# CO2-MEA SIMULATION by Aspen Plus

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*CONTENTS*

# 1 Background

This document deals solely with the calculation of CO2-MEA absorption and desorption using Aspen Plus.

It is taken as basic fact that the reboiler duty of a stripper in a CO2-MEA -unit, with "conventional" design is 4 MJ/kg CO2 captured.[1]

The CO2-MEA -package published by AspenTech on its support pages in February 2008 predicts a reboiler duty of about 30 % larger. This discrepancy the motivation of this study.

# 2 Aspen Plus CO2-MEA

In January 2008 Aspen Plus published - and in February revised - a (Aspen Plus 2006.5) CO2-MEA - model in Support Solution ID 122271.

In September 2010 Aspen Plus published an updated (Aspen Plus V7.2) CO2-MEA - model in Support Solution ID 129521.

## 2.1 Comparison - I

In the two Aspen+ models (2006.5 and V7.2) the same unit with the same feed is simulated.

The amine recirculation is not closed in the simulation. The results are presented in Table 1.

| 2006.5 | | CO2 | ABSORBER | | CO2 | STRIPPER | |
|---|---|---|---|---|---|---|---|
| PurePara | 21 | FG,IN | 3.40 | kmol/h | QR | 247.48 | kW |
| her BinPara | 21 | FG,OUT | 1.20 | kmol/h | QR/CO2 | 9.08 | MW/kg |
| Henry | 21 | | | | | | |
| NRTL | 21 | Capture | 2.20 | kmol/h | OUT | 2.23 | kmol/h |
| ElecPara | 21 | Capture | 64.79 | % | Recovery | 101.30 | % |
| CHEM+REA | 21 | | | | | | |
| Columns | 21 | FG,OUT | 0.064 | %-vol | CO2OUT | 100.00 | kg/h |
| **V7.2** | | **CO2** | ABSORBER | | **CO2** | STRIPPER | |
| PurePara | 24 | FG,IN | 3.40 | kmol/h | QR | 152.53 | kW |
| her BinPara | 24 | FG,OUT | 1.04 | kmol/h | QR/CO2 | 5.83 | MW/kg |
| Henry | 24 | | | | | | |
| NRTL | 24 | Capture | 2.36 | kmol/h | OUT | 2.14 | kmol/h |
| ElecPara | 24 | Capture | 69.30 | % | Recovery | 90.92 | % |
| CHEM+REA | 24 | | | | | | |
| Columns | 24 | FG,OUT | 0.054 | %-vol | CO2OUT | 96.00 | kg/h |

Table 1: Results I

For the absorber the results are essentially the same: The capture fractions of feed for 2006.5 and V7.2 are 65 % and 69 % and the CO2 exit concentrations are 6.4 mole-% and 5.4 mole-%, respectively.

[1] For Example: Wheeldon, D., Review of CO2-Capture Development Activities for Coal-Fired Power Generation Plants, ELECTRIC POWER RESEARCH INSTITUTE, 2007, p. 3-1:
"Fluor Daniel has investigated improvements to its technology and is offering it commercially. In addition to a standard design they offer to integrate the CO2-recovery stage into the process in a manner that minimizes energy consumption. Econamine FG PlusSM was investigated as part of the Canadian Clean Power Coalition study in which it was retrofitted to a PC boiler fired on lignite and shown to reduce energy consumption by a third from 4,070 kJ/kg to 2,760 kJ/kg of CO2 captured (1,750 Btu/lb to 1,180 Btu/lb).See Reference 3-1. [...]
3-1. “Evaluation of Advanced Coal Technologies with CO2 Capture: Canadian CPC Phase 1 Studies of Coal Technologies with CO2 Capture”, EPRI Report 1004880, April 2004."

For the stripper the results are significantly different. The reboiler duties for 2006.5 and V7.2 are 9.1 MJ/kg $CO_2$ captured and 5.8 MJ/kg $CO_2$ captured, respectively. The V7.2 value is 64 % of the 2006.5 value.

The recovery fraction (of the $CO_2$ captured) of V7.2 is 91 % only, however, whereas in 2006.5 the recovery is over 100 %.

### 2.1.1 Absorber

The temperatures and flow rates are essentially the same:

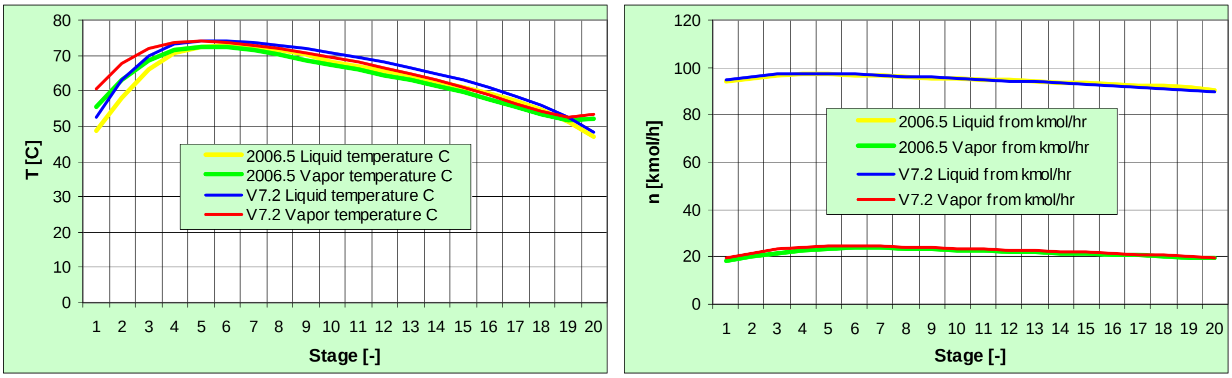



Figure 1: Absorber profiles I

### 2.1.2 Stripper

There are significant differences in the temperatures and flow profiles:

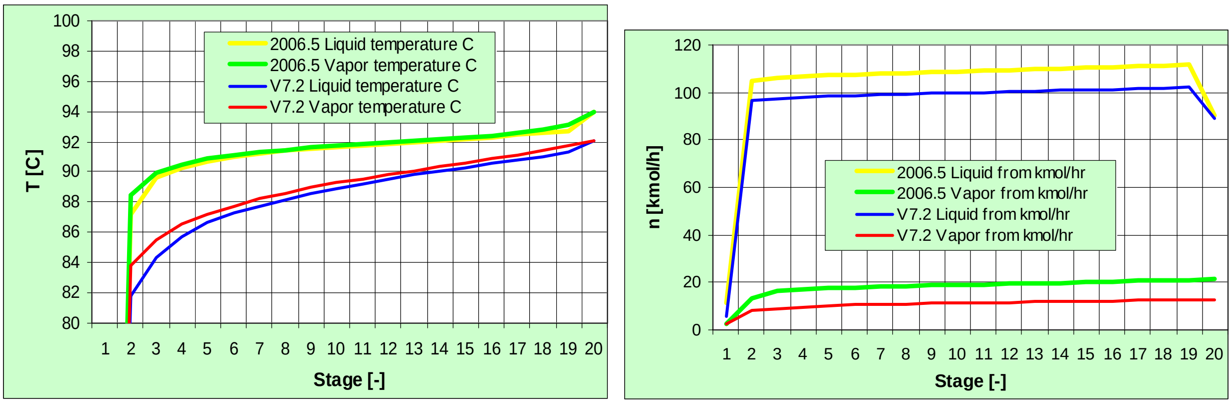



Figure 2:Stripper profiles I

In the new (V7.2) version the temperatures and the flow rates in the stripper are lower. In the 2006.5 model the mean vapor flow rate is 18 kmol/h, whereas in the V7.2. model the mean vapor flow rate is 11 kmol/h (with reboiler duty of 5.8 MJ/kg $CO_2$ captured), which is 60 % of the 2006.5 value.

## 2.2 Comparison - II

In the original - as supplied by AspenTech - two Aspen+ models (2006.5 and V7.2) the same unit with the same feed is simulated. The amine recirculation is not closed in the simulation. This leads to the recovery not being 100 %.

Thus with a design spec to get a 100 % recovery was added. The new results are presented in Table 2.

| 2006.5 | | CO2 | ABSORBER | | CO2 | STRIPPER | |
|---|---|---|---|---|---|---|---|
| PurePara | 21 | FG,IN | 3.40 | kmol/h | QR | 238.04 | kW |
| her BinPara | 21 | FG,OUT | 1.20 | kmol/h | QR/CO2 | 8.85 | MW/kg |
| Henry | 21 | | | | | | |
| NRTL | 21 | Capture | 2.20 | kmol/h | OUT | 2.20 | kmol/h |
| ElecPara | 21 | Capture | 64.79 | % | Recovery | 100.00 | % |
| CHEM+REA | 21 | | | | | | |
| Columns | 21 | FG,OUT | 0.064 | %-vol | CO2OUT | 98.71 | kg/h |
| **V7.2** | | **CO2** | ABSORBER | | **CO2** | STRIPPER | |
| PurePara | 24 | FG,IN | 3.40 | kmol/h | QR | 194.27 | kW |
| her BinPara | 24 | FG,OUT | 1.04 | kmol/h | QR/CO2 | 6.75 | MW/kg |
| Henry | 24 | | | | | | |
| NRTL | 24 | Capture | 2.36 | kmol/h | OUT | 2.36 | kmol/h |
| ElecPara | 24 | Capture | 69.30 | % | Recovery | 100.00 | % |
| CHEM+REA | 24 | | | | | | |
| Columns | 24 | FG,OUT | 0.054 | %-vol | CO2OUT | 105.58 | kg/h |

Table 2: Results II

For the absorber the results are the same.

For the stripper for 2006.5 the results are essentially the same as with no design spec but for V7.2 the result are significantly different: The reboiler duty for V7.2 is now 6.8 MJ/kg CO2 captured, which is 76 % of the 2006.5 new value of 8.9 MJ/kg CO2 captured.

### 2.2.1 Stripper

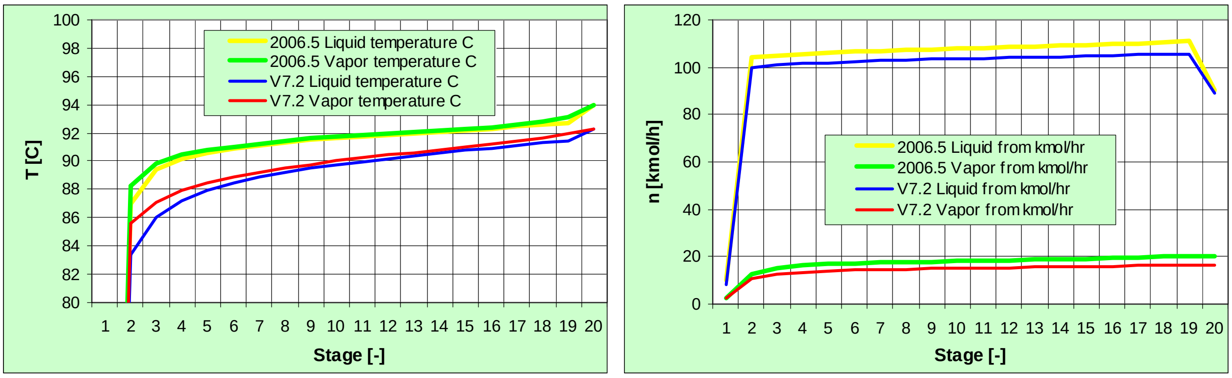



Figure 3:Stripper profiles II

In the new (V7.2) version the temperatures and the flow rates in the stripper are lower. In the 2006.5 model the mean vapor flow rate is 18 kmol/h, whereas in the V7.2. model the mean vapor flow rate is 15 kmol/h (with reboiler duty of 6.8 MJ/kg CO2 captured), which is 83 % of the 2006.5 value.

# 3 The Changes

The changes from 2006.5 to V7.2 include:

1. Physical properties:
   - o Changes in the Pure Component Parameters
   - o Changes in the Binary Interaction Parameters (including HENRY-1 and NRTL-1)
   - o Changes in Electrolyte Pair Parameters.
2. Reactions:
   - o The calculation of reaction equilibria (in Chemistry and in Reactions) through Gibbs energies and not by user given expressions. The change of kinetic parameters
3. Columns:
   - o Changes in packing calculation specification in the two columns

# 4 Test of Effect of Changes

## 4.1 Physical Properties

### 4.1.1 Pure Component Parameters

The use of the Pure Component Parameters of V7.2. in the 2006.5 causes no significant changes in the results. The results are presented in Table 3.

| 2006.5 | | CO2 | ABSORBER | | CO2 | STRIPPER | |
|---|---|---|---|---|---|---|---|
| PurePara | 21 | FG,IN | 3.40 | kmol/h | QR | 238.04 | kW |
| her BinPara | 21 | FG,OUT | 1.20 | kmol/h | QR/CO2 | 8.85 | MW/kg |
| Henry | 21 | | | | | | |
| NRTL | 21 | Capture | 2.20 | kmol/h | OUT | 2.20 | kmol/h |
| ElecPara | 21 | Capture | 64.79 | % | Recovery | 100.00 | % |
| CHEM+REA | 21 | | | | | | |
| Columns | 21 | FG,OUT | 0.064 | %-vol | CO2OUT | 98.71 | kg/h |

| 2006.5 | | CO2 | ABSORBER | | CO2 | STRIPPER | |
|---|---|---|---|---|---|---|---|
| PurePara | 24 | FG,IN | 3.40 | kmol/h | QR | 238.99 | kW |
| her BinPara | 21 | FG,OUT | 1.19 | kmol/h | QR/CO2 | 8.85 | MW/kg |
| Henry | 21 | | | | | | |
| NRTL | 21 | Capture | 2.21 | kmol/h | OUT | 2.21 | kmol/h |
| ElecPara | 21 | Capture | 64.99 | % | Recovery | 100.00 | % |
| CHEM+REA | 21 | | | | | | |
| Columns | 21 | FG,OUT | 0.063 | %-vol | CO2OUT | 99.01 | kg/h |

Table 3: Results

### 4.1.2 + Binary Interaction Parameters

The use of the Pure Component Parameters and Binary Interaction Parameters of V7.2. in the 2006.5 causes an increase of the capture fraction and an increase in the reboiler duty per CO2 recovered; a change in the wrong direction. The results are presented in Table 4.

| 2006.5 | | CO2 | ABSORBER | | CO2 | STRIPPER | |
|---|---|---|---|---|---|---|---|
| PurePara | 21 | FG,IN | 3.40 | kmol/h | QR | 238.04 | kW |
| her BinPara | 21 | FG,OUT | 1.20 | kmol/h | QR/CO2 | 8.85 | MW/kg |
| Henry | 21 | | | | | | |
| NRTL | 21 | Capture | 2.20 | kmol/h | OUT | 2.20 | kmol/h |
| ElecPara | 21 | Capture | 64.79 | % | Recovery | 100.00 | % |
| CHEM+REA | 21 | | | | | | |
| Columns | 21 | FG,OUT | 0.064 | %-vol | CO2OUT | 98.71 | kg/h |
| **2006.5** | | **CO2** | ABSORBER | | **CO2** | STRIPPER | |
| PurePara | 24 | FG,IN | 3.40 | kmol/h | QR | 256.09 | kW |
| her BinPara | 24 | FG,OUT | 1.13 | kmol/h | QR/CO2 | 9.24 | MW/kg |
| Henry | 24 | | | | | | |
| NRTL | 24 | Capture | 2.27 | kmol/h | OUT | 2.27 | kmol/h |
| ElecPara | 21 | Capture | 66.71 | % | Recovery | 100.00 | % |
| CHEM+REA | 21 | | | | | | |
| Columns | 21 | FG,OUT | 0.060 | %-vol | CO2OUT | 101.63 | kg/h |

Table 4: Results

### 4.1.3 + Electrolyte Pair Parameters

The use of the Pure Component Parameters and Binary Interaction Parameters and Electrolyte Pair Parameters of V7.2. in the 2006.5 causes an increase of the capture fraction and a dramatic increase in the reboiler duty per CO2 recovered; a change in the wrong direction. The results are presented in Table 5.

| 2006.5 | | CO2 | ABSORBER | | CO2 | STRIPPER | |
|---|---|---|---|---|---|---|---|
| PurePara | 21 | FG,IN | 3.40 | kmol/h | QR | 238.04 | kW |
| her BinPara | 21 | FG,OUT | 1.20 | kmol/h | QR/CO2 | 8.85 | MW/kg |
| Henry | 21 | | | | | | |
| NRTL | 21 | Capture | 2.20 | kmol/h | OUT | 2.20 | kmol/h |
| ElecPara | 21 | Capture | 64.79 | % | Recovery | 100.00 | % |
| CHEM+REA | 21 | | | | | | |
| Columns | 21 | FG,OUT | 0.064 | %-vol | CO2OUT | 98.71 | kg/h |
| **2006.5** | | **CO2** | ABSORBER | | **CO2** | STRIPPER | |
| PurePara | 24 | FG,IN | 3.40 | kmol/h | QR | 568.17 | kW |
| her BinPara | 24 | FG,OUT | 0.83 | kmol/h | QR/CO2 | 18.10 | MW/kg |
| Henry | 24 | | | | | | |
| NRTL | 24 | Capture | 2.57 | kmol/h | OUT | 2.57 | kmol/h |
| ElecPara | 24 | Capture | 75.57 | % | Recovery | 100.00 | % |
| CHEM+REA | 21 | | | | | | |
| Columns | 21 | FG,OUT | 0.042 | %-vol | CO2OUT | 115.12 | kg/h |

Table 5: Results

## 4.2 Reactions

The use of the Chemistry and Reactions - in addition of the use of the Parameters - of V7.2. in the 2006.5 causes an increase of the capture fraction and a dramatic decrease in the reboiler duty per CO2 recovered; a change in the right direction, but a change too large. The results are presented in Table 6.

| 2006.5 | | CO2 | ABSORBER | | CO2 | STRIPPER | |
|---|---|---|---|---|---|---|---|
| PurePara | 21 | FG,IN | 3.40 | kmol/h | QR | 238.04 | kW |
| her BinPara | 21 | FG,OUT | 1.20 | kmol/h | QR/CO2 | 8.85 | MW/kg |
| Henry | 21 | | | | | | |
| NRTL | 21 | Capture | 2.20 | kmol/h | OUT | 2.20 | kmol/h |
| ElecPara | 21 | Capture | 64.79 | % | Recovery | 100.00 | % |
| CHEM+REA | 21 | | | | | | |
| Columns | 21 | FG,OUT | 0.064 | %-vol | CO2OUT | 98.71 | kg/h |
| **2006.5** | | **CO2** | ABSORBER | | **CO2** | STRIPPER | |
| PurePara | 24 | FG,IN | 3.40 | kmol/h | QR | 169.27 | kW |
| her BinPara | 24 | FG,OUT | 0.93 | kmol/h | QR/CO2 | 5.61 | MW/kg |
| Henry | 24 | | | | | | |
| NRTL | 24 | Capture | 2.47 | kmol/h | OUT | 2.47 | kmol/h |
| ElecPara | 24 | Capture | 72.63 | % | Recovery | 100.00 | % |
| CHEM+REA | 24 | | | | | | |
| Columns | 21 | FG,OUT | 0.048 | %-vol | CO2OUT | 110.65 | kg/h |
| **V7.2** | | **CO2** | ABSORBER | | **CO2** | STRIPPER | |
| PurePara | 24 | FG,IN | 3.40 | kmol/h | QR | 194.27 | kW |
| her BinPara | 24 | FG,OUT | 1.04 | kmol/h | QR/CO2 | 6.75 | MW/kg |
| Henry | 24 | | | | | | |
| NRTL | 24 | Capture | 2.36 | kmol/h | OUT | 2.36 | kmol/h |
| ElecPara | 24 | Capture | 69.30 | % | Recovery | 100.00 | % |
| CHEM+REA | 24 | | | | | | |
| Columns | 24 | FG,OUT | 0.054 | %-vol | CO2OUT | 105.58 | kg/h |

Table 6: Results

# 4.3 Columns

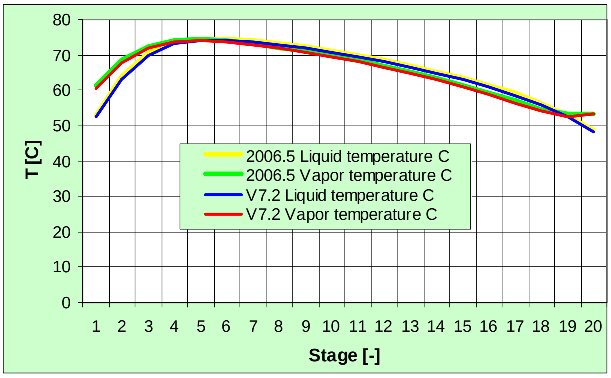
The use of the columns - in addition to the use of the Parameters and the Chemistry and Reactions - of V7.2. in the 2006.5 causes no significant changes. The results are presented in Table 7.

| 2006.5 | | CO2 | ABSORBER | | CO2 | STRIPPER | |
|---|---|---|---|---|---|---|---|
| PurePara | 21 | FG,IN | 3.40 | kmol/h | QR | 238.04 | kW |
| her BinPara | 21 | FG,OUT | 1.20 | kmol/h | QR/CO2 | 8.85 | MW/kg |
| Henry | 21 | | | | | | |
| NRTL | 21 | Capture | 2.20 | kmol/h | OUT | 2.20 | kmol/h |
| ElecPara | 21 | Capture | 64.79 | % | Recovery | 100.00 | % |
| CHEM+REA | 21 | | | | | | |
| Columns | 21 | FG,OUT | 0.064 | %-vol | CO2OUT | 98.71 | kg/h |
| **2006.5** | | **CO2** | ABSORBER | | **CO2** | STRIPPER | |
| PurePara | 24 | FG,IN | 3.40 | kmol/h | QR | 158.99 | kW |
| her BinPara | 24 | FG,OUT | 1.09 | kmol/h | QR/CO2 | 5.62 | MW/kg |
| Henry | 24 | | | | | | |
| NRTL | 24 | Capture | 2.31 | kmol/h | OUT | 2.31 | kmol/h |
| ElecPara | 24 | Capture | 68.07 | % | Recovery | 100.00 | % |
| CHEM+REA | 24 | | | | | | |
| Columns | 24 | FG,OUT | 0.055 | %-vol | CO2OUT | 103.70 | kg/h |
| **V7.2** | | **CO2** | ABSORBER | | **CO2** | STRIPPER | |
| PurePara | 24 | FG,IN | 3.40 | kmol/h | QR | 194.27 | kW |
| her BinPara | 24 | FG,OUT | 1.04 | kmol/h | QR/CO2 | 6.75 | MW/kg |
| Henry | 24 | | | | | | |
| NRTL | 24 | Capture | 2.36 | kmol/h | OUT | 2.36 | kmol/h |
| ElecPara | 24 | Capture | 69.30 | % | Recovery | 100.00 | % |
| CHEM+REA | 24 | | | | | | |
| Columns | 24 | FG,OUT | 0.054 | %-vol | CO2OUT | 105.58 | kg/h |

Table 7: Results

## 4.3.1 Absorber

The temperatures and flow rates are the same:



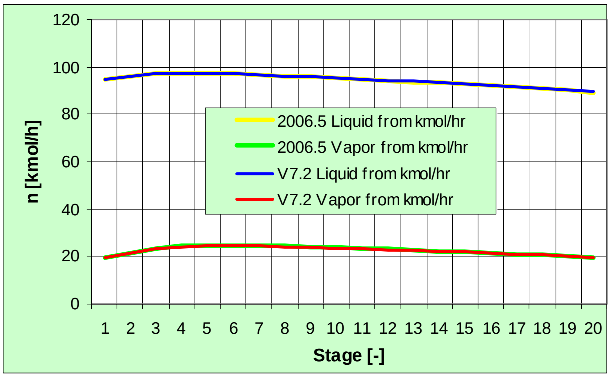




Figure 4: Absorber profiles

## 4.3.2 Stripper

There are small but significant differences in the temperatures and flow profiles:

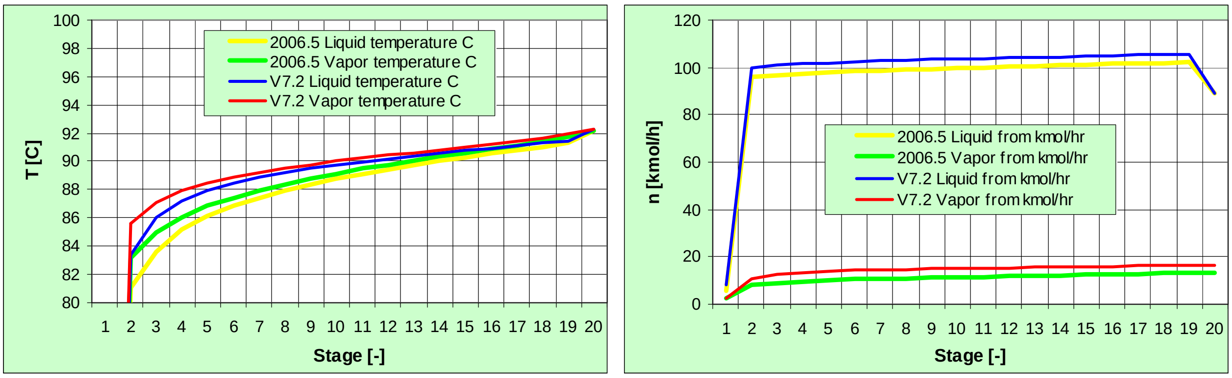



Figure 5:Stripper profiles

# 5 Summary and Conclusions

The summary of results is presented in Table 8.

| | 2006.5 | 2006.5 | 2006.5 | 2006.5 | 2006.5 | 2006.5 | V7.2 | |
|---|---|---|---|---|---|---|---|---|
| PurePara | 2006.5 | V7.1 | V7.2 | V7.2 | V7.2 | V7.2 | V7.2 | |
| BinPara | 2006.5 | 2006.5 | V7.2 | V7.2 | V7.2 | V7.2 | V7.2 | |
| ElecPara | 2006.5 | 2006.5 | 2006.5 | V7.2 | V7.2 | V7.2 | V7.2 | |
| CHEM+REA | 2006.5 | 2006.5 | 2006.5 | 2006.5 | V7.2 | V7.2 | V7.2 | |
| Columns | 2006.5 | 2006.5 | 2006.5 | 2006.5 | 2006.6 | V7.2 | V7.2 | |
| Capture | 2.20 | 2.21 | 2.27 | 2.57 | 2.47 | 2.31 | 2.36 | kmol/h |
| Capture | 64.79 | 64.99 | 66.71 | 75.57 | 72.63 | 68.07 | 69.30 | % |
| QR | 238.04 | 238.99 | 256.09 | 568.17 | 169.27 | 159.00 | 194.27 | kW |
| QR/CO2 | 8.85 | 8.85 | 9.24 | 18.10 | 5.61 | 5.62 | 6.75 | MW/kg |

Table 8: Result Summary

It is seen that:

- Pure component and binary interaction parameters have only a minor effect and that in the wrong direction (i.e. increasing QR/CO2).
- Electrolyte pair parameters have a dramatic effect and that in the wrong direction (i.e. increasing QR/CO2).
- The calculation of reaction equilibria through Gibbs energies as in V7.2 - and not through given equations - has a dramatic effect and that in the right direction (i.e. decreasing QR/CO2).
- The column specifications have only a minor effect.

Given the very complicated calculations involved it seems a miracle that the dramatic increasing effect (with respect to QR/CO2) of the electrolyte pair parameters and the dramatic decreasing effect of the parameters affecting the Gibbs free energy change (used in the calculation of reaction equilibria) combined give a QR/CO2 quite near the desired value.

The very complicated calculations are also make it rather difficult - or arduous, at least - to investigate the relationships.

The AspenTech document "Rate-Based Model of the CO2 Capture Process by MEA using Aspen Plus" gives the following on p. 7 (for the electrolyte pair parameters):

> The interaction energy parameters between H2O and (MEAH+, HCO3 -) and those parameters between H2O and (MEAH+, MEACOO-), GMELCC, are regressed using the absorption heat data from Kim et al. (2007)[12], heat capacity data from Weiland et al. (1996)[13] and VLE data from Lee at al. (1976)[14] and Jou et al. (1995)[15].
>
> The interaction energy parameters between H2O and (MEAH+, HS-), GMELCC and GMELCD, are obtained from the works of Austgen et al. (1988)[2].

and on p. 15 (for the reactions):

> The equilibrium constants for reactions 1-5 in **MEA** are calculated from the standard Gibbs free energy change. DGAQFM. DHAQFM and CPAQ0 of MEAH+ and MEACOO-, which are used to calculate the standard MEAH+ and MEACOO Gibbs free energy, are determined in this work. The DGAQFM (or DGFORM), DHAQFM (or DHFORM) and CPAQ0 (or CPIG) parameters of the other components can be obtained from the databank of Aspen Plus. The equilibrium constants for reactions 6-7 in **MEA** are obtained from Austgen et al. (1988) [2].

The key phrase is "are determined in this work" without reference to other sources. Further study is needed, if the data and methods used in the "work" referred to, are deemed worth the effort.

**Appendix 1: Simulations and Files**

## Simulations

All simulations done with V7.2.

## 5.1 Databases

In 2006.5 the existing databases are kept, because in V7.2. PURE20 is defined to be used. Thus the pure databanks are the same.

Why in V7.2. PURE20 is defined to be used, has been asked from AspenTech on the 2011-09-12.

## 5.2 2006.5

### 5.2.1 Rate_Based_MEA_Model.bkp

- Rate_Based_MEA_Model.bkp and Rate-Based MEA Model.pdf from http://support.aspentech.com/, Solution ID 122271
- Files renamed to 2006.5_Rate_Based_MEA_Model.bkp and 2006.5_Rate_Based_MEA_Model.pdf
- Open with V7.2
- Keep existing databanks
- Reinit, Run, Converged.
- Convergence
    - Delete components: N2, O2
    - Delete empty column estimates for N2, O2
    - Run, Stripper not converged.

### 5.2.2 2006.5_MEA_MPE-01.bkp

- Copied from 2006.5_Rate_Based_MEA_Model.bkp
- Open with V7.2
- Keep existing databanks
- Chemistry MEA renamed CHEM-21
- Reactions MEA-REA renamed REA-21
- Remove mass from stream report options.
- Unit set US-KPA-01 imported, defaulted in Setup/Global. (Existing specs not changed.)
- Import CHEM-24, REA-24
- Clear Fash Error Tol speck (was equal to default = 0.0001), Clear Valid Phases speck
- Add design spec for CO2 out to equal the captured CO2
- Run, Converged, Saved.

### 5.2.3 2006.5_MEA_MPE-02.bkp

- Copied from 2006.5_MEA_MPE-01.bkp
- Delete and Copy (i.e. import) Pure Params from V7.2

### 5.2.4 2006.5_MEA_MPE-03.bkp

- Copied from 2006.5_MEA_MPE-02.bkp

- Clear and Copy (i.e. import) all (incl. HENRY and NRTL) Binary Params from V7.2

### 5.2.5 2006.5_MEA_MPE-04.bkp

- Copied from 2006.5_MEA_MPE-03.bkp
- Clear and Copy (i.e. import) Elec Params from V7.2
- In design Spec increase the upper limit to 120 kg/h

### 5.2.6 2006.5_MEA_MPE-05.bkp

- Copied from 2006.5_MEA_MPE-04.bkp
- Use CHEM-24, REA-24

### 5.2.7 2006.5_MEA_MPE-06.bkp

- Copied from 2006.5_MEA_MPE-05.bkp
- Delete end Copy (i.e. import) columns from V7.2

## 5.3 V7.2

### 5.3.1 Original

- Rate_Based_MEA_Model.bkp and Rate-Based MEA Model.pdf from a zip-file from http://support.aspentech.com/, Solution ID 129521
    - Files renamed to V7.2_Rate_Based_MEA_Model.bkp and V7.2_Rate_Based_MEA_Model.pdf

### 5.3.2 V7.2_MEA_MPE-01.bkp

- Copied from V7.2_Rate_Based_MEA_Model.bkp
- Components: Delete H2 and CO. Arrange as in 2006.5
- Parameters: Delete empty columns for H2 and CO in HENRY-1.
- Unit set US-KPA-01 imported, defaulted in Setup/Global. (Existing specs not changed.)
- CPAQ0-1 unit set SET-2 → SI.[2]
- Rename stream GASOUT -> PUREGAS
- Chemistry MEA renamed CHEM-24
- Reactions MEA-REA renamed REA-24
- Import CHEM-21, REA-21
- Add design spec for CO2 out to equal the captured CO2
- Run, Converged, Saved.

### 5.3.3 V7.2_Blanko_MEA_MPE-01.bkp

- Open blank simulation
- Import unit set US-KPA-0, defaulted in Setup/Global.
- Import V7.2 components
- Define ELECNRTL
- Import V7.2 Henry components "MEA"
- Define Henry components "MEA"
- Run ElecWizard
    - Select all but O2 and N2

[2] SET-2 not defined in 2006.5

   - No salt formation
   - "Set up global property ...": ELECNRTL
   - New Henry Comps GLOBAL: Equal to MEA
   - Chemistry GLOBAL: Equilibrium k's by equation (not Gibbs)
   - Open (and thus accept) parameter values
- Import REA-24
- Copy flowsheet from V7.2_MEA_MPE-01.bkp
   - 2 error messages. Chemistry CHEM-24 not found for the stripper
- Define Chemistry GLOBAl for the striper stages a and 20.
- Run: Not converged. Abso convergence too slow.
- Import CHEM-24.
- Define CHEM-24 to be used
- Reinit, Run: Flash failures. Severe errors! Stopped.

#### 5.3.4 V7.2_Blanko_MEA_MPE-02.bkp

- Open blank simulation
- Import unit set US-KPA-1, defaulted in Setup/Global.
- Import V7.2 components
- Import V7.2 Henry components "MEA"
- Define Henry components "MEA"
- Import CHEM-24, REA-24
- Define ELECNRTL, Henry MEA, Chemistry CHEM-24
- Import all V7.2 parameters
   - Error in NRTL-1: Both H2O-MEA and MEA-H2O
   - Clear NRTL-1
   - Import V7.2 NRTL-1
- Define stream 1 and 1 and block B1, Run, Global data visible.
- Copy flowsheet from V7.2_MEA_MPE-01.bkp,
- Run: Abso converged. Stripper not. Global data not visible.
- Reduce Stripper Equilibrium max iterations to 10.
- Run: Converged. Results essentially equal to the original. Global data not visible.