0,17	0,1141	45,03606	0,17	0,1156	45,326555	0,1438	0,109288	45,53804	0,13	0,10465	46,78343	0,1	0,0761	49,10508
15	10	0,14	0,0939	43,5555	0,14	0,0952	43,895712	0,1331	0,101156	44,285826	0,12	0,0966	45,80341	0,1	0,0761	48,72899
14	11	0,11	0,0738	42,06904	0,11	0,0748	42,45902	0,1223	0,092948	42,926887	0,11	0,08855	44,75239	0,1	0,0761	48,30878
13	12	0,08	0,0537	40,6472	0,08	0,0544	41,087216	0,1115	0,08474	41,461972	0,1	0,0805	43,63769	0,1	0,0761	47,83926
12	13	0,05	0,0336	39,36715	0,055	0,0374	39,856939	0,1007	0,076532	39,897602	0,09	0,07245	42,46943	0,1	0,0761	47,31309
11	14	0,0475	0,0319	38,31365	0,0525	0,0357	38,814125	0,09	0,0684	38,212142	0,08	0,0644	41,25999	0,1	0,0761	46,72341
10	15	0,045	0,0302	37,31795	0,05	0,0340	37,847421	0,01	0,0076	36,409475	0,07	0,05635	40,02409	0,1	0,0761	46,05962
9	16	0,0425	0,0285	36,36103	0,0475	0,0323	36,853094	0,01	0,0076	35,202827	0,06	0,0483	38,77978	0,1	0,0761	45,30973
8	17	0,04	0,0268	35,40799	0,045	0,0306	35,850149	0,01	0,0076	34,325948	0,05	0,04025	37,51217	0,1	0,0761	44,45984
7	18	0,0375	0,0252	34,43906	0,0425	0,0289	34,817489	0,01	0,0076	33,639361	0,04	0,0322	36,26933	0,1	0,0761	43,49247
6	19	0,035	0,0235	33,44131	0,04	0,0272	33,740492	0,01	0,0076	33,063529	0,03	0,02415	35,07892	0,1	0,0761	42,38661
5	20	0,0001	0,0001	32,40377	0,0001	0,0001	32,605354	0,01	0,0076	32,551638	0,02	0,0161	33,97429	0,1	0,0761	41,1158
4	21	0,0001	0,0001	31,6643	0,0001	0,0001	31,799405	0,01	0,0076	32,072696	0,01	0,00805	32,99398	0,1	0,0761	39,64469
3	22	0,0001	0,0001	31,12427	0,0001	0,0001	31,211752	0,01	0,0076	31,608348	0,01	0,00805	32,18628	0,1	0,0761	37,92874
2	23	0,0001	0,0001	30,72278	0,0001	0,0001	30,774157	0,01	0,0076	31,145663	0,01	0,00805	31,4781	0,1	0,0761	35,85459
1	24	0,0001	0,0001	30,41848	0,0001	0,0001	30,441574	0,01	0,0076	30,6743	0,01	0,00805	30,82119	0,1	0,0761	33,33372

Calculated efficiency	94,8338	85,2487	#	94,5630	85,2151		92,4054	85,2513	#	90,9594	85,1453	#	92,0234	85,0377	
simulated efficiency	90,12	83,51	#	89,94	83,5		88,28	83,54	#	89,54	83,51	#	90,77	83,49	
difference	4,713805	1,7387035	#	4,6229585	1,71514		4,125385	1,711287	#	1,419447	1,63526	#	1,253356	1,5476706	

Table I.5: Data from simulation of scenario F17 in Aspen HYSYS (Kent-Eisenberg)

Appendix J – Data from simulation with estimated Murphree efficiency (Plus)

Scenario H14

Scenario H14		SF1*0.995 (90,05%)				SF2*1.005 (89,98%)				Zhu*1.120 (90.05%)				Lin *1.170 (90,00%)				0.1 *1.100 (90.03%)		
		Removal grade		90,12		Removal grade		89,94		Removal grade		90		Removal grade		90		Removal grade		90,01
		Rich loading		0,4936		Rich loading		0,4931		Rich loading		0,4933		Rich loading		0,4885		Rich loading		0,4427
Height (m)	Step	EM	EM	T		EM	EM	T		EM	EM	T		EM	EM	T		EM	EM	T
24	1	0,245	0,244	48,0479		0,24	0,241	48,0322		0,23	0,258	47,9127		0,17	0,1989	47,849		0,1	0,1100	46,8969
23	2	0,2425	0,241	51,5593		0,235	0,236	51,5426		0,2192	0,246	51,3808		0,17	0,1989	51,3963		0,1	0,1100	50,4122
22	3	0,24	0,239	52,266		0,23	0,231	52,2572		0,2085	0,234	52,0643		0,17	0,1989	52,2095		0,1	0,1100	51,4071
21	4	0,2375	0,236	52,0289		0,225	0,226	52,0406		0,1977	0,221	51,8184		0,17	0,1989	52,1283		0,1	0,1100	51,5771
20	5	0,235	0,234	51,3817		0,22	0,221	51,436		0,1869	0,209	51,1961		0,17	0,1989	51,7012		0,1	0,1100	51,4735
19	6	0,2325	0,231	50,4389		0,215	0,216	50,5718		0,18	0,202	50,3458		0,16	0,1872	51,0667		0,1	0,1100	51,2654
18	7	0,23	0,229	49,1798		0,23	0,231	49,4525		0,1762	0,197	49,2756		0,15	0,1755	50,2806		0,1	0,1100	51,0019
17	8	0,2	0,199	47,5244		0,2	0,201	47,8998		0,1546	0,173	47,9347		0,14	0,1638	49,3527		0,1	0,1100	50,6949
16	9	0,17	0,169	45,5971		0,17	0,171	46,0646		0,1438	0,161	46,409		0,13	0,1521	48,2808		0,1	0,1100	50,344
15	10	0,14	0,139	43,5139		0,14	0,141	44,0616		0,1331	0,149	44,67		0,12	0,1404	47,0622		0,1	0,1100	49,9446
14	11	0,11	0,109	41,416		0,11	0,111	42,0229		0,1223	0,137	42,7273		0,11	0,1287	45,6983		0,1	0,1100	49,4897
13	12	0,08	0,080	39,4438		0,08	0,080	40,0854		0,1115	0,125	40,636		0,1	0,117	44,1985		0,1	0,1100	48,9707
12	13	0,05	0,050	37,7052		0,055	0,055	38,3669		0,1007	0,113	38,4925		0,09	0,1053	42,5834		0,1	0,1100	48,3768
11	14	0,0475	0,047	36,2848		0,0525	0,053	36,9196		0,09	0,101	36,3987		0,08	0,0936	40,8878		0,1	0,1100	47,6952
10	15	0,045	0,045	35,0123		0,05	0,050	35,5924		0,01	0,011	34,3986		0,07	0,0819	39,1587		0,1	0,1100	46,9099
9	16	0,0425	0,042	33,8159		0,0475	0,048	34,3256		0,01	0,011	33,0556		0,06	0,0702	37,4479		0,1	0,1100	46,0012
8	17	0,04	0,040	32,6626		0,045	0,045	33,0944		0,01	0,011	32,0599		0,05	0,0585	35,7994		0,1	0,1100	44,9447
7	18	0,0375	0,037	31,5333		0,0425	0,043	31,8838		0,01	0,011	31,2532		0,04	0,0468	34,2426		0,1	0,1100	43,7096
6	19	0,035	0,035	30,4128		0,04	0,040	30,6799		0,01	0,011	30,5482		0,03	0,0351	32,793		0,1	0,1100	42,2579
5	20	0,0001	0,000	29,2767		0,0001	0,000	29,4565		0,01	0,011	29,8941		0,02	0,0234	31,4618		0,1	0,1100	40,5437
4	21	0,0001	0,000	28,4308		0,0001	0,000	28,5511		0,01	0,011	29,2589		0,01	0,0117	30,2676		0,1	0,1100	38,5169
3	22	0,0001	0,000	27,782		0,0001	0,000	27,8593		0,01	0,011	28,6209		0,01	0,0117	29,2551		0,1	0,1100	36,1343
2	23	0,0001	0,000	27,2725		0,0001	0,000	27,3175		0,01	0,011	27,9636		0,01	0,0117	28,3319		0,1	0,1100	33,3737
1	24	0,0001	0,000	26,8625		0,0001	0,000	26,8822		0,01	0,011	27,2706		0,01	0,0117	27,4366		0,1	0,1100	30,2124
Calculated efficiency		94,83380484	94,747378 %			94,56295847	94,65050401 %			92,4054	94,6178564 %			90,95945	94,20941 %			92,02336	93,89957 %	
simulated efficiency		90,12	90,05 %			89,94	89,98 %			90	90,05 %			90	90 %			90,01	90,03 %	
difference		4,713804836	4,6973783			4,62295847	4,670504012		0	2,40538	4,56785642		0	0,959447	4,209407		0	2,013356	3,869574	

Rate based (IAF=1) (88,82%)
88,82
0,4894
54,4007
52,0345
52,1856
51,7759
51,4076
50,9679
50,4612
49,8871
49,2292
48,4911
47,6571
46,7325
45,7046
44,5816
43,3554
42,0418
40,6432
39,1879
37,6946
36,2078
34,7614
33,4075
32,1762
31,101
30,1823
29,4207
28,7907
28,2788
27,8569
27,5147
27,2299
26,9983
26,8029
26,6439
26,508
26,3979
26,3024
26,226
26,1587
26,1059
26,0584
26,0224
25,9892
25,9653
25,9424
25,9274
25,9122
25,9045
25,8984
25,9097
24,73440003

Table J.1: Data from simulation of scenario H14 in Aspen Plus (eNRTL & Rate-based)

Scenario 6w

Scenario 6w		SF1*0,603 (78,98%)			SF2*0,612 (79,03%)			Zhu*0,680 (78,92%)			Lin*0,722 (79,03%)			0.1*0,680 (79,07%)		
		Removal grade		78,98	Removal grade		79,03	Removal grade		78,92	Removal grade		79,03	Removal grade		79,07
		Rich loading		0,4426	Rich loading		0,4426	Rich loading		0,4426	Rich loading		0,4427	Rich loading		0,4426
Height (m)	Step	EM (H14)	EM*0,603	T	EM(H14)	EM*0,612	T	EM(H14)	EM*0,68	T	EM	EM*0,722	T	EM	EM*0,680	T
24	1	0,245	0,1477	46,4959	0,24	0,1469	46,4914	0,23	0,1564	46,3661	0,17	0,1227	46,3046	0,1	0,0680	45,2186
23	2	0,2425	0,1462	49,5581	0,235	0,1438	49,5559	0,2192	0,149056	49,3737	0,17	0,1227	49,402	0,1	0,0680	48,2375
22	3	0,24	0,1447	50,1567	0,23	0,1408	50,1645	0,2085	0,14178	49,9427	0,17	0,1227	50,1041	0,1	0,0680	49,1326
21	4	0,2375	0,1432	49,8718	0,225	0,1377	49,9005	0,1977	0,134436	49,6474	0,17	0,1227	49,9573	0,1	0,0680	49,2594
20	5	0,235	0,1417	49,2137	0,22	0,1346	49,2801	0,1869	0,127092	49,0107	0,17	0,1227	49,4733	0,1	0,0680	49,1065
19	6	0,2325	0,1402	48,3259	0,215	0,1316	48,455	0,18	0,1224	48,1968	0,16	0,1155	48,8044	0,1	0,0680	48,8409
18	7	0,23	0,1387	47,2284	0,23	0,1408	47,4587	0,1762	0,119816	47,2386	0,15	0,1083	48,0228	0,1	0,0680	48,5176
17	8	0,2	0,1206	45,8889	0,2	0,1224	46,1829	0,1546	0,105128	46,1161	0,14	0,1011	47,1509	0,1	0,0680	48,1533
16	9	0,17	0,1025	44,4026	0,17	0,1040	44,7505	0,1438	0,097784	44,9024	0,13	0,0939	46,1957	0,1	0,0680	47,7514
15	10	0,14	0,0844	42,8294	0,14	0,0857	43,2313	0,1331	0,090508	43,5739	0,12	0,0866	45,1599	0,1	0,0680	47,3102
14	11	0,11	0,0663	41,2283	0,11	0,0673	41,6865	0,1223	0,083164	42,1173	0,11	0,0794	44,0466	0,1	0,0680	46,8258
13	12	0,08	0,0482	39,6686	0,08	0,0490	40,187	0,1115	0,07582	40,5219	0,1	0,0722	42,8586	0,1	0,0680	46,2932
12	13	0,05	0,0302	38,2356	0,055	0,0337	38,8174	0,1007	0,068476	38,7782	0,09	0,0650	41,6003	0,1	0,0680	45,7057
11	14	0,0475	0,0286	37,0364	0,0525	0,0321	37,6382	0,09	0,0612	36,8723	0,08	0,0578	40,2786	0,1	0,0680	45,0558
10	15	0,045	0,0271	35,9243	0,05	0,0306	36,5176	0,01	0,0068	34,7642	0,07	0,0505	38,9025	0,1	0,0680	44,3336
9	16	0,0425	0,0256	34,8267	0,0475	0,0291	35,39	0,01	0,0068	33,3427	0,06	0,0433	37,486	0,1	0,0680	43,5276
8	17	0,04	0,0241	33,7044	0,045	0,0275	34,2182	0,01	0,0068	32,292	0,05	0,0361	36,0448	0,1	0,0680	42,6228
7	18	0,0375	0,0226	32,5321	0,0425	0,0260	32,9783	0,01	0,0068	31,4487	0,04	0,0289	34,6002	0,1	0,0680	41,6
6	19	0,035	0,0211	31,2893	0,04	0,0245	31,6462	0,01	0,0068	30,7213	0,03	0,0217	33,1808	0,1	0,0680	40,4342
5	20	0,0001	0,0001	29,9461	0,0001	0,0001	30,1843	0,01	0,0068	30,055	0,02	0,0144	31,8244	0,1	0,0680	39,0913
4	21	0,0001	0,0001	28,9518	0,0001	0,0001	29,1106	0,01	0,0068	29,4149	0,01	0,0072	30,584	0,1	0,0680	37,5233
3	22	0,0001	0,0001	28,1889	0,0001	0,0001	28,2913	0,01	0,0068	28,7767	0,01	0,0072	29,528	0,1	0,0680	35,6597
2	23	0,0001	0,0001	27,5873	0,0001	0,0001	27,6473	0,01	0,0068	28,1224	0,01	0,0072	28,566	0,1	0,0680	33,3904
1	24	0,0001	0,0001	27,0992	0,0001	0,0001	27,1262	0,01	0,0068	27,4338	0,01	0,0072	27,6365	0,1	0,0680	30,5261

Calculated efficiency	94,8338	81,1911		94,5630	81,1672		92,4054	81,1847		90,9594	81,0858		92,0234	80,7753	
simulated efficiency	90,02	78,98		89,88	79,03		89,60	78,92		88,91	79,03		89,72	79,07	
difference	4,813805	2,211092		4,682958	2,1372		2,805385	2,26466		2,049447	2,055797		2,303356	1,705271	

Rate based (IAF=0,29) (79,04%)
79,04
0,487
42,5532
46,1021
48,0197
48,9304
49,2977
49,3901
49,3462
49,233
49,0828
48,9103
48,7226
48,5227
48,3122
48,0911
47,8599
47,618
47,3655
47,1018
46,8268
46,5398
46,2406
45,9288
45,6039
45,2653
44,9128
44,5456
44,1634
43,7655
43,3516
42,9209
42,4729
42,0069
41,5223
41,0184
40,4944
39,9494
39,3826
38,793
38,1795
37,5409
36,876
36,1831
35,4609
34,7079
33,9221
33,1013
32,2426
31,3432
30,3996
29,4079

Table J.2: Data from simulation of scenario 6w in Aspen Plus (eNRTL & Rate-based)

Scenario 2B5

Scenario 2B5		SF1*0,887 (87,29%)			SF2*0,900 (87,29%)			Zhu*1,008 (87,31%)			Lin*1,004 (87,30%)			0.1*1,008 (87,30%)		
		Removal grade		87,29	Removal grade		87,29	Removal grade		87,31	Removal grade		87,3	Removal grade		87,3
		Rich loading		0,4891	Rich loading		0,4891	Rich loading		0,4892	Rich loading		0,4891	Rich loading		0,4891
Height (m)	Step	EM (H14)	EM*0,887	T	EM(H14)	EM*0,9	T	EM(H14)	EM*1,008	T	EM	EM*1,004	T	EM	EM*1,008	T
24	1	0,245	0,2173	47,8166	0,24	0,2160	47,8146	0,23	0,23184	47,7536	0,17	0,1707	47,7309	0,1	0,1008	47,2108
23	2	0,2425	0,2151	50,857	0,235	0,2115	50,8571	0,2192	0,220954	50,7561	0,17	0,1707	50,8287	0,1	0,1008	50,3592
22	3	0,24	0,2129	51,3287	0,23	0,2070	51,3379	0,2085	0,210168	51,1978	0,17	0,1707	51,4107	0,1	0,1008	51,1323
21	4	0,2375	0,2107	50,9731	0,225	0,2025	51,0041	0,1977	0,199282	50,8266	0,17	0,1707	51,2118	0,1	0,1008	51,1932
20	5	0,235	0,2084	50,2578	0,22	0,1980	50,3317	0,1869	0,188395	50,1294	0,17	0,1707	50,7127	0,1	0,1008	51,0318
19	6	0,2325	0,2062	49,2769	0,215	0,1935	49,4268	0,18	0,18144	49,2305	0,16	0,1606	50,0246	0,1	0,1008	50,7857
18	7	0,23	0,2040	48,0111	0,23	0,2070	48,2927	0,1762	0,17761	48,1332	0,15	0,1506	49,1988	0,1	0,1008	50,4914
17	8	0,2	0,1774	46,3928	0,2	0,1800	46,7603	0,1546	0,155837	46,7898	0,14	0,1406	48,245	0,1	0,1008	50,1558
16	9	0,17	0,1508	44,5563	0,17	0,1530	44,9941	0,1438	0,14495	45,2963	0,13	0,1305	47,1643	0,1	0,1008	49,7775
15	10	0,14	0,1242	42,6178	0,14	0,1260	43,1121	0,1331	0,134165	43,6312	0,12	0,1205	45,9579	0,1	0,1008	49,3514
14	11	0,11	0,0976	40,7097	0,11	0,0990	41,2412	0,1223	0,123278	41,8159	0,11	0,1104	44,6329	0,1	0,1008	48,8711
13	12	0,08	0,0710	38,961	0,08	0,0720	39,5088	0,1115	0,112392	39,9172	0,1	0,1004	43,2046	0,1	0,1008	48,3286
12	13	0,05	0,0444	37,4672	0,055	0,0495	38,0193	0,1007	0,101506	38,0378	0,09	0,0904	41,7012	0,1	0,1008	47,7145
11	14	0,0475	0,0421	36,2999	0,0525	0,0473	36,8136	0,09	0,09072	36,2801	0,08	0,0803	40,1651	0,1	0,1008	47,0175
10	15	0,045	0,0399	35,2945	0,05	0,0450	35,7459	0,01	0,01008	34,6891	0,07	0,0703	38,6479	0,1	0,1008	46,2242
9	16	0,0425	0,0377	34,3869	0,0475	0,0428	34,7654	0,01	0,01008	33,7252	0,06	0,0602	37,2031	0,1	0,1008	45,3183
8	17	0,04	0,0355	33,552	0,045	0,0405	33,8545	0,01	0,01008	33,0783	0,05	0,0502	35,8748	0,1	0,1008	44,281
7	18	0,0375	0,0333	32,7793	0,0425	0,0383	33,0081	0,01	0,01008	32,5978	0,04	0,0402	34,6888	0,1	0,1008	43,0905
6	19	0,035	0,0310	32,0635	0,04	0,0360	32,2227	0,01	0,01008	32,2068	0,03	0,0301	33,6571	0,1	0,1008	41,7238
5	20	0,0001	0,0001	31,3937	0,0001	0,0001	31,4873	0,01	0,01008	31,8647	0,02	0,0201	32,7833	0,1	0,1008	40,1611
4	21	0,0001	0,0001	30,98	0,0001	0,0001	31,0344	0,01	0,01008	31,5495	0,01	0,0100	32,0726	0,1	0,1008	38,3976
3	22	0,0001	0,0001	30,7207	0,0001	0,0001	30,7511	0,01	0,01008	31,2491	0,01	0,0100	31,5409	0,1	0,1008	36,4626
2	23	0,0001	0,0001	30,5564	0,0001	0,0001	30,5718	0,01	0,01008	30,957	0,01	0,0100	31,1078	0,1	0,1008	34,4289
1	24	0,0001	0,0001	30,4448	0,0001	0,0001	30,4507	0,01	0,01008	30,6625	0,01	0,0100	30,7233	0,1	0,1008	32,3765

Calculated efficiency	94,8338	89,4175		94,5630	89,4306		92,4054	89,4033		90,9594	89,3142		92,0234	89,2101	
simulated efficiency	90,12	87,29		89,94	87,29		88,28	87,31		88,91	87,3		89,97	87,3	
difference	4,713805	2,127526		4,622958	2,140555		4,125385	2,093253		2,049447	2,0141963		2,053356	1,910121	

Rate based (IAF=1) (86,14%)
86,14
0,4857
54,2651
50,8566
51,2477
50,662
50,2149
49,6563
49,0256
48,3131
47,5079
46,6129
45,6183
44,5307
43,3452
42,076
40,7294
39,3329
37,9102
36,5089
35,1725
33,9602
32,9111
32,0585
31,3961
30,9098
30,558
30,3153
30,144
30,0308
29,9504
29,9002
29,8634
29,8427
29,8261
29,8191
29,8117
29,8109
29,8077
29,8097
29,8084
29,8115
29,8111
29,8148
29,8147
29,8186
29,8187
29,8228
29,8234
29,8291
29,8356
29,865

Table J.3: Data from simulation of scenario 2B5 in Aspen Plus (eNRTL & Rate-based)

Scenario Goal1

Scenario Goal1		SF1*0,896 (90,11%)			SF2*0,910 (90,11%)			Zhu*1,015 (90,12%)			Lin*1,074 (90,12%)			0.1*1,025 (90,09%)		
		Removal grade		90,11	Removal grade		90,11	Removal grade		90,12	Removal grade		90,12	Removal grade		90,09
		Rich loading		0,487	Rich loading		0,487	Rich loading		0,4871	Rich loading		0,4871	Rich loading		0,4869
Height (m)	Step	EM (H14)	EM*0,896	T	EM(H14)	EM*0,91	T	EM	EM*1,015	T	EM	EM*1,074	T	EM	EM*1,025	T
24	1	0,245	0,2195	47,3613	0,24	0,2184	47,3587	0,23	0,23345	47,259	0,17	0,1826	47,2302	0,1	0,1025	46,4696
23	2	0,2425	0,2173	50,1803	0,235	0,2139	50,179	0,2192	0,222488	50,0396	0,17	0,1826	50,0885	0,1	0,1025	49,3283
22	3	0,24	0,2150	50,591	0,23	0,2093	50,5973	0,2085	0,211628	50,4253	0,17	0,1826	50,5911	0,1	0,1025	49,9963
21	4	0,2375	0,2128	50,2682	0,225	0,2048	50,293	0,1977	0,200666	50,0908	0,17	0,1826	50,4006	0,1	0,1025	50,036
20	5	0,235	0,2106	49,6335	0,22	0,2002	49,6955	0,1869	0,189704	49,4752	0,17	0,1826	49,95	0,1	0,1025	49,8861
19	6	0,2325	0,2083	48,7625	0,215	0,1957	48,8926	0,18	0,1827	48,6833	0,16	0,1718	49,3323	0,1	0,1025	49,6646
18	7	0,23	0,2061	47,6287	0,23	0,2093	47,8791	0,1762	0,178843	47,712	0,15	0,1611	48,5893	0,1	0,1025	49,4012
17	8	0,2	0,1792	46,1536	0,2	0,1820	46,4849	0,1546	0,156919	46,5111	0,14	0,1504	47,7263	0,1	0,1025	49,1008
16	9	0,17	0,1523	44,4406	0,17	0,1547	44,8462	0,1438	0,145957	45,161	0,13	0,1396	46,7403	0,1	0,1025	48,7614
15	10	0,14	0,1254	42,5662	0,14	0,1274	43,046	0,1331	0,135097	43,6207	0,12	0,1289	45,6289	0,1	0,1025	48,3781
14	11	0,11	0,0986	40,6252	0,11	0,1001	41,1771	0,1223	0,124135	41,8736	0,11	0,1181	44,3906	0,1	0,1025	47,9447
13	12	0,08	0,0717	38,7375	0,08	0,0728	39,3561	0,1115	0,113173	39,9227	0,1	0,1074	43,0297	0,1	0,1025	47,4537
12	13	0,05	0,0448	37,0379	0,055	0,0501	37,7171	0,1007	0,102211	37,7984	0,09	0,0967	41,5549	0,1	0,1025	46,8959
11	14	0,0475	0,0426	35,6728	0,0525	0,0478	36,3452	0,09	0,09135	35,5781	0,08	0,0859	39,9842	0,1	0,1025	46,2602
10	15	0,045	0,0403	34,4313	0,05	0,0455	35,0578	0,01	0,01015	33,3454	0,07	0,0752	38,3475	0,1	0,1025	45,5332
9	16	0,0425	0,0381	33,239	0,0475	0,0432	33,7933	0,01	0,01015	32,026	0,06	0,0644	36,6851	0,1	0,1025	44,698
8	17	0,04	0,0358	32,0723	0,045	0,0410	32,5376	0,01	0,01015	31,1435	0,05	0,0537	35,0484	0,1	0,1025	43,7337
7	18	0,0375	0,0336	30,9302	0,0425	0,0387	31,2943	0,01	0,01015	30,4785	0,04	0,0430	33,4895	0,1	0,1025	42,6137
6	19	0,035	0,0314	29,8158	0,04	0,0364	30,0741	0,01	0,01015	29,9229	0,03	0,0322	32,0556	0,1	0,1025	41,304
5	20	0,0001	0,0001	28,721	0,0001	0,0001	28,8722	0,01	0,01015	29,421	0,02	0,0215	30,7877	0,1	0,1025	39,7612
4	21	0,0001	0,0001	28,0421	0,0001	0,0001	28,1303	0,01	0,01015	28,9433	0,01	0,0107	29,7222	0,1	0,1025	37,931
3	22	0,0001	0,0001	27,6113	0,0001	0,0001	27,6611	0,01	0,01015	28,4733	0,01	0,0107	28,9109	0,1	0,1025	35,7531
2	23	0,0001	0,0001	27,3336	0,0001	0,0001	27,3591	0,01	0,01015	28,002	0,01	0,0107	28,2311	0,1	0,1025	33,1843
1	24	0,0001	0,0001	27,1449	0,0001	0,0001	27,1549	0,01	0,01015	27,5161	0,01	0,0107	27,61	0,1	0,1025	30,2409

Calculated efficiency		94,8338	91,6846	#	94,5630	91,6593		92,4054	94,1292		90,9594	91,6139		92,0234	94,0620	
simulated efficiency		90,3	90,11	#	90,02	90,11		90,2	90,12		89,91	90,12		89,97	90,09	
difference		4,533805	1,574602	#	4,542958	1,549294		2,205385	4,00917		1,049447	1,493906		2,053356	3,971972	

Rate based [0,51] (90,11%)
90,11 0,487
48,8326
50,8846
50,9133
50,791
50,6474
50,492
50,3213
50,1374
49,9361
49,7194
49,4832
49,2293
48,9537
48,658
48,3383
47,9964
47,628
47,2352
46,8141
46,3664
45,8887
45,3828
44,8453
44,2784
43,6791
43,05
42,3886
41,6981
40,9765
40,2277
39,4508
38,6507
37,8277
36,9884
36,1351
35,276
34,4157
33,5646
32,7293
31,9218
31,1494
30,4241
29,7521
29,1424
28,5971
28,1199
27,7076
27,3593
27,0694
26,837

Table J.4: Data from simulation of scenario Goal1 in Aspen Plus (eNRTL & Rate-based)

Scenario F17

Scenario F17		SF1*0,772 (83,51%)			SF2*0,732 (83,49%)			Zhu*0,818 (83,49%)			Lin*0,863 (83,51%)			0.1*1,1 (83,50%)		
		Removal grade		83,51	Removal grade		83,49	Removal grade		83,49	Removal grade		83,51	Removal grade		83,5
		Rich loading		0,4837	Rich loading		0,4836	Rich loading		0,4836	Rich loading		0,4837	Rich loading		0,4836
Height (m)	Step	EM (H14)	EM*0,772	T	EM(H14)	EM*0,732	T	EM(H14)	EM*0,818	T	EM	EM*0,863	T	EM	EM*1,1	T
24	1	0,245	0,1891	47,6719	0,24	0,1757	47,6682	0,23	0,18814	47,6049	0,17	0,14671	47,5929	0,1	0,11	47,0789
23	2	0,2425	0,1872	50,3556	0,235	0,1720	50,3538	0,2192	0,179306	50,2486	0,17	0,14671	50,3387	0,1	0,11	49,8924
22	3	0,24	0,1853	50,6487	0,23	0,1684	50,6564	0,2085	0,170553	50,5122	0,17	0,14671	50,7421	0,1	0,11	50,5008
21	4	0,2375	0,1834	50,2124	0,225	0,1647	50,2418	0,1977	0,161719	50,0637	0,17	0,14671	50,4554	0,1	0,11	50,4844
20	5	0,235	0,1814	49,4706	0,22	0,1610	49,541	0,1869	0,152884	49,3447	0,17	0,14671	49,9107	0,1	0,11	50,2808
19	6	0,2325	0,1795	48,508	0,215	0,1574	48,6488	0,18	0,14724	48,4653	0,16	0,13808	49,2043	0,1	0,11	50,0065
18	7	0,23	0,1776	47,3125	0,23	0,1684	47,571	0,1762	0,144132	47,4301	0,15	0,12945	48,3859	0,1	0,11	49,6909
17	8	0,2	0,1544	45,8303	0,2	0,1464	46,1598	0,1546	0,126463	46,2005	0,14	0,12082	47,4674	0,1	0,11	49,3391
16	9	0,17	0,1312	44,1826	0,17	0,1244	44,571	0,1438	0,117628	44,8658	0,13	0,11219	46,4524	0,1	0,11	48,9499
15	10	0,14	0,1081	42,4548	0,14	0,1025	42,8968	0,1331	0,108876	43,4004	0,12	0,10356	45,3434	0,1	0,11	48,5192
14	11	0,11	0,0849	40,7378	0,11	0,0805	41,2268	0,1223	0,100041	41,8031	0,11	0,09493	44,1459	0,1	0,11	48,0422
13	12	0,08	0,0618	39,1342	0,08	0,0586	39,661	0,1115	0,091207	40,0967	0,1	0,0863	42,8709	0,1	0,11	47,5128
12	13	0,05	0,0386	37,742	0,055	0,0403	38,2994	0,1007	0,082373	38,3273	0,09	0,07767	41,5344	0,1	0,11	46,9239
11	14	0,0475	0,0367	36,6599	0,0525	0,0384	37,1957	0,09	0,07362	36,5674	0,08	0,06904	40,16	0,1	0,11	46,2671
10	15	0,045	0,0347	35,7099	0,05	0,0366	36,1962	0,01	0,00818	34,8755	0,07	0,06041	38,7809	0,1	0,11	45,5324
9	16	0,0425	0,0328	34,8276	0,0475	0,0348	35,247	0,01	0,00818	33,9248	0,06	0,05178	37,4349	0,1	0,11	44,7079
8	17	0,04	0,0309	33,9921	0,045	0,0329	34,3341	0,01	0,00818	33,3226	0,05	0,04315	36,1619	0,1	0,11	43,7793
7	18	0,0375	0,0290	33,1994	0,0425	0,0311	33,4596	0,01	0,00818	32,89	0,04	0,03452	34,9979	0,1	0,11	42,7296
6	19	0,035	0,0270	32,451	0,04	0,0293	32,6286	0,01	0,00818	32,5415	0,03	0,02589	33,9723	0,1	0,11	41,5387
5	20	0,0001	0,0001	31,7397	0,0001	0,0001	31,8351	0,01	0,00818	32,2351	0,02	0,01726	33,1047	0,1	0,11	40,1844
4	21	0,0001	0,0001	31,3422	0,0001	0,0001	31,3931	0,01	0,00818	31,9497	0,01	0,00863	32,4115	0,1	0,11	38,6449
3	22	0,0001	0,0001	31,1167	0,0001	0,0001	31,1429	0,01	0,00818	31,6747	0,01	0,00863	31,9168	0,1	0,11	36,9079
2	23	0,0001	0,0001	30,9873	0,0001	0,0001	30,9996	0,01	0,00818	31,4047	0,01	0,00863	31,5235	0,1	0,11	34,9886
1	24	0,0001	0,0001	30,9098	0,0001	0,0001	30,9142	0,01	0,00818	31,1345	0,01	0,00863	31,1807	0,1	0,11	32,9464

Calculated efficiency	94,8338	85,2487	#	94,5630	85,2151		92,4054	85,2513	#	90,9594	85,1453	#	92,0234	85,0377	
simulated efficiency	90,12	83,51	#	89,94	83,49		88,28	83,49	#	89,54	83,51	#	90,77	83,5	
difference	4,713805	1,7387035	#	4,6229585	1,72514		4,125385	1,761287	#	1,419447	1,63526	#	1,253356	1,5376706	

Rate based (0,51) (83.48%)
83,48
0,4836
48,7205
51,0303
51,1265
50,9802
50,8001
50,6067
50,3986
50,1777
49,9411
49,6904
49,4227
49,1397
48,8385
48,5208
48,1838
47,8293
47,4547
47,0617
46,6479
46,2152
45,7614
45,2884
44,7941
44,2808
43,7467
43,1944
42,6226
42,0341
41,4283
40,8086
40,1748
39,5311
38,8782
38,2212
37,5618
36,9058
36,256
35,6192
34,9988
34,402
33,8326
33,2975
32,7996
32,3448
31,9337
31,5698
31,2509
30,9776
30,7457
30,5542

Table J.5: Data from simulation of scenario F17 in Aspen Plus (eNRTL & Rate-based)

Appendix K – Comparison of Rate-based and Equilibrium-stage in HYSYS and Plus

Scenario H14

	Comparison HYSYS and Plus - Scenario H14											
	SF1		SF2		Zhu		Lin		0.1		Rate-based	
	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	Plus	
EM-Factor	1.0	0.995	1.0	1.005	1.106	1.120	1.159	1.170	1.101	1.100	IAF = 1	
Removal grade[9	90,12	90,05	89,94	89,98	90	90,05	90,01	90	90,01	90,03	8882,00 %	
Rich loading	0,4936	0,4929	0,4931	0,4929	0,4932	0,4929	0,4933	0,4928	0,4932	0,4928	0,4894	
Temp-profile	46,43	48,05	46,41	48,03	45,59	47,91	45,53	47,85	44,79	46,90	54,401	29,4
	49,81	51,56	49,78	51,54	48,58	51,38	48,60	51,40	47,82	50,41	52,035	28,8
	50,59	52,27	50,58	52,26	49,21	52,06	49,37	52,21	48,75	51,41	52,186	28,3
	50,39	52,03	50,41	52,04	48,96	51,82	49,30	52,13	48,93	51,58	51,776	27,9
	49,72	51,38	49,79	51,44	48,32	51,20	48,86	51,70	48,83	51,47	51,408	27,5
	48,72	50,44	48,89	50,57	47,43	50,35	48,20	51,07	48,61	51,27	50,968	27,2
	47,37	49,18	47,70	49,45	46,32	49,28	47,37	50,28	48,33	51,00	50,461	27
	45,65	47,52	46,10	47,90	44,94	47,93	46,40	49,35	48,00	50,69	49,887	26,8
	43,69	45,60	44,25	46,06	43,40	46,41	45,29	48,28	47,62	50,34	49,229	26,6
	41,61	43,51	42,26	44,06	41,69	44,67	44,04	47,06	47,19	49,94	48,491	26,5
	39,58	41,42	40,28	42,02	39,80	42,73	42,67	45,70	46,70	49,49	47,657	26,4
	37,72	39,44	38,42	40,09	37,84	40,64	41,20	44,20	46,13	48,97	46,733	26,3
	36,12	37,71	36,80	38,37	35,92	38,49	39,61	42,58	45,49	48,38	45,705	26,2
	34,80	36,28	35,43	36,92	34,12	36,40	37,98	40,89	44,76	47,70	44,582	26,2
	33,64	35,01	34,20	35,59	32,50	34,40	36,35	39,16	43,92	46,91	43,355	26,1
	32,60	33,82	33,08	34,33	31,32	33,06	34,79	37,45	42,96	46,00	42,042	26,1
	31,63	32,66	32,03	33,09	30,39	32,06	33,34	35,80	41,85	44,94	40,643	26
	30,72	31,53	31,05	31,88	29,63	31,25	32,00	34,24	40,58	43,71	39,188	26
	29,85	30,41	30,11	30,68	28,97	30,55	30,79	32,79	39,13	42,26	37,695	26
	29,02	29,28	29,20	29,46	28,38	29,89	29,70	31,46	37,40	40,54	36,208	25,9
	28,32	28,43	28,46	28,55	27,81	29,26	28,73	30,27	35,42	38,52	34,761	25,9
	27,73	27,78	27,82	27,86	27,26	28,62	27,87	29,26	33,21	36,13	33,408	25,9
	27,20	27,27	27,26	27,32	26,70	27,96	27,08	28,33	30,82	33,37	32,176	25,9
	26,73	26,86	26,76	26,88	26,14	27,27	26,31	27,44	28,29	30,21	31,101	25,9
											30,182	25,9
											29,421	24,7

Table K.1: Comparison of Rate-based (Aspen Plus) and Equilibrium (Aspen Plus & HYSYS) for Scenario H14

Scenario 2B5

	Comparison HYSYS and Plus - Scenario 2B5											
	SF1		SF2		Zhu		Lin		0.1		Rate-based	
	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	Plus	
EM-Factor	0,778	0,887	0,79	0,9	0,88	1,008	0,935	1,005	0,886	1,008	IAF = 1	
Removal grade[%	87,3	87,29	87,31	87,29	87,29	87,31	87,32	87,3	87,29	87,3	86,14	
Rich loading	0,4635	0,48909	0,4635	0,48909	0,4634	0,48916	0,4635	0,489123	0,4634	0,4891	0,4857	
Temp-profile	46,44	47,82	46,45	47,81	46,36	47,75	46,31	47,73	45,55	47,21	54,27	30,32
	49,42	50,86	49,44	50,86	49,31	50,76	49,33	50,83	48,55	50,36	50,86	30,14
	50,02	51,33	50,05	51,34	49,88	51,20	50,02	51,41	49,41	51,13	51,25	30,03
	49,78	50,97	49,83	51,00	49,63	50,83	49,90	51,21	49,54	51,19	50,66	29,95
	49,17	50,26	49,27	50,33	49,05	50,13	49,47	50,71	49,42	51,03	50,21	29,90
	48,33	49,28	48,49	49,43	48,28	49,23	48,85	50,02	49,19	50,79	49,66	29,86
	47,26	48,01	47,53	48,29	47,35	48,13	48,12	49,20	48,91	50,49	49,03	29,84
	45,93	46,39	46,26	46,76	46,25	46,79	47,28	48,25	48,60	50,16	48,31	29,83
	44,44	44,56	44,83	44,99	45,04	45,30	46,35	47,16	48,24	49,78	47,51	29,82
	42,88	42,62	43,30	43,11	43,71	43,63	45,33	45,96	47,85	49,35	46,61	29,81
	41,31	40,71	41,78	41,24	42,26	41,82	44,22	44,63	47,41	48,87	45,62	29,81
	39,83	38,96	40,33	39,51	40,71	39,92	43,05	43,20	46,92	48,33	44,53	29,81
	38,46	37,47	39,02	38,02	39,03	38,04	41,82	41,70	46,37	47,71	43,35	29,81
	37,35	36,30	37,91	36,81	37,27	36,28	40,55	40,17	45,76	47,02	42,08	29,81
	36,34	35,29	36,88	35,75	35,46	34,69	39,27	38,65	45,07	46,22	40,73	29,81
	35,38	34,39	35,87	34,77	34,28	33,73	37,93	37,20	44,29	45,32	39,33	29,81
	34,43	33,55	34,86	33,85	33,46	33,08	36,63	35,87	43,42	44,28	37,91	29,81
	33,49	32,78	33,84	33,01	32,82	32,60	35,38	34,69	42,43	43,09	36,51	29,81
	32,54	32,06	32,81	32,22	32,30	32,21	34,20	33,66	41,30	41,72	35,17	29,82
	31,60	31,39	31,76	31,49	31,84	31,86	33,14	32,78	40,02	40,16	33,96	29,82
	30,95	30,98	31,06	31,03	31,42	31,55	32,22	32,07	38,56	38,40	32,91	29,82
	30,50	30,72	30,57	30,75	31,01	31,25	31,50	31,54	36,85	36,46	32,06	29,82
	30,19	30,56	30,22	30,57	30,61	30,96	30,88	31,11	34,85	34,43	31,40	29,83
	29,96	30,44	29,97	30,45	30,67	30,66	30,32	30,72	32,51	32,38	30,91	29,84
											30,56	29,87

Table K.2: Comparison of Rate-based (Aspen Plus) and Equilibrium (Aspen Plus & HYSYS) for Scenario 2B5

Scenario 6w

	Comparison HYSYS and Plus - Scenario 6w											
	SF1		SF2		Zhu		Lin		0.1		Rate-based	
	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	Plus	
EM-Factor	0,591	0,603	0,599	0,612	0,669	0,68	0,708	0,722	0,664	0,68	IAF = 0.29	
Removal grade[%]	79	78,98	79,01	79,03	79,02	78,92	79,04	79,03	79,04	79,07	79,04	
Rich loading	0,4426	0,4418	0,4426	0,4420	0,4426	0,4413	0,4427	0,4419	0,4426	0,4420	0,4870	
Temp-profile	45,34	46,50	45,33	46,49	45,26	46,37	46,31	46,30	44,16	45,22	42,55	44,55
	48,31	49,56	48,30	49,56	48,17	49,37	49,33	49,40	47,04	48,24	46,10	44,16
	48,99	50,16	48,99	50,16	48,82	49,94	50,02	50,10	48,00	49,13	48,02	43,77
	48,77	49,87	48,79	49,90	48,59	49,65	49,90	49,96	48,19	49,26	48,93	43,35
	48,15	49,21	48,20	49,28	47,99	49,01	49,47	49,47	48,07	49,11	49,30	42,92
	47,28	48,33	47,39	48,46	47,19	48,20	48,85	48,80	47,81	48,84	49,39	42,47
	46,20	47,23	46,41	47,46	46,25	47,24	48,12	48,02	47,49	48,52	49,35	42,01
	44,89	45,89	45,16	46,18	45,15	46,12	47,28	47,15	47,11	48,15	49,23	41,52
	43,47	44,40	43,78	44,75	43,96	44,90	46,35	46,20	46,70	47,75	49,08	41,02
	41,98	42,83	42,34	43,23	42,69	43,57	45,33	45,16	46,25	47,31	48,91	40,49
	40,49	41,23	40,89	41,69	41,32	42,12	44,22	44,05	45,75	46,83	48,72	39,95
	39,06	39,67	39,50	40,19	39,85	40,52	43,05	42,86	45,21	46,29	48,52	39,38
	37,72	38,24	38,24	38,82	38,29	38,78	41,82	41,60	44,61	45,71	48,31	38,79
	36,58	37,04	37,11	37,64	36,57	36,87	40,55	40,28	43,95	45,06	48,09	38,18
	35,52	35,92	36,05	36,52	34,73	34,76	39,27	38,90	43,22	44,33	47,86	37,54
	34,50	34,83	35,00	35,39	33,39	33,34	37,93	37,49	42,40	43,53	47,62	36,88
	33,46	33,70	33,92	34,22	32,34	32,29	36,63	36,04	41,50	42,62	47,37	36,18
	32,39	32,53	32,80	32,98	31,47	31,45	35,38	34,60	40,48	41,60	47,10	35,46
	31,27	31,29	31,60	31,65	30,71	30,72	34,20	33,18	39,33	40,43	46,83	34,71
	30,08	29,95	30,32	30,18	30,00	30,06	33,14	31,82	38,02	39,09	46,54	33,92
	29,12	28,95	29,29	29,11	29,33	29,41	32,22	30,58	36,52	37,52	46,24	33,10
	28,31	28,19	28,43	28,29	28,65	28,78	31,50	29,53	34,76	35,66	45,93	32,24
	27,61	27,59	27,69	27,65	27,96	28,12	30,88	28,57	32,60	33,39	45,60	31,34
	26,98	27,10	27,01	27,13	27,21	27,43	30,32	27,64	29,92	30,53	45,27	30,40
											44,91	29,41

Table K.3: Comparison of Rate-based (Aspen Plus) and Equilibrium (Aspen Plus & HYSYS) for Scenario 6w

Scenario Goal1

	Comparison HYSYS and Plus - Scenario Goal1											
	SF1		SF2		Zhu		Lin		0.1		Rate-based	
	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	HYSYS	Plus	Plus	
EM-Factor	0,92	0,896	0,891	0,91	0,995	1,015	1,055	1,074	1,015	1,025	IAF = 0,51	
Removal grade[%]	90,1	90,11	90.11	90,11	90.10	90,12	90,11	90,11	90,09	90,09	90,11	
Rich loading	0.4904	0,487	0.4874	0,487	0.4873	0,4871	0.4875	0,4871	0,4872	0,4869	0,4870	
Temp-profile	44,98	47,36	44,88	47,36	44,82	47,26	44,78	47,23	44,07	46,47	48,83	43,05
	47,43	50,18	47,31	50,18	47,20	50,04	47,24	50,09	46,52	49,33	50,88	42,39
	47,90	50,59	47,76	50,60	47,62	50,43	47,78	50,59	47,22	50,00	50,91	41,70
	47,67	50,27	47,53	50,29	47,36	50,09	47,68	50,40	47,36	50,04	50,79	40,98
	47,10	49,63	47,00	49,70	46,81	49,48	47,30	49,95	47,30	49,89	50,65	40,23
	46,28	48,76	46,24	48,89	46,06	48,68	46,74	49,33	47,17	49,66	50,49	39,45
	45,17	47,63	45,26	47,88	45,13	47,71	46,04	48,59	46,99	49,40	50,32	38,65
	43,70	46,15	43,90	46,48	43,96	46,51	45,22	47,73	46,76	49,10	50,14	37,83
	41,99	44,44	42,31	44,85	42,65	45,16	44,27	46,74	46,49	48,76	49,94	36,99
	40,15	42,57	40,59	43,05	41,17	43,62	43,19	45,63	46,18	48,38	49,72	36,14
	38,26	40,63	38,85	41,18	39,53	41,87	42,00	44,39	45,80	47,94	49,48	35,28
	36,45	38,74	37,15	39,36	37,73	39,92	40,71	43,03	45,37	47,45	49,23	34,42
	34,84	37,04	35,65	37,72	35,79	37,80	39,33	41,55	44,86	46,90	48,95	33,56
	33,55	35,67	34,39	36,35	33,82	35,58	37,91	39,98	44,27	46,26	48,66	32,73
	32,41	34,43	33,24	35,06	31,92	33,35	36,40	38,35	43,59	45,53	48,34	31,92
	31,38	33,24	32,15	33,79	30,70	32,03	34,90	36,69	42,79	44,70	48,00	31,15
	30,42	32,07	31,11	32,54	29,87	31,14	33,46	35,05	41,86	43,73	47,63	30,42
	29,54	30,93	30,11	31,29	29,27	30,48	32,11	33,49	40,78	42,61	47,24	29,75
	28,74	29,82	29,18	30,07	28,80	29,92	30,90	32,06	39,52	41,30	46,81	29,14
	28,01	28,72	28,30	28,87	28,41	29,42	29,85	30,79	38,07	39,76	46,37	28,60
	27,53	28,04	27,73	28,13	28,08	28,94	28,99	29,72	36,34	37,93	45,89	28,12
	27,23	27,61	27,35	27,66	27,77	28,47	28,34	28,91	34,32	35,75	45,38	27,71
	27,06	27,33	27,13	27,36	27,49	28,00	27,81	28,23	32,03	33,18	44,85	27,36
	26,95	27,14	26,98	27,15	27,20	27,52	27,34	27,61	29,51	30,24	44,28	27,07
											43,68	26,84

Table K.4: Comparison of Rate-based (Aspen Plus) and Equilibrium (Plus & HYSYS) for Scenario Goal1

Scenario F17

	Comparison HYSYS and Plus - Scenario F17											
	SF1		**SF2**		**Zhu**		**Lin**		**0.1**		**Rate-based**	
	HYSYS	**Plus**	**HYSYS**	**Plus**	**HYSYS**	**Plus**	**HYSYS**	**Plus**	**HYSYS**	**Plus**	**Plus**	
EM-Factor	0,92	0,896	0,891	0,91	0,995	1,015	1,055	1,074	1,015	1,025	IAF = 0,51	
Removal grade[%]	83,51	83,51	83,5	83,49	83,54	83,49	83,51	83,51	83,49	83,5	83,48	
Rich loading	0,4354	0,4837	0,4353	0,4836	0,4354	0,4836	0,4353	0,4837	0,4353	0,4836	0,4836	
Temp-profile	46,56	47,67	46,54	47,67	46,46	47,60	46,41	47,59	45,88	47,08	48,72	43,19
	49,70	50,36	49,66	50,35	49,54	50,25	49,58	50,34	49,10	49,89	51,03	42,62
	50,38	50,65	50,35	50,66	50,20	50,51	50,36	50,74	50,09	50,50	51,13	42,03
	50,17	50,21	50,16	50,24	49,98	50,06	50,28	50,46	50,29	50,48	50,98	41,43
	49,58	49,47	49,60	49,54	49,40	49,34	49,85	49,91	50,20	50,28	50,80	40,81
	48,75	48,51	48,84	48,65	48,65	48,47	49,24	49,20	50,00	50,01	50,61	40,17
	47,72	47,31	47,90	47,57	47,75	47,43	48,51	48,39	49,74	49,69	50,40	39,53
	46,45	45,83	46,68	46,16	46,69	46,20	47,69	47,47	49,44	49,34	50,18	38,88
	45,04	44,18	45,33	44,57	45,54	44,87	46,78	46,45	49,11	48,95	49,94	38,22
	43,56	42,45	43,90	42,90	44,29	43,40	45,80	45,34	48,73	48,52	49,69	37,56
	42,07	40,74	42,46	41,23	42,93	41,80	44,75	44,15	48,31	48,04	49,42	36,91
	40,65	39,13	41,09	39,66	41,46	40,10	43,64	42,87	47,84	47,51	49,14	36,26
	39,37	37,74	39,86	38,30	39,90	38,33	42,47	41,53	47,31	46,92	48,84	35,62
	38,31	36,66	38,81	37,20	38,21	36,57	41,26	40,16	46,72	46,27	48,52	35,00
	37,32	35,71	37,85	36,20	36,41	34,88	40,02	38,78	46,06	45,53	48,18	34,40
	36,36	34,83	36,85	35,25	35,20	33,92	38,78	37,43	45,31	44,71	47,83	33,83
	35,41	33,99	35,85	34,33	34,33	33,32	37,51	36,16	44,46	43,78	47,45	33,30
	34,44	33,20	34,82	33,46	33,64	32,89	36,27	35,00	43,49	42,73	47,06	32,80
	33,44	32,45	33,74	32,63	33,06	32,54	35,08	33,97	42,39	41,54	46,65	32,34
	32,40	31,74	32,61	31,84	32,55	32,24	33,97	33,10	41,12	40,18	46,22	31,93
	31,66	31,34	31,80	31,39	32,07	31,95	32,99	32,41	39,64	38,64	45,76	31,57
	31,12	31,12	31,21	31,14	31,61	31,67	32,19	31,92	37,93	36,91	45,29	31,25
	30,72	30,99	30,77	31,00	31,15	31,40	31,48	31,52	35,85	34,99	44,79	30,98
	30,42	30,91	30,44	30,91	30,67	31,13	30,82	31,18	33,33	32,95	44,28	30,75
											43,75	30,55

Table K.5: Comparison of Rate-based (Aspen Plus) and Equilibrium (Aspen Plus & HYSYS) for Scenario F17

Appendix L – Data from simulation with default Murphree efficiency (HYSYS)

Default efficiencies of each scenario, compared with estimated Murphree efficiencies										
SCENARIO	H14		2B5		6w		Goal1		F17	
Performance										
Removal grade	90.0	%	87.3	%	79.0	%	90.1	%	83.5	%
rich loading	0.48		0.50		0.46		0.50		0.48	
Simulation										
Removal grade	89.64	%	86.80	%	79.80	%	90.39	%	82.80	%
rich loading	0.4921		0.4619		0.4446		0.4883		0.4332	
number of stages	**14**		**10**		**8**		**13**		**8**	
From the top	EM	Temp	EM	Temp	EM	Temp	EM	Temp	EM	Temp
stage 1	0,2281	44,7420	0,2288	45,1199	0,2204	43,2570	0,2321	44,5271	0,2316	44,6293
stage 2	0,2327	47,5736	0,2370	47,7228	0,2249	45,3781	0,2360	46,7850	0,2388	47,0896
stage 3	0,2318	48,1973	0,2361	48,0537	0,2211	45,4028	0,2343	47,0592	0,2351	47,2408
stage 4	0,2279	47,9273	0,2300	47,4268	0,2115	44,3041	0,2300	46,5992	0,2271	46,2780
stage 5	0,2219	47,2082	0,2202	46,2509	0,1969	42,4206	0,2236	45,7525	0,2149	44,5751
stage 6	0,2136	46,1629	0,2066	44,6176	0,1775	39,8190	0,2148	44,5842	0,1963	42,1847
stage 7	0,2026	44,8054	0,1888	42,5241	0,1537	36,4545	0,2028	43,0755	0,1716	39,0642
stage 8	0,1883	43,1245	0,1670	39,9692	0,1263	32,1137	0,1870	41,1959	0,1426	35,1543
stage 9	0,1708	41,1260	0,1423	36,9582			0,1661	38,9476		
stage 10	0,1511	38,8131	0,1175	33,5340			0,1420	36,3798		
stage 11	0,1315	36,2787					0,1188	33,6217		
stage 12	0,1137	33,6392					0,0998	30,8545		
stage 13	0,0987	30,9876					0,0856	28,2022		
stage 14	0,0866	28,3315								

Table L.1: Data from simulation of all scenarios with default Murphree efficiencies (HYSYS, Kent-Eisenberg)

Appendix M – Data from simulation with different Amine Packages (HYSYS)

Scenario H14

SF1 (90,12%)			
EM	90,12	89,76	92,4
	0,4936	0,4925	0,4994
	K-E	L-M	A-G
0,245	46,4342258	46,375271	48,2461886
0,2425	49,8081863	49,7342237	51,78971
0,24	50,5942462	50,5205212	52,5506441
0,2375	50,3916977	50,3274063	52,4021596
0,235	49,7221879	49,6784739	51,8765501
0,2325	48,717496	48,7132793	51,0893233
0,23	47,3740912	47,4405605	50,0220597
0,2	45,64572	45,8305971	48,6051231
0,17	43,6919687	44,0351228	46,9209835
0,14	41,6084485	42,1485705	45,0376821
0,11	39,5754089	40,2934553	43,0464597
0,08	37,7206045	38,5666054	41,0696074
0,05	36,1177076	37,0377215	39,2542841
0,0475	34,7967801	35,7595895	37,7537596
0,045	33,6428227	34,6115189	36,3722083
0,0425	32,5978031	33,5349374	35,0252761
0,04	31,6304739	32,4991771	33,6751182
0,0375	30,7194473	31,4857051	32,3036075
0,035	29,852258	30,480374	30,8994102
0,0001	29,0155655	29,4694028	29,4465191
0,0001	28,3244528	28,6472166	28,3838979
0,0001	27,7288275	27,9528013	27,5642882
0,0001	27,2037386	27,3439944	26,9035992
0,0001	26,7299504	26,7966397	26,3483613

SF2 (89,94%)			
EM	89,94	89,55	92,12
	0,4931	0,4919	0,4986
	K-E	L-M	A-G
0,24	46,4113685	46,3431799	48,2162529
0,235	49,7839479	49,6961117	51,752214
0,23	50,5815423	50,489371	52,5156987
0,225	50,407563	50,3177753	52,3806515
0,22	49,7927544	49,7138016	51,8873336
0,215	48,8857809	48,8304612	51,1645391
0,23	47,7042106	47,6939947	50,210008
0,2	46,1033341	46,1824434	48,8819033
0,17	44,2540034	44,4649699	47,2895943
0,14	42,2624546	42,6761226	45,5065485
0,11	40,2756708	40,8585492	43,6198219
0,08	38,4241064	39,157909	41,7420489
0,055	36,7998207	37,6462777	40,0088318
0,0525	35,4279717	36,3524216	38,5148982
0,05	34,202939	35,1660927	37,0940872
0,0475	33,0791142	34,0360983	35,6776956
0,045	32,0309215	32,9366462	34,2373797
0,0425	31,0455979	31,8521395	32,7618493
0,04	30,1060051	30,7701351	31,2454384
0,0001	29,1991052	29,6772334	29,6749331
0,0001	28,4550561	28,7939661	28,5379972
0,0001	27,8190383	28,0538746	27,6640677
0,0001	27,259634	27,4068143	26,9623044
0,0001	26,7562372	26,8263997	26,37277

Zhu*1,106 (90,00%)			
EM	90	89,64	92,14
	0,4932	0,4922	0,4986
	K-E	L-M	A-G
0,2544	45,5944732	45,5226925	47,244311
0,2424	48,5798781	48,491851	50,3915384
0,2306	49,2122628	49,1254149	51,0035465
0,2187	48,9628532	48,8854323	50,7954208
0,2067	48,3200054	48,2605762	50,263583
0,1991	47,4315337	47,402061	49,5367493
0,1949	46,3151667	46,3333785	48,6206317
0,171	44,9382058	45,02989	47,4774334
0,159	43,3962696	43,5854605	46,171319
0,1472	41,6926451	42,0027997	44,6644414
0,1353	39,8032042	40,2688013	42,9345308
0,1233	37,8416443	38,4499175	40,9717039
0,1114	35,9157309	36,6094998	38,7811946
0,0995	34,1213457	34,8109839	36,3917526
0,0111	32,5014427	33,0929277	33,8578673
0,0111	31,3176839	31,852152	32,2315027
0,0111	30,3944828	30,8889038	31,1053444
0,0111	29,633161	30,0917737	30,2526249
0,0111	28,9731376	29,3943022	29,5351991
0,0111	28,376442	28,7545898	28,8711183
0,0111	27,8119185	28,1444996	28,2128189
0,0111	27,2559137	27,5315307	27,5316798
0,0111	26,6968454	26,9004847	26,8099251
0,0111	26,1352527	26,2467091	26,0152418

Lin*1,159 (90,01%)			
EM	90,01	89,63	91,85
	0,4933	0,4922	0,4977
	K-E	L-M	A-G
0,197	45,5320875	45,4506475	47,1908803
0,197	48,5994623	48,4980007	50,4116948
0,197	49,3691855	49,2651499	51,1371241
0,197	49,2950103	49,1932886	51,067633
0,197	48,8591013	48,7636835	50,6961444
0,1854	48,1980825	48,1154456	50,1460617
0,1739	47,3738681	47,3127945	49,4638142
0,1623	46,4034553	46,3748567	48,6554694
0,1507	45,2906169	45,3098147	47,715692
0,1391	44,0421069	44,126284	46,6383209
0,1275	42,6713357	42,8388432	45,4196878
0,1159	41,2026646	41,4702824	44,0616085
0,1043	39,610637	40,0065247	42,5739669
0,0927	37,9776636	38,5034235	40,9754415
0,0811	36,3542442	36,9927776	39,2908635
0,0695	34,7941013	35,5073346	37,5207097
0,058	33,3362422	34,074093	35,7271286
0,0464	32,0000833	32,7115544	33,9720087
0,0348	30,7886265	31,4311958	32,3070409
0,0232	29,6978804	30,2425144	30,7720015
0,0116	28,7251112	29,1601539	29,4031197
0,0116	27,8722519	28,2101949	28,2501178
0,0116	27,0762598	27,3161221	27,1949969
0,0116	26,3114794	26,4403434	26,1650436

0.1 *1,101 (90,01%)			
EM	90,01	89,87	91,92
	0,4932	0,4928	0,498
	K-E	L-M	A-G
0,1101	44,7875923	44,6188325	46,1441072
0,1101	47,8157598	47,6108184	49,3022913
0,1101	48,7530004	48,5468479	50,1825108
0,1101	48,9316644	48,730695	50,3308709
0,1101	48,8307824	48,6356862	50,2387658
0,1101	48,6135331	48,4242047	50,0545142
0,1101	48,3322484	48,1493883	49,8203502
0,1101	48,0007417	47,826357	49,5456983
0,1101	47,6211323	47,4566592	49,2297736
0,1101	47,1882573	47,0365621	48,8681068
0,1101	46,6955688	46,5597929	48,4542549
0,1101	46,1344955	46,0183666	47,9808822
0,1101	45,4936315	45,4027192	47,4395034
0,1101	44,7609489	44,7016003	46,8195179
0,1101	43,9217992	43,9018557	46,1069869
0,1101	42,9590958	42,9882033	45,2919077
0,1101	41,853358	41,943239	44,3438617
0,1101	40,5836482	40,7474721	43,2288232
0,1101	39,1285389	39,3807524	41,9066487
0,1101	37,3972112	37,7739185	40,3247269
0,1101	35,4216904	35,9237264	38,4110083
0,1101	33,2139572	33,8043621	36,0671237
0,1101	30,8240497	31,4027426	33,1652772
0,1101	28,2918834	28,6937152	29,5667061

Table M.1: Data from simulation of scenario H14 with different Amine Packages

Scenario 2B5

SF1*0,778 (87,30%)			
EM	87,3	86,63	87,86
	0,4635	0,4615	0,4643
	K-E	L-M	A-G
0,1906	46,441007	46,3885456	48,1312483
0,1887	49,4236972	49,3477662	51,2277414
0,1867	50,0198783	49,9253846	51,7390509
0,1848	49,7774947	49,6628621	51,445848
0,1828	49,1734784	49,0364376	50,8276609
0,1809	48,3323143	48,1718446	49,9893316
0,1789	47,2631248	47,0809453	48,9237246
0,1556	45,931612	45,7344767	47,578342
0,1323	44,4431562	44,2424027	46,0505158
0,1089	42,8760513	42,6849608	44,4080677
0,0856	41,3094649	41,1394403	42,7244139
0,0622	39,8277853	39,6864726	41,0875956
0,0389	38,4620532	38,3516877	39,5987746
0,037	37,3480952	37,2664801	38,3540403
0,035	36,3421048	36,2892808	37,1670017
0,0331	35,3798548	35,3550823	36,0153919
0,0311	34,4330242	34,4332076	34,8771972
0,0292	33,4893668	33,5090894	33,7297326
0,0272	32,5443261	32,5756312	32,5553376
0,0001	31,5955494	31,6282358	31,3451681
0,0001	30,9511987	30,9809803	30,6017399
0,0001	30,5038654	30,5272413	30,1256751
0,0001	30,1884188	30,2032298	29,8124311
0,0001	29,9577506	29,9652496	29,6013419

SF2*0,79 (87,31%)			
EM	87,31	86,66	87,89
	0,4635	0,4615	0,4644
	K-E	L-M	A-G
0,1896	46,4528457	46,3902322	48,1363314
0,1857	49,4429024	49,3535033	51,2366594
0,1817	50,0508443	49,9426338	51,756439
0,1778	49,8309519	49,7032307	51,4816434
0,1738	49,2664763	49,1173018	50,8978701
0,1699	48,4909811	48,3186412	50,1182969
0,1817	47,5270866	47,3310834	49,1449549
0,158	46,2619845	46,0474832	47,8560978
0,1343	44,8258867	44,6032501	46,376499
0,1106	43,3041856	43,0860336	44,7814504
0,0869	41,7788294	41,5753222	43,1488718
0,0632	40,3344017	40,1496696	41,5716345
0,0435	39,0169936	38,8523811	40,1549555
0,0415	37,9077695	37,7604472	38,954263
0,0395	36,8771631	36,7499039	37,7976501
0,0375	35,8687128	35,7656556	36,6092443
0,0356	34,8599919	34,7822801	35,3754476
0,0336	33,8415271	33,7877113	34,0988214
0,0316	32,8105327	32,7757308	32,7824065
0,0001	31,7648129	31,7410843	31,4297002
0,0001	31,0581827	31,041637	30,6210297
0,0001	30,568844	30,5574196	30,1232934
0,0001	30,2239266	30,2166767	29,8075801
0,0001	29,9725265	29,9686618	29,5997539

Zhu*0,88 (87,29%)			
EM	87,29	86,63	87,88
	0,4634	0,4615	0,4643
	K-E	L-M	A-G
0,2026	46,3648186	46,3052196	48,0200398
0,1931	49,3087064	49,2232304	51,0769353
0,1837	49,880093	49,7759566	51,564373
0,1742	49,6285977	49,5056076	51,2615279
0,1647	49,0451389	48,9028478	50,6624294
0,1586	48,2781527	48,116243	49,8941806
0,1552	47,3525779	47,1718717	48,9656676
0,1362	46,2464573	46,0500628	47,8468784
0,1267	45,03704	44,8297568	46,6062393
0,1173	43,7083583	43,4975411	45,2113813
0,1078	42,2612189	42,0562054	43,6464078
0,0982	40,7085823	40,5204729	41,904677
0,0887	39,031628	38,8729558	39,987515
0,0793	37,2715299	37,1543188	37,9070715
0,00881	35,4570228	35,3857155	35,6981673
0,00881	34,2832297	34,2399579	34,4521268
0,00881	33,4555502	33,4300243	33,650953
0,00881	32,8225638	32,8080394	33,0456133
0,00881	32,3005316	32,2930278	32,5209455
0,00881	31,8415612	31,8386149	32,0242444
0,00881	31,4172168	31,4175469	31,5303615
0,00881	31,0106397	31,0128331	31,0269104
0,00881	30,6098907	30,6131921	30,5154959
0,00881	30,6742999	30,6626694	30,2674148

Lin*0,935 (87,32%)			
EM	87,32	86,7	87,85
	0,4635	0,4616	0,4644
	K-E	L-M	A-G
0,1589	46,3130173	46,2676696	47,9584959
0,1589	49,3306149	49,2687619	51,0916443
0,1589	50,0175141	49,9450814	51,6924194
0,1589	49,9034911	49,8201806	51,5237663
0,1589	49,4705413	49,3753423	51,0721347
0,1496	48,8547514	48,7462523	50,456433
0,1403	48,1185332	47,9965775	49,7268771
0,1309	47,28099	47,1460148	48,8942065
0,1216	46,3490499	46,2023947	47,9588257
0,1122	45,3277477	45,1719708	46,9199877
0,1029	44,2246911	44,0630487	45,778774
0,0935	43,0498061	42,8874444	44,5396339
0,0842	41,8185302	41,6608525	43,2117626
0,0748	40,5488139	40,4026249	41,8099528
0,0655	39,2655097	39,1349421	40,3553567
0,0561	37,9347622	37,8274465	38,8754645
0,0468	36,6303532	36,5492683	37,4032271
0,0374	35,377165	35,3218506	35,9759447
0,0281	34,2037029	34,1711095	34,6337269
0,0187	33,1410069	33,1268718	33,4200298
0,00935	32,224969	32,2237414	32,3810077
0,00935	31,4970727	31,5031355	31,5665284
0,00935	30,878545	30,8868942	30,8457383
0,00935	30,3171294	30,3227955	30,1493016

0.1 *0,886 (87,29%)			
EM	87,29	86,78	87,87
	0,4634	0,4618	0,4643
	K-E	L-M	A-G
0,0886	45,5525108	45,5039813	47,1953991
0,0886	48,5492183	48,4833169	50,3115086
0,0886	49,4088242	49,3343814	51,0869835
0,0886	49,5389144	49,4575479	51,1620856
0,0886	49,4152003	49,3269403	51,0188998
0,0886	49,1911869	49,0957344	50,7938716
0,0886	48,9145356	48,8115434	50,524247
0,0886	48,5983026	48,4874711	50,2184641
0,0886	48,2439683	48,1250842	49,8761442
0,0886	47,8489547	47,7217863	49,4937958
0,0886	47,4087231	47,2731511	49,066356
0,0886	46,9177701	46,7735924	48,5876172
0,0886	46,3692159	46,2164912	48,0500444
0,0886	45,7553564	45,5941048	47,4446383
0,0886	45,0666389	44,8973846	46,7604745
0,0886	44,2915368	44,1157294	45,9841766
0,0886	43,4166252	43,236671	45,0991946
0,0886	42,4265238	42,2455041	44,084631
0,0886	41,3031108	41,1249148	42,9136967
0,0886	40,0239147	39,8545039	41,5511908
0,0886	38,5627541	38,4108805	39,9501452
0,0886	36,8488477	36,7255726	38,0462604
0,0886	34,8505171	34,7690935	35,749635
0,0886	32,5074239	32,47582	32,936282

Table M.2: Data from simulation of scenario 2B5 with different Amine Packages

Scenario 6w

SF1*0,591 (79,00%)			
EM	79	78,28	79,53
	0,4426	0,4406	0,4433
	K-E	L-M	A-G
0,1448	45,3437118	45,2631779	46,7942146
0,1433	48,3076912	48,1960163	49,865542
0,1418	48,991069	48,8630434	50,4320044
0,1404	48,7715543	48,6303382	50,1126804
0,1389	48,1460258	47,9925078	49,4171982
0,1374	47,2750391	47,1107877	48,4840047
0,1359	46,19534	46,0237151	47,3273269
0,1182	44,8943392	44,7212793	45,9170423
0,1005	43,4679217	43,2998683	44,3474394
0,0827	41,9805287	41,8232126	42,6830827
0,0650	40,4917605	40,3494266	40,9938435
0,0473	39,0628727	38,9380336	39,3626651
0,0296	37,7215397	37,6173635	37,8877099
0,0281	36,5797838	36,4955298	36,6733357
0,0266	35,5247169	35,461203	35,5601651
0,0251	34,4962868	34,454081	34,4672481
0,0236	33,4594765	33,4382001	33,350652
0,0222	32,3909416	32,3890547	32,1834049
0,0207	31,270301	31,2851332	30,9425386
0,0001	30,0780343	30,1054608	29,6107093
0,0001	29,1162154	29,1502026	28,617918
0,0001	28,313683	28,3493127	27,8349126
0,0001	27,6109263	27,6423627	27,186772
0,0001	26,9770221	26,9954868	26,6276587

SF2*0,599 (79,01%)			
EM	79,01	78,29	79,53
	0,4426	0,4406	0,4433
	K-E	L-M	A-G
0,1438	45,3322283	45,2652914	46,8029346
0,1408	48,2975408	48,2053022	49,8812852
0,1374	48,990846	48,8854131	50,4591364
0,1348	48,7920002	48,6755497	50,1595434
0,1318	48,2034636	48,0760846	49,4972693
0,1288	47,3928806	47,2548307	48,6162837
0,1378	46,4072978	46,2596449	47,5373351
0,1198	45,1646008	45,0128168	46,1716883
0,1018	43,7840802	43,6343779	44,6419853
0,0839	42,3390496	42,196992	43,0178905
0,0659	40,890929	40,7602306	41,3653155
0,0479	39,5031955	39,3845283	39,7636551
0,0329	38,2443328	38,1338264	38,3087753
0,0314	37,1120166	37,0100712	37,0778513
0,0300	36,0493776	35,9543076	35,9322039
0,0285	34,9971777	34,9091872	34,798271
0,0270	33,9210665	33,841569	33,6353187
0,0255	32,7967101	32,7278334	32,4163451
0,0240	31,6028618	31,5468692	31,1181409
0,0001	30,3159409	30,2741906	29,7195629
0,0001	29,2853878	29,2549567	28,6879879
0,0001	28,4301764	28,4083385	27,8762571
0,0001	27,6854437	27,6701914	27,2080248
0,0001	27,0134156	27,0051424	26,6302252

Zhu*0,669 (79,02%)			
EM	79,02	78,31	79,54
	0,4426	0,4407	0,4433
	K-E	L-M	A-G
0,1539	45,25502	45,1889499	46,7207597
0,1466	48,1695055	48,07833	49,7527581
0,1395	48,823279	48,7188827	50,2988355
0,1323	48,5938195	48,4786321	49,9788395
0,1250	47,9902671	47,8650401	49,3176562
0,1204	47,1920118	47,0578482	48,4758725
0,1179	46,2459956	46,104753	47,482228
0,1034	45,1462898	45,0008109	46,3187206
0,0962	43,9646225	43,8178943	45,0542222
0,0890	42,6897286	42,5458012	43,6632122
0,0818	41,31775	41,1818853	42,1279489
0,0746	39,8493473	39,7277874	40,4340609
0,0674	38,2872102	38,1863032	38,5703815
0,0602	36,5675692	36,4950325	36,5331441
0,0067	34,7259576	34,6824282	34,3397735
0,0067	33,3862389	33,3569268	32,9151299
0,0067	32,3396052	32,3170878	31,9059262
0,0067	31,4696893	31,450551	31,1037173
0,0067	30,7060679	30,6882374	30,3917663
0,0067	30,0025178	29,9846197	29,7095413
0,0067	29,3258112	29,3094432	29,0243594
0,0067	28,6517656	28,6386793	28,3291446
0,0067	27,9553033	27,9462268	27,6212814
0,0067	27,2084945	27,2030309	26,8942388

Lin*0,708 (79,04%)			
EM	79,04	78,37	79,52
	0,4427	0,4408	0,4433
	K-E	L-M	A-G
0,1204	46,3130173	45,0955887	46,6507817
0,1204	49,3306149	48,0664352	49,772315
0,1204	50,0175141	48,8404505	50,4496308
0,1204	49,9034911	48,7500155	50,2747684
0,1204	49,4705413	48,2887921	49,7625448
0,1133	48,8547514	47,623756	49,0648838
0,1062	48,1185332	46,8385712	48,2518386
0,0991	47,28099	45,9643216	47,3440889
0,0920	46,3490499	45,0139812	46,3456464
0,0850	45,3277477	43,9949632	45,2540518
0,0779	44,2246911	42,9136369	44,0675999
0,0708	43,0498061	41,7768631	42,7903056
0,0637	41,8185302	40,5922545	41,4359688
0,0566	40,5488139	39,3700275	40,0271508
0,0496	39,2655097	38,1220432	38,58896
0,0425	37,9347622	36,8201814	37,1424978
0,0354	36,6303532	35,5081354	35,6841558
0,0283	35,377165	34,1976277	34,2262282
0,0212	34,2037029	32,905907	32,7933928
0,0142	33,1410069	31,6574102	31,4199383
0,0071	32,224969	30,4853055	30,154347
0,0071	31,4970727	29,435411	29,0680473
0,0071	30,878545	28,444433	28,0732392
0,0071	30,3171294	27,4436153	27,1051908

0.1*0,664 (79,04%)			
EM	79,04	78,52	79,46
	0,4426	0,4412	0,4431
	K-E	L-M	A-G
0,0664	44,1550848	44,0969364	45,661799
0,0664	47,0423852	46,9671529	48,7475005
0,0664	48,0020429	47,9215931	49,6357498
0,0664	48,1890552	48,105133	49,745914
0,0664	48,0670004	47,9790373	49,5772316
0,0664	47,8113356	47,7187385	49,2967588
0,0664	47,486445	47,3889914	48,9589
0,0664	47,1146521	47,0123662	48,5810842
0,0664	46,7023967	46,5953279	48,1675304
0,0664	46,2496339	46,1378397	47,7157669
0,0664	45,7534053	45,6368019	47,2194375
0,0664	45,2089762	45,0872786	46,6684248
0,0664	44,6100848	44,4829865	46,0491678
0,0664	43,9490777	43,8160184	45,3470561
0,0664	43,2171802	43,0781125	44,5537955
0,0664	42,4040147	42,2605744	43,6840513
0,0664	41,4969942	41,3515402	42,721644
0,0664	40,4802149	40,3351691	41,6425412
0,0664	39,3325018	39,1908347	40,4176162
0,0664	38,0249324	37,8913778	39,0103994
0,0664	36,5183162	36,399074	37,3613211
0,0664	34,760174	34,6609781	35,3984399
0,0664	32,5989153	32,5277923	33,0121639
0,0664	29,9185772	29,8810104	30,0273898

Table M.3: Data from simulation of scenario 6w with different Amine Packages

Scenario Goal1

SF1*0,920 (90,10%)			
EM	90,1 0.4904	90,68 0,4893	92,05 0,4929
	K-E	L-M	A-G
0,2254	44,9779401	44,9379624	46,6847171
0,2231	47,4347861	47,3783518	49,3250486
0,2208	47,8960614	47,8286209	49,7752346
0,2185	47,6653619	47,5876681	49,5617952
0,2162	47,1041637	47,0164426	49,0590056
0,2139	46,281642	46,1857659	48,327636
0,2116	45,1693562	45,0726728	47,3331033
0,1840	43,7002175	43,6169794	45,9972403
0,1564	41,9928303	41,9436655	44,4128445
0,1288	40,1505045	40,1591454	42,6500056
0,1012	38,2616467	38,380063	40,7980861
0,0736	36,4507913	36,6496654	38,9742742
0,0460	34,8424734	35,1246358	37,3161229
0,0437	33,5486787	33,9026305	35,9563097
0,0414	32,413141	32,823603	34,6621803
0,0391	31,375659	31,8196231	33,3801842
0,0368	30,4180192	30,8644636	32,0966338
0,0345	29,5379079	29,950282	30,8095522
0,0322	28,7376377	29,0768318	29,5226176
0,0001	28,0098154	28,2388844	28,2406836
0,0001	27,5333107	27,6842268	27,4908626
0,0001	27,2322907	27,3285391	27,0548123
0,0001	27,0571941	27,1127452	26,8108132
0,0001	26,9544896	26,9790573	26,6788942

SF2*0,891 (90,11%)			
EM	90.11 0.4874	89,74 0.4861	91,06 0,4896
	K-E	L-M	A-G
0,2138	44,8793681	44,8494604	46,5900126
0,2094	47,3062286	47,2638402	49,2029522
0,2049	47,7569433	47,7062133	49,6395975
0,2005	47,5309706	47,471605	49,4218792
0,1960	46,9971955	46,9296166	48,9312623
0,1916	46,2398449	46,1663058	48,2416008
0,2049	45,2587235	45,180249	47,3343775
0,1782	43,8981501	43,8269808	46,0623313
0,1515	42,3061294	42,2572186	44,552207
0,1247	40,5866815	40,5766388	42,8815258
0,0980	38,8482964	38,8918954	41,1374791
0,0713	37,1538648	37,2649324	39,4269617
0,0490	35,6464823	35,822848	37,8735876
0,0468	34,3887608	34,6229926	36,5454319
0,0446	33,2420634	33,5244612	35,2446902
0,0423	32,1532519	32,4691783	33,9121307
0,0401	31,1094595	31,4374455	32,5436698
0,0379	30,1146925	30,4252931	31,1475882
0,0356	29,177987	29,4349929	29,7405867
0,0001	28,3041803	28,4693514	28,339363
0,0001	27,7273369	27,833722	27,5381895
0,0001	27,3541989	27,4191801	27,0801659
0,0001	27,1262676	27,1620223	26,8258377
0,0001	26,984001	26,9988784	26,686691

Zhu*0,995 (90,10%)			
EM	90.10 0.4873	89,73 0,4861	91,07 0,4896
	K-E	L-M	A-G
0,22885	44,8166129	44,7688424	46,4661818
0,218104	47,2047233	47,1371099	49,0381832
0,207458	47,6188174	47,5393514	49,4467381
0,196712	47,3584857	47,2683316	49,2056117
0,185966	46,8068503	46,7036618	48,7051668
0,1791	46,0642476	45,9484655	48,034534
0,175319	45,1288884	45,0056676	47,1867441
0,153827	43,9624416	43,8380935	46,1201796
0,143081	42,6511186	42,5331918	44,9009869
0,132435	41,1734539	41,0732087	43,4861612
0,121689	39,5345887	39,4673548	41,8508441
0,110943	37,7260293	37,7155918	39,9809732
0,100197	35,7939369	35,8606674	37,8764188
0,08955	33,8216876	33,9573291	35,5658971
0,00995	31,9173983	32,0746298	33,1324199
0,00995	30,7031359	30,8751988	31,7700644
0,00995	29,8729591	30,0503208	30,9008938
0,00995	29,2687517	29,4412091	30,2505542
0,00995	28,7976576	28,9628942	29,6923635
0,00995	28,4114933	28,5665053	29,1708518
0,00995	28,0753035	28,2162406	28,6631515
0,00995	27,770395	27,8878476	28,1610235
0,00995	27,4864077	27,5728054	27,6600285
0,00995	27,1968992	27,2444606	27,1430787

Lin*1,055 (90,11%)			
EM	90,11 0.4875	89,76 0,4862	91 0,4894
	K-E	L-M	A-G
0,17935	44,775511	44,7260847	47,1860194
0,17935	47,2415561	47,1759786	49,7706575
0,17935	47,7809333	47,7067805	50,3306534
0,17935	47,6762569	47,5942571	50,2119412
0,17935	47,3001513	47,2093661	49,8058813
0,1688	46,7420617	46,6418116	49,2071112
0,15825	46,0447875	45,9379324	48,4645187
0,1477	45,2200932	45,1087207	47,5897003
0,13715	44,2692302	44,1575556	46,5862212
0,1266	43,1947684	43,0886024	45,4584756
0,11605	42,0039218	41,9099724	44,2150209
0,1055	40,7095432	40,6355635	42,8705194
0,09495	39,3329507	39,2872184	41,4480154
0,0844	37,9061285	37,8988587	39,983296
0,07385	36,3987211	36,4438838	38,4482974
0,0633	34,9015766	35,0009348	36,9259863
0,05275	33,4559369	33,6039535	35,4521709
0,0422	32,1078435	32,2891812	34,0650862
0,03165	30,896945	31,0897785	32,7997163
0,0211	29,8514418	30,0343751	31,6862657
0,01055	28,9923407	29,1500808	30,7533352
0,01055	28,3417778	28,4711369	30,0370494
0,01055	27,8106674	27,905625	29,4404343
0,01055	27,3375407	27,3901138	28,89657

0.1*1,015 (90,09%)			
EM	90,09 0,4872	89,89 0,4865	91,19 0,49
	K-E	L-M	A-G
0,1015	44,0736494	43,9954806	45,6793363
0,1015	46,5170678	46,4198811	48,2937903
0,1015	47,2181831	47,1160161	48,9787139
0,1015	47,3567212	47,25172	49,1078273
0,1015	47,3030662	47,1953142	49,0601213
0,1015	47,1692086	47,058352	48,9404138
0,1015	46,9866651	46,8725001	48,7770545
0,1015	46,7620265	46,6443555	48,5758376
0,1015	46,4937481	46,3723165	48,3352229
0,1015	46,1767925	46,0520554	48,0507671
0,1015	45,8047132	45,6783666	47,7162815
0,1015	45,3699629	45,2444144	47,3242209
0,1015	44,8634205	44,7387549	46,8652805
0,1015	44,273304	44,1476778	46,3283199
0,1015	43,5864227	43,4623204	45,6994204
0,1015	42,7878788	42,672476	44,96148
0,1015	41,8596702	41,7565673	44,0930184
0,1015	40,7801055	40,6910387	43,0664776
0,1015	39,5245217	39,4591566	41,8460242
0,1015	38,066861	38,0396024	40,3838158
0,1015	36,3391925	36,3704924	38,6164847
0,1015	34,3241662	34,4321152	36,4600375
0,1015	32,0255487	32,2006486	33,8095528
0,1015	29,5100701	29,6789934	30,5339106

Table M.4: Data from simulation of scenario Goal1 with different Amine Packages

Scenario F17

SF1*0,671 (83,51%)			
EM	83,51	82,9	83,88
	0,4354	0,4336	0,4356
	K-E	**L-M**	**A-G**
0,1644	46,5638618	46,4854016	47,9924756
0,1627	49,6986308	49,5917898	51,2001989
0,161	50,3824386	50,2599244	51,7697829
0,1594	50,1724243	50,0357465	51,4756909
0,1577	49,5803863	49,4296086	50,8317086
0,156	48,7539877	48,5902769	49,9628817
0,1543	47,7170617	47,5438532	48,8734133
0,1342	46,4454712	46,2683737	47,5250763
0,1141	45,0360559	44,8621755	46,0106167
0,0939	43,555496	43,392556	44,3948272
0,0738	42,0690391	41,9231949	42,7512572
0,0537	40,6471963	40,5219419	41,1710137
0,0336	39,3671511	39,2623539	39,7603713
0,0319	38,3136512	38,2239963	38,628372
0,0302	37,3179524	37,2456168	37,5960907
0,0285	36,3610336	36,3044699	36,5828629
0,0268	35,4079878	35,3663172	35,5506857
0,0252	34,4390604	34,4112929	34,4796465
0,0235	33,4413121	33,4264668	33,3560828
0,0001	32,4037723	32,4004089	32,1713108
0,0001	31,6643048	31,666889	31,3896857
0,0001	31,124269	31,1291999	30,8337113
0,0001	30,7227815	30,7275356	30,4017676
0,0001	30,4184839	30,421212	30,0368103

SF2*0,68 (83,50%)			
EM	83,5	82,88	83,86
	0,4353	0,4336	0,4355
	K-E	**L-M**	**A-G**
0,1632	46,535464	46,4776756	48,0273314
0,1598	49,6647088	49,5855025	51,2448118
0,1564	50,3548189	50,2627904	51,8244221
0,153	50,1623581	50,0582998	51,547797
0,1496	49,6043633	49,487762	50,9344696
0,1462	48,8366427	48,7074821	50,1161668
0,1564	47,8950067	47,7545231	49,1038917
0,136	46,6846617	46,536264	47,7981451
0,1156	45,3265549	45,1755207	46,3202641
0,0952	43,8957117	43,7476838	44,7397886
0,0748	42,45902	42,3194243	43,1267863
0,0544	41,0872163	40,9598112	41,5674946
0,0374	39,8569386	39,7428672	40,1663906
0,0357	38,8141252	38,7120075	39,0030522
0,034	37,8474214	37,7566023	37,9235853
0,0323	36,8530941	36,77536	36,8558094
0,0306	35,8501492	35,7856108	35,7635162
0,0289	34,8174888	34,7663636	34,6260133
0,0272	33,7404919	33,7030527	33,4280315
0,0001	32,6053542	32,5811609	32,15898
0,0001	31,7994047	31,7840343	31,3309559
0,0001	31,2117521	31,2020814	30,7502649
0,0001	30,7741566	30,7686296	30,3196983
0,0001	30,4415741	30,438958	29,9815875

Zhu*0,76 (83,54%)			
EM	83,54	82,93	83,9
	0,4354	0,4337	0,4357
	K-E	**L-M**	**A-G**
0,1748	46,4550151	46,4010113	47,944278
0,1666	49,5413384	49,4648729	51,1168142
0,1585	50,1973398	50,1069257	51,6660093
0,1503	49,9772862	49,8733151	51,3681991
0,142	49,4048791	49,2875214	50,752249
0,1368	48,6495041	48,5186813	49,966058
0,1339	47,7481282	47,6043851	49,0296368
0,1175	46,6864649	46,532325	47,92041
0,1093	45,5380399	45,3754901	46,706707
0,1012	44,2858262	44,1200209	45,3616385
0,093	42,9268867	42,7625435	43,8692544
0,0847	41,4619722	41,3058416	42,2175821
0,0765	39,897602	39,7557832	40,397179
0,0684	38,2121419	38,1210266	38,4052637
0,0076	36,4094747	36,333694	36,2642712
0,0076	35,2028267	35,1350044	34,980192
0,0076	34,325948	34,2646745	34,1204863
0,0076	33,6393613	33,5837006	33,4622302
0,0076	33,0635289	33,0130211	32,8939554
0,0076	32,5516376	32,5058619	32,3613589
0,0076	32,0726962	32,0335292	31,8369005
0,0076	31,6083483	31,5773318	31,3154307
0,0076	31,145663	31,124176	30,7938302
0,0076	30,6742999	30,6626694	30,2674148

Lin*0,81 (83,51%)			
EM	83,51	82,94	83,84
	0,4353	0,4337	0,4355
	K-E	**L-M**	**A-G**
0,1368	46,4120033	46,3403595	47,9047755
0,1368	49,5803871	49,4845026	51,1640905
0,1368	50,3581506	50,249813	51,8348802
0,1368	50,2767697	50,1574115	51,6741672
0,1368	49,8508306	49,7198823	51,2025611
0,1288	49,2366859	49,0939199	50,5598837
0,1208	48,5072525	48,3531565	49,8071437
0,1127	47,6865202	47,5222156	48,9606599
0,1047	46,7834318	46,6108161	48,0233602
0,0966	45,8034134	45,6251025	46,9922072
0,0886	44,7523903	44,5715096	45,8638725
0,0805	43,6376874	43,4581269	44,6398395
0,0725	42,4694337	42,2952229	43,3322264
0,0644	41,2599885	41,0952971	41,963928
0,0564	40,0240882	39,8731098	40,5617403
0,0483	38,779784	38,6456494	39,1520414
0,0403	37,5121675	37,4325099	37,7424452
0,0322	36,269328	36,1991215	36,352975
0,0242	35,0789163	35,023104	35,0155157
0,0161	33,9742898	33,9324938	33,7744185
0,0081	32,9939789	32,964676	32,6870931
0,0081	32,1862812	32,1666602	31,8239186
0,0081	31,4780987	31,4656231	31,0796848
0,0081	30,8211877	30,8145532	30,3905617

0.1 *0,761 (83,49%)			
EM	83,49	83,13	83,93
	0,4353	0,4342	0,4357
	K-E	**L-M**	**A-G**
0,1	45,8819901	45,4913291	47,0134148
0,1	49,1022207	48,5962461	50,2598217
0,1	50,0925831	49,5443602	51,1242514
0,1	50,2883746	49,7086995	51,2232898
0,1	50,199762	49,586717	51,0717089
0,1	49,9985325	49,3493598	50,8257731
0,1	49,7403572	49,0535228	50,5311422
0,1	49,4415376	48,716744	50,1995217
0,1	49,1050804	48,3427747	49,8318964
0,1	48,7289884	47,9302664	49,425523
0,1	48,3087823	47,475696	48,9759706
0,1	47,8392575	46,9742839	48,4776535
0,1	47,313085	46,4202276	47,9238115
0,1	46,7234073	45,8066327	47,306327
0,1	46,0596165	45,1253213	46,6153605
0,1	45,3097279	44,3665237	45,8388492
0,1	44,4598402	43,5184288	44,961796
0,1	43,492469	42,5665731	43,9651988
0,1	42,3866082	41,4928943	42,8244857
0,1	41,1157985	40,2746669	41,5070232
0,1	39,6446902	38,8821631	39,9682498
0,1	37,9287428	37,2754473	38,1449078
0,1	35,8545875	35,3990736	35,9428175
0,1	33,3337217	33,0816047	33,2135459

Table M.5: Data from simulation of scenario F17 with different Amine Packages