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Benchmarking and comparing first and second generation post combustion CO_2 capture technologies

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Abstract

The Octavius FP7 project focuses on demonstration of CO_2 capture for zero emission power generation. As part of this work many partners are involved using different rate based simulation tools to develop tomorrow's new power plants. A benchmarking is performed, in order to synchronize accuracy and quality control the used modeling tools.

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The aim is to have 6 independent partners produce results on simulation tasks which are well defined in this work. The results show the performance of a typical simulation tool ranging from in-house process simulator to Aspen Plus® and combination of the two, using CAPE-Open. Definitions of the models are outlined describing the used assumptions on mass transfer correlations, hydraulics, thermodynamic models, kinetics, and property packages.
A sensitivity study is carried out for absorption and desorption which shows the performance of capture percentage, specific reboiler duties, loading of rich and lean solutions, pressure drop, flooding, concentration and temperature profiles, product purity, and condenser performance.
The overall conclusion is that most predicted properties vary in the order of 5-10% percent, often more than accuracy in experimental pilot plant measurements. There is a general good resemblance between modeling results.
A few important properties like specific reboiler duty and reboiler temperature plus concentration and temperature profiles vary more than expected. Also high flooding scenarios in the stripper are difficult cases.
Efficiencies are discussed as part of the summary. Recommendations for modeling principles and best practice are given.

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Keywords: CO2 capture proces simulation; modelling; bechmarking; rate based software; absorption and desorption; stripping; comparison;

1. Introduction

This work is performed in relation to the OCTAVIUS FP7 project. The overall aim is to demonstrate integrated concepts for zero emission power plants covering all the components needed for power generation as well as CO_2 capture and compression. Pilot scale experiments of first and second generation post combustion processes are demonstrated by TNO, EnBW, and ENEL.

A task of the Octavius project is to perform a benchmarking of two power plants to estimate the energy foot print. The work entails several subcategories of tasks covering everything from process development, simulation extensions, optimizations, validation, evaluation, and control. An iterative procedure is applied between simulation and pilot scale testing. Knowledge is to flow from simulation and optimization into the pilot scale experiment and vice versa in order to benefit from several different types of information. The combined results will contribute to improving the capture units and the power integration.

It is not a trivial task to perform and therefore several partners are involved in validation and development of the process models. These partners have different preferences when it comes to modeling tool usage. Internal model synchronization is important in order to guarantee the correctness of the comparison in a later stage of the project. The work needs to be harmonized to secure the similarity of the produced results. The simulation benchmarking will show to which degree of accuracy the various properties can be modeled. It is expected that some variables will be very accurate, but others will tend to be less reliable. This is very important to the further work in OCTAVIUS but also to the general interpretation of the simulation results. It is vital that the partners are aware of which properties poses higher uncertainty. This is especially important when comparing results or carrying knowledge from one task to the other. It would not be beneficial to blindly trust already known inaccurate calculations. But at the same expectedly accurate results should also be appreciated and trusted which would greatly improve the application of the findings.

The core aim of this work is to prove the similarity of modeling principles spanning several different simulation tools. It is a quality control of the models to secure that the produced results are equivalent and do not deviate from expected behavior and from each other. A further aim is to outline which type of model results would often be accurate and which would tend to be less accurate.

The model comparison will be performed by SINTEF (Norway), TUHH (Germany), DTU (Denmark), IFPEN (France), EDF (France), TNO (Netherlands). It comprises anything from in house simulators to commercial tools.

2. The benchmarking

2.1. Benchmarking Basis

The basis of the benchmarking in this work builds on the knowledge of the European Benchmarking Task Force – EBTF [1] from the CESAR, CAESAR, and DECARBit projects. These groups developed a detailed description of capture and power plant cases which enabled them to construct similar and comparable results in terms of energy penalty and cost for specific power plant types using different CCS technologies. The focus on degradation, emission, operability and flexibility in OCTAVIUS requires additional criteria are used for the comparison. A new and proper reference capture process is established using criteria which are both of qualitative and of quantitative nature.

Two definitions are given in the OCTAVIUS benchmarking: The power plant base cases and the capture reference case. In this work the capture cases will be the main focus. Further simulation of the integrated first and second generation power base cases are bound for calculation through the next period in the OCTAVIUS project, a brief outline is given below, even though.

The benchmarking description is a very detailed documentation of the required information to perform the power simulations. It contains tables and notes on air composition and conditions plus fuel compositions. The outline is as follows.

2.2. The power plant base cases

Two new build base cases will be considered for the benchmarking in OCTAVIUS, an 800 MWe Bituminous Pulverised Coal and a 430 MWe Natural Gas Combined Cycle (NGCC) case.

The pulverized coal case has a net cycle efficiency of 45.5% while the specific CO_2 emission is 763 g/kWh_{net} without post-combustion CO_2 capture. The steam turbines have extraction points, which deliver steam for nine feed water heaters. The live steam parameters are 300 bar at 600 °C, the parameters of the reheated steam are 60 bar at 620°C. For the control of combustion product emissions, the power plant is equipped with SCR DeNOx plant, electrostatic precipitators and a wet limestone based desulphurization plant.

The NGCC case is based on a gas turbine where the exhaust gas is led to a heat recovery steam generator (HRSG), feeding its steam to a steam turbine. The net cycle efficiency is 58.1% while the specific CO_2 emission is 354 g/kWh_{net} without post-combustion CO_2 capture.

The produced flue gases from the two power plants are very different and two non-similar capture setups need to be construction in connection to these two units.

2.3. Simulation synchronization methodology

The Benchmarking requires the simulation tools are reasonably well synchronized. To perform this, one of the Octavius partners described a flowsheet with relatively specific conditions for a basic CO_2 capture facility. It was a standard solvent based setup comprising a well-defined absorber and desorber using a typical heat exchange of the rich and lean solutions. 30 wt% MEA should be used as solvent, applying lean vapor recompression (LVC) and no absorber intercooling. This decision was taken based on the results of the CESAR FP7 project which showed that intercooling had no effect on the energy penalty of the MEA process. The project also showed that intercooling had positive effect on other solvents. The intent was to compare the calculated results.

Reasonably specific conditions were defined - everybody thought. Quickly problems arose when the partners set out to compare. Everybody had performed the simulation differently, and everybody tried to match the results of the one partner who originally produced a set of results. Some varied the height of the columns, other varied the reboiler temperature to match the heat duty. Even closing the loop of the solvent cycle posed room for interpretation. Some did not even try to match the reboiler duties but matched other properties. The group had basically produced 6 incomparable simulations using many different techniques and assumptions. It looked like almost any result could be produced, if the right variable where tuned accordingly. This is a noteworthy conclusion. Simulation results appearing in the open literature may very well describe and show results of specific reboiler duty, but even small differences in simulation design specification can give variations in the conclusions. Even missing information on packing type, column heights, temperature approaches etc. open room for unnecessary fatal interpretation.

The main conclusion was to create an extremely well-defined CO_2 capture simulation task, to establish the synchronization of the models. This meant that definitions needed to include information on flow input, what to compare for output, and which variables to fix. The capture plant was completely split up. The task was no longer to close the loop and prove a calculation of a flowsheet. The task was to perform an absorber calculation, and secondly to perform a desorber calculation. All room for interpretation and complexity was removed in order to secure that everybody were benchmarking the same information.

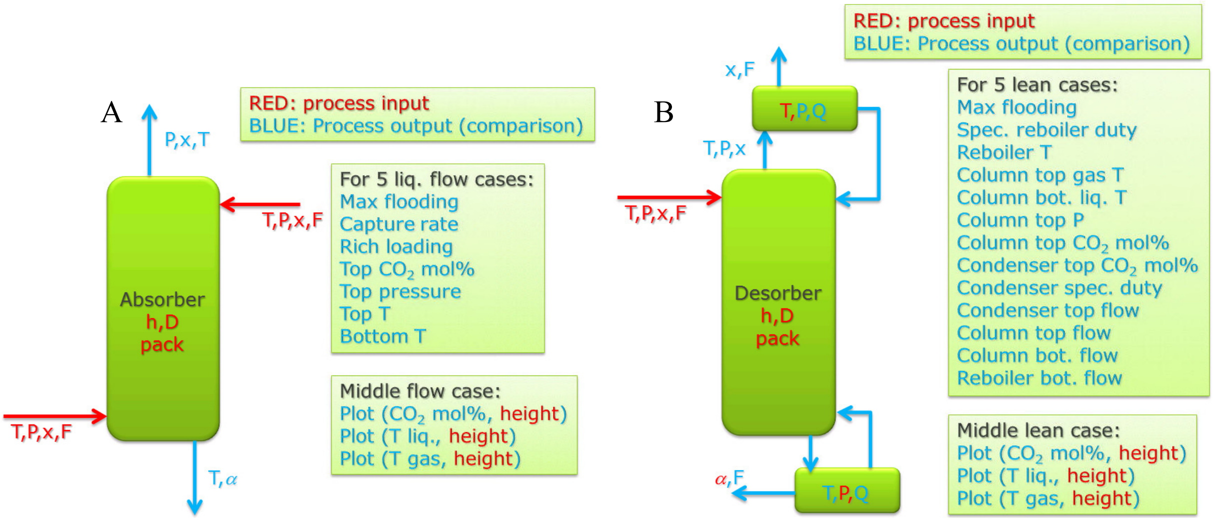

Fig. 1. (A) Absorber input and output specifications; (B) Desorber input and output specifications

The outline of the comparison is shown in Fig. 1. It contains the definition of input variables in red and calculated output results. As indicated in the figure, the absorber is supposed to be run at 5 lean flow rates, *F*, to study the effect of clean flue gas and the rich properties like loading ,(mol CO_2/mol MEA) α, temperature, *T*, and pressure *P*. Also maximum flooding % for a given height in the column was to be determined together with capture %. For the middle flow rate an additional analysis on column interior CO_2 mol% and temperatures were to be plotted. The column had a fixed height, *h*, diameter, *D*, and packing type. The inlet streams were given at fixed, *T*, *P*, *F* and compositions, *x*.

Similar conditions were defined for the desorber, except that flowsheet iteration had to applied for the calculations to succeed. The reason is that the partners decided, a bit unorthodox, to specify lean loading and calculate temperature and energy input to the reboiler, *Q*, instead of specifying them Similar to the absorber calculations, the middle lean specifications, was expected to present results on CO_2 mol% and temperatures as function of height. Note that LVC is not applied in this calculation scheme, in order to reduce the complexity, preventing partners to come up with new flowsheet assumptions. For the same reason wash sections for absorption and desorption were not included.

The second comparison was performed different to the first session. The intent was to perform a kind of round robin test where partners would go and perform calculations; DTU would collect and present the obtained results. In practice the testing was not completely blinded and some partners distributed the information internally before the final comparison.

The intent of this comparison was not to optimize or develop the CO_2 capture technology. The aim was to conclude if any of the partners modeling tools were giving unexpected results in core calculations of CO_2 capture.

2.4. The capture reference

The input variables defined above is summarized in the tables below. It contains detailed information in order to reproduce the results presented below. It has a general set of process criteria; an outline is given in table 1 for the absorber and desorber columns. It shows design specifications of the solvent type, packing, and dimensions.

Table 1. Absorber & desorber design specifications.

Parameter	**Fixed values**
Solvent	30 wt% MEA (CO_2 free)
Packing material (absorber & desorber)	Sulzer Mellapak 2X
Absorber height	20 m
Absorber diameter	13 m
Desorber height	13 m
Desorber diameter	8 m

Table 2. Absorber inlet flows specifications.

Parameter	**Fixed values**
Gas Inlet	
Temperature	43.5 °C
Pressure	104.5 kPa
CO_2 mole fraction	0.141
H_2O mole fraction	0.073
Inert mole fraction	0.786
Flow rate	46861.9 kmol/hr
Liquid inlet	
Temperature	40 °C
Pressure	102 kPa
CO_2 mol fraction	0.023
H_2O mol fraction	0.8675
MEA mol fraction	0.1095
Flow rate	180000 kmol/hr
CO_2 loading	0.21

Additional information is given in table 2 on inlet flows specifications for the absorber. It shows the variables on temperature, pressure, flow, and composition. The sensitivity carried out on lean flow rate is performed for 5 cases: 0%, ±10% and ±20% of the value given in table 2. The values were chosen according to the Octavius benchmarking definition.

Desorber design specifications are found in table 3. It contains definitions outlined in Fig. 1. The inlet pressure is defined as high pressure to prevent flashing in the pipes which would naturally occur at these conditions. No separate flash tank is used in this simulation and all flashing is expected to occur in the column. Pressure is defined in the reboiler at 190 kPa absolute. The pressure drop is considered upwards in the column. These properties together with the temperature in the condenser originate from the Octavius benchmarking definition.

The sensitivity of the lean loading is performed for 5 cases: -20%, - 15%, 0 %, 15%, and 30%. Originally -30% was used in the sensitivity but early calculation showed that some partners reached flooding at these conditions, therefore it was changed.

Table 3. Desorber inlet flow and design specifications.

Parameter	**Fixed values**
Rich feed solution	
Temperature	98 °C
Pressure	300 kPa (above bubble point)
CO_2 mol fraction	0.0578
H_2O mol fraction	0.8246
MEA mol fraction	0.1176
Flow rate	177400 kmol/hr
Rich loading (mol/mol)	0.4915 mol CO_2/mol MEA
Utilities(Condenser/Reboiler)	
Condenser temperature	30 °C
Reboiler pressure	190 kPa
Lean loading	0.21 mol CO_2/mol MEA

Table 4. Description of used simulation tools and setup.

	SINTEF	**DTU**	**EDF**	**TUHH**	**IFPEN**	**TNO**
Used tool	CO2SIM – in-house SINTEF simulator	DTU - CAPCO2 in Aspen Plus	Aspen Plus Standard Package	Aspen Plus V7.3	In-house model with ASPEN Plus V 8.4	Aspen Plus V8.2
Used simulation context	In-house flow sheet simulator with thermodynamic, kinetic, and unit operation models	Columns are DTU Cape-open modules in Aspen Plus. Other units Aspen Plus.	All Aspen plus.	All Aspen Plus. Columns Rad-Frac.	All Aspen Plus. Columns RateSep with kinetic models for absorber and desorber	All Aspen Plus. Columns Rad-Frac.
Modeling approach	Rate based columns. Other units: Equilibrium.	Rate based, identical column models. Other units: Equilibrium.	Rate based columns. Desorber: only transfer limitation, due to very fast kinetics. Other units: Equilibrium.	Rate based columns. Other units: Equilibrium.	Rate based, identical column models.	Rate based, identical column models. Internal reboiler and cond.
Solution approach	Columns are solved as BVPs using an adaptive collocation method.	Columns are solved as a BVP. Dynamic height discretization with min 30 steps and max 300.	Fixed 40 steps discretization for absorber, 30 for desorber. 10 steps for the liquid film of absorber, no desorber film discretization.	Fixed 30 step discretization; non linear 15 step film discretization; default convergence options	Discretization of columns heights in 20 stages. Maximum number of iterations 30.	20 stages for both absorber and desorber, standard initialization. Sequential modular approach.
Thermodynamic model	Astarita-model [3-5] Henry parameter [6]. Heat of absorption [7]. Ideality of gas phase is assumed	Extended UNIQUAC for liquid phase and thermal properties. Ideality of gas phase is assumed.	ELEC-NRTL for liquid phase and thermal properties. Ideality of gas phase is assumed	ELEC-NRTL for liquid phase and thermal properties. Ideality of gas phase is assumed.	ELEC-NRTL for liquid phase and thermal properties. Ideality of gas phase is assumed.	ENRTL-RK and PC-SAFT. Henry's law for solubility of supercritical gases.

There are a number of additional detailed specifications for wash sections, coolers, pumps, and compressors and economy in the Octavius benchmarking document which is not relevant for this study.

2.5. Used simulation tools

The six partners involved in the comparison study used anything from pure in-house software to fully commercial solutions, but also principles in-between. SINTEF applied a fully in-house software package which constitutes a flowsheet simulator. DTU used a mixture of in-house and Aspen Plus. This means the core rate based columns where developed by DTU which applies to the CAPE-Open standard and the modules can be used in other process simulators implementing CAPE-Open. The remaining partners used Aspen Plus. IFPEN applied an external property package to Aspen Plus. Based on the description in table 4 it can be seen how EDF used a more fine-tuned version, and TNO took advantage of the work by Zhang et al. [2].

Table 5. Description of used simulation properties and correlations

	SINTEF	**DTU**	**EDF**	**TUHH**	**IFPEN**	**TNO**
Chemical properties	Correlations [5]	Correlations [8]	Aspen Plus DB	Aspen default settings	ASPEN PLUS Library (v 8.4)	Documented in [2]
Mass transfer model	Rocha et al. [9] mass transfer correlations	Rocha et al. [9] mass transfer correlations	Bravo et al. [12]	Bravo et al. [11]	Bravo et al. [12]	Bravo et al. [12]
Hydraulic model	Rocha et al. [10]. Holdup corrections for Sultzer packing	Rocha et al. [10]	Bravo et al [12]	Bravo et al. [11]	Bravo et al. [11]	Bravo et al. [11]
Heat transfer model	Chilton-Colburn analogy [13]	Chilton Colburn analogy	Chilton Colburn analogy	Chilton Colburn analogy	Chilton Colburn analogy	Chilton Colburn analogy
Reaction kinetics	Second order, Versteeg et al. [14].	Second order, Versteeg et al. [14] – zwitterion reaction mechanism	Second order. [19] derived from pseudo-first order assumption	Second order Plaza et al.[15] using Aboudheir [16] and Rochelle et al. [17]	[18]	Documented in [2]
Reaction rate constant	[14]	[14]	Hikita et al. [19]	Plaza et al.[15]	[14], modified by [18]	Documented in [2]
Kinetic model/approach	Enhancement factor based. penetration model in the absorber, instantaneous reversible model in the desorber.	General method enhancement factor based on the two-film theory	Resolution of diffusion reaction equation through the liquid film	Two film model with reactions taking place only in the liquid phase	Liquid Film discretization (6 points). No vapor phase discretization	Diffusion resistance and reaction in discretised (5) liquid film, diffusion resistance in vapor film
Other assumptions	MEA is considered non-volatile. Liquid side mass-transfer resistance of the volatile solvent is neglected. Adiabatic column. No pressure drop.	MEA is considered non-volatile. Liquid side mass-transfer resistance of the volatile solvent is neglected. Adiabatic column.	MEA is volatile. All species can transfer MEA, H_2O, CO_2 and N_2. Adiabatic column.	Diffusion resistance in liquid and vapour film, reactions in liquid phase only		Stages: liquid phase well mixed, vapour is plug flow. Adiabatic column. MEA volatility not ignored.

In general all models used where rate based. SINTEF and EDF treated the absorber and desorber modelling principles differently. All applied an advanced activity coefficient model for the thermodynamic calculations. Some took more care to model the vapour phase. Note that the simulation are carried out at low pressure < 5bar. The simulation used equilibrium approaches for condenser and reboiler. TNO seem to have applied the principles slightly different compared to the other partners and decided to run columns with integrated units, even though this should not make a difference. There is a great variance on the detail for the solution and discretization of the model as outlined in the table.

Table 5 presents details of the simulation principles. The mass transfer correlations applied are reasonably the same, but the kinetic properties vary to a great extent. The theory applied for the enhancement factor is of cause very locked in Aspen Plus, where clearly there is more room for variety when the in-house software is applied.

3. Synchronization comparison and discussion

In practice the comparison study was performed as a two-step process. First the absorber calculations were performed and evaluated and secondly the desorber calculations were performed. Based on the discussions and the comparison of the results it was concluded that IFPEN deviated a bit due to misplaced definitions of the condenser specifications and similar issues. IFPEN therefore produced new improved results. Furthermore SINTEF wanted to improve the equilibrium modeling based on the comparison and they set out to improve the thermodynamic description and they were therefore allowed to produce new results as part of the test.

The results were constructed early 2014.

The discussion of calculations outcome is presented for the absorption and desorption process simulation below. It will be clear that some of the assumption outlined in table 4 and 5 are visible in the result and discussions below.

3.1. Absorption synchronization comparison

In absorption, one of the important variables for this study is the calculated capture percentage. It is a key property which is often compared to pilot scale tests. Model performance is often determined on its capability to reproduce this exact property. Fig. 2A indicates that a model output is ±10% accurate, even with almost identical modeling basis in Aspen Plus. Remember, pilot campaigns often strive to measure this property very accurately by making sure to close the mass balances.

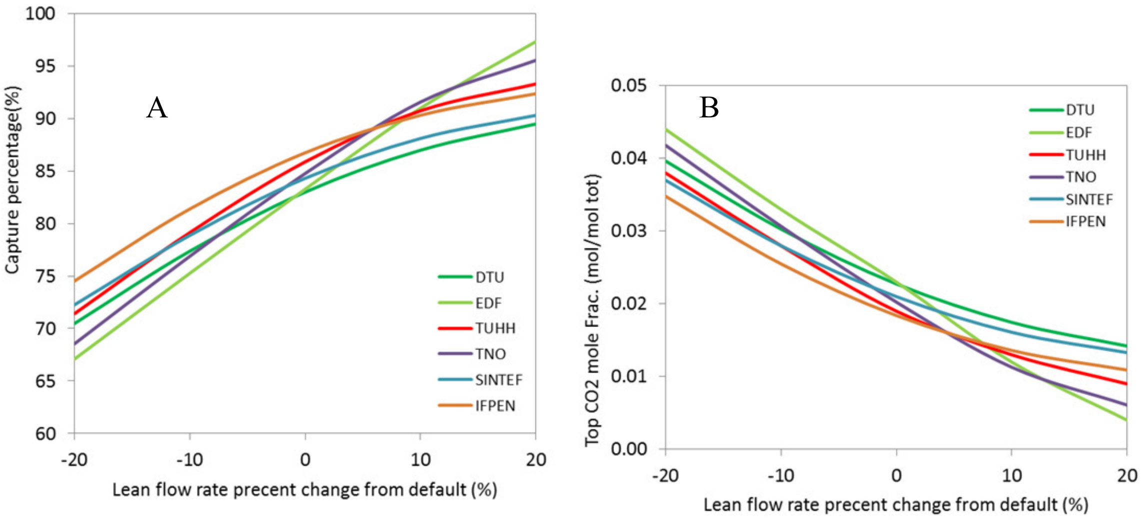

Fig. 2. (A) Absorber capture percentage; (B) absorber top gas phase mole fraction of CO_2 before washing.

The conclusion is that a model result of this kind is expected to be intermediate accurate. The results are as expected within the range of 70 to 95% capture corresponding to typical requirements for a CO_2 capture facility. The figure indicates that the results of EDF end IFPEN are outliers but nothing out of the ordinary. Fig. 2B supports the same conclusions and is basically a reflection of the same property because of mass balance conservation. It shows the top gas composition. The same variation is observed, ±10%.

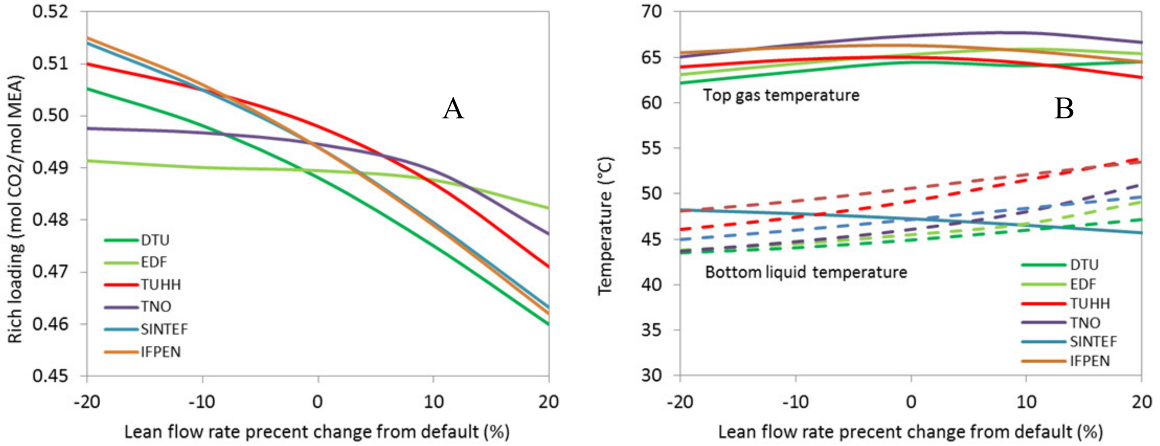

Fig. 3. (A) Absorber bottom rich loading; (B) Absorber top and bottom outlet temperatures.

The variation in capture percentage is not reflected in the bottom rich loading though, shown in figure 3A. It can be concluded that the obtained results of the partners are very similar and are reproduceable, within 4-5% accuracy. The typical equilibrium condition for these temperatures is approximately 0.52 in loading. This means the rich loading is not far from equilibrium. The main variation is most likely caused by the variability in the bottom temperaures shown in figure 3B. It shows a low predicted bottom liquid temperature of EDF and DTU. Figure 3A shows a low range rich loading. One would actually expect the opposite, that the low temperature would cause a high loading. The explanation is probably the thermodynamic model behind the calculations. It may have a tendency to give reasonbly high CO_2 partial pressures at low temperature for these two partners.

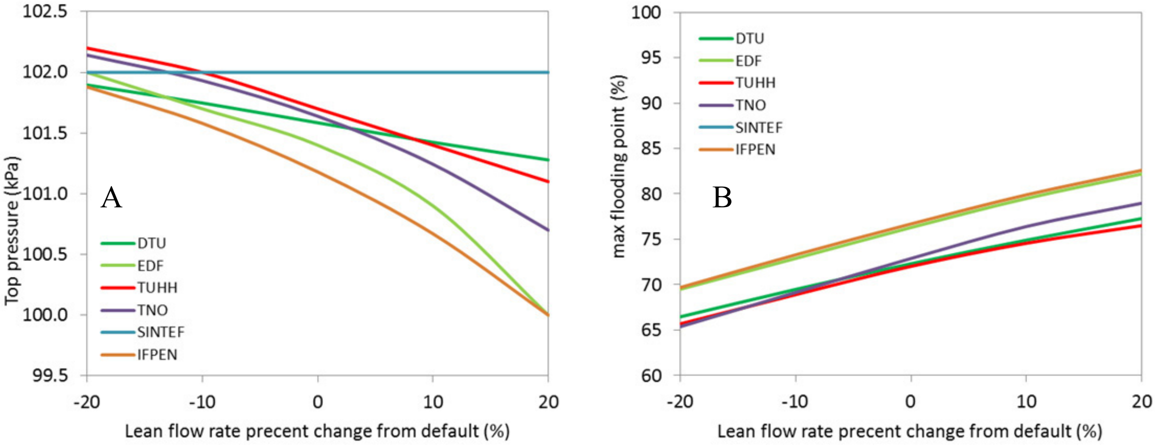

Fig. 4. (A) Absorber pressure at the top outlet; (B) Desorber input and output specifications

A conclusion on temperature accuracy can be drawn from figure 3B. In general the models seem to predict oulet temperatures within ±5 °C. This is also important to be aware off when comparing estimated temperaures. Later it can be seen that lower accuracy should be expected for temperaure profiles as function of column height.

The pressure drop is illustrated in figure 4A. SINTEF do no consider pressure drop as indicated. The inlet flue gas pressure is 104.5 kPa and the inlet liquid pressure is 102.0 kPa. A top outlet pressure of approximately 101.5 kPa is therefore a drop of 3 kPa over the 20 m. Only a small variation should be observed in pressure calculations of ±1%. It is closely linked to the amount of flooding presented in figure 4B. Here shown for the maximum flooding oberserved for any height in the column. Note flooding is not considered by SINTEF.

There seem to be two catagories of floodnig calculations. EDF and IFPEN in one group and the remaining in the other group. Table 5 summarises the hydrodynamic model used. It can not explain why here is a difference. TNO and TUHH uses the same model as IFPEN for this property, but the results are different.

Finally the gas concentration and liquid temperature profiles are shown in figure 5A and B. Liquid temperatuers are not shown but they are very similar to figure 5B. There is a direct link between 5A and B. As the gas flows upwards in the column, CO_2 is absorbed. The EDF calculations show at 12 m there is decrease in the CO_2 concentration which results in an increase of temperature. This is a well know phenomenon: The heat of absorption gives rise to temperature. It is a question of how quick the CO_2 is absorber. A high rate results in noticeable temperature increase. The CO_2 profiles by EDF and TNO indicates a high absorption efficiency in the top 8 m. The lower part of the column indicate that the bottom section is not efficient. The trend from these two calculations are similar. This is explainable from table 5, as the two partners use the same mass transfer correlation. DTU and SINTEF also use the same mass transfer correlation, even though, the temperature profile by SINTEF has a slightly different tendency in the range 0 to 2m. This could be water condensation from the gas phase which in the calculations could be slightly super-saturated.

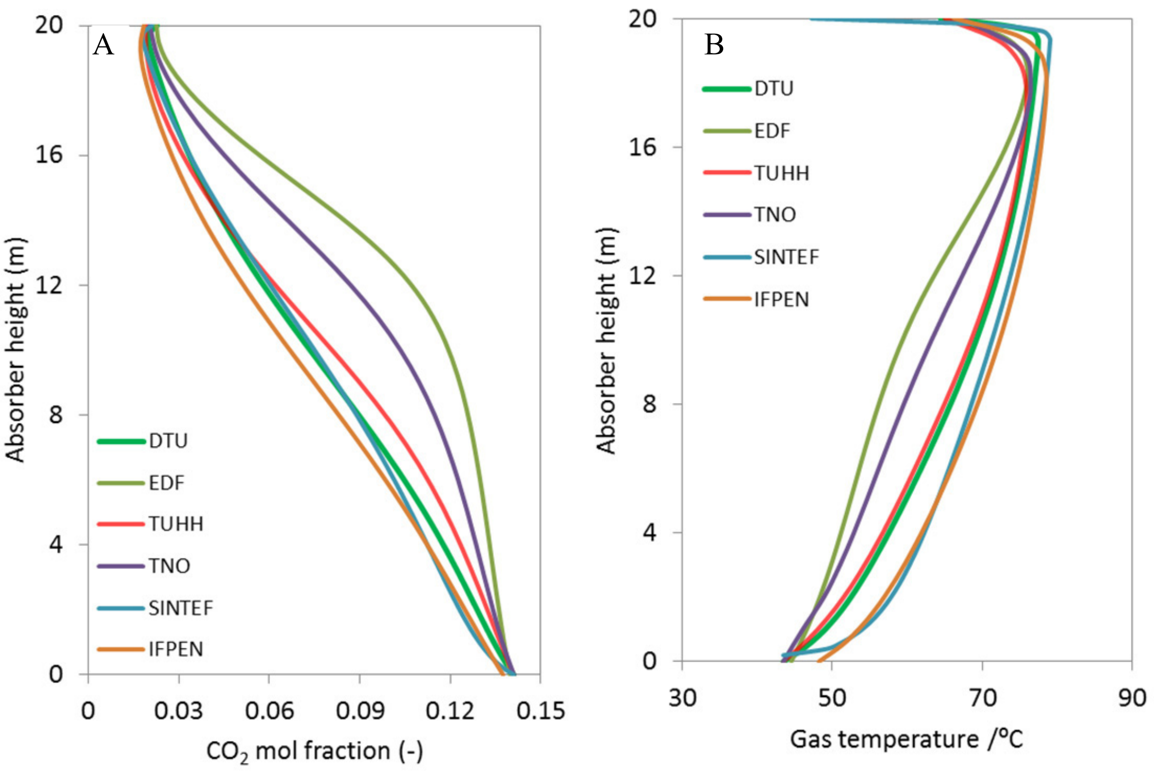

Fig. 5. (A) Absorber input and output specifications; (B) Desorber input and output specifications

It can be concluded that the majority of simulations for this specific problem gives linear concentration profiles as shown in figure 5A. There is obviously a great difference in the predicted concentrations, ±6%, in the mid column section, but the overall capture is the same, which is also substantiated by the results of figure 3A. There are no great outliers in the calculations.

The conclusions on the temperature profile are similar to the concentration profiles. The variation is greater in the mid section The properties are directly linked through the heat of absorption and the behaviour is therefore expected. Similar to the conclusions on the capture % above, it is noteworthy that many model validations in the literature are performed using pilot plant data showing plots similar to 5B. The observed termperature variance is in the order of ±10 °C. The experimental accuracy is expectedly in the order of 1-5 °C. This means that comparison of mid column temperature profiles may not be trustworthy to some extend and deviations should be expected.

The general conclusion is that reaonably similar and accepted results are obtained from the 6 partners. Variation are observed for column mid sections temperature, CO_2 concentrationsm, and capture % determinations. This is noteworthy during a comparison to experimental data. Further it can be concluded that even though 4 partners use Aspen Plus, off the shelf, the results are similar, but not in anyway identical.

3.2. Desorption synchronization comparison

The property most important to CO_2 capture is the specific reboiler duty (SRD), a variable determining the cost of operation. Figure 6A gives an outline of the obtained values. There is a high degree of variability, 10-15%. Some partners indicate a minimum in the energy consumption at 0% sensitivity. The calculations by TUHH and SINTEF seem to disprove this existence. The behavior of the SRD is reasonably homogenous, ±5%, for the 0 to 30% sensitivity. There is an indication that the TNO results give an energy consumption which could be 5% too high.

Pilot plant test often struggle to indicate reliable and accurate SRD values, where the truth is more likely that the modeling results are accurate to ±5-10%. The values are as expected in the order of 4 GJ/ton CO_2 which is comparable to the 3.9 GJ/ton CO_2 obtained in the CASTOR project.

In general the comparison is acceptable. The reason is found in figure 6B. The flooding results show that the sensitivity case -20 to 0 % gives flooding of the column close to 100%. Basically the majority of cases >70% flooding are not interesting from an industrial point of view. It would not be beneficial to operate the column at these conditions. The scatter observed in figure 6A is therefore not industrially interesting. SINTEF has not calculated flooding.

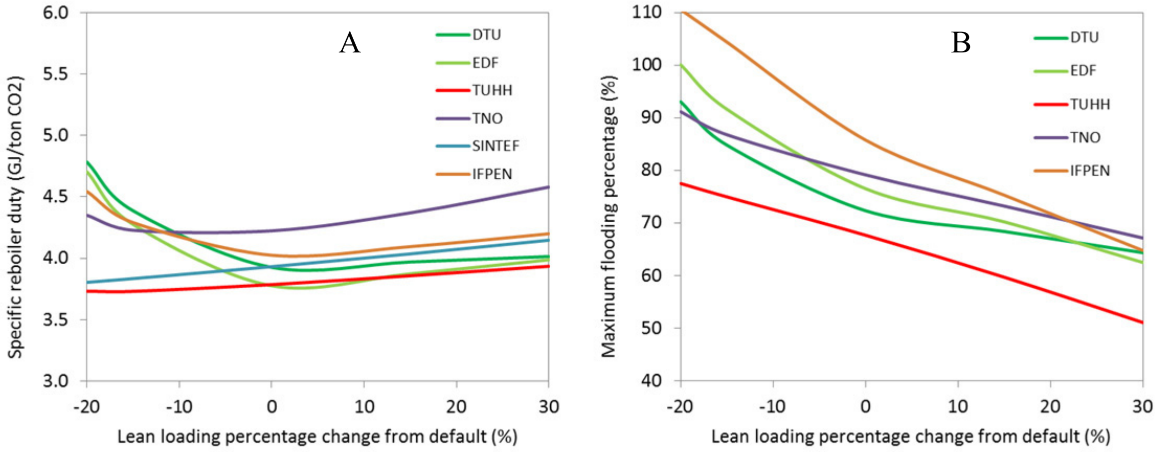

Fig. 6. (A) Reboiler specific heat duty; (B) Desorber flooding. Maximum indicates the maximum value, obtained at any height of the column.

It can be concluded that there is an unreasonably high variability in the SRD for cases close to flooding. A relative consistent reproduction is observed for lower flooding. A scatter in the order of 5% should be expected and results within this window should be seen as accurate. A comparison of model and pilot plant date would expectedly be accurate to 5%, based on these results.

The flooding calculations by IFPEN, performed with Aspen plus and KG Tower softwares, show that the column is flooded for the lean loading sensitivity cases <0%. Therefore they are unable to determine pressure loss of the column as indicated in figure 7A. SINTEF is not considering pressure loss and their stripper top pressure is the same as the reboiler pressure. A low pressure loss is calculated by most partners. Only IFPEN seem to calculate a reasonbly high pressure loss, but their calculations also indicate a realtive high degree of flooding, figure 6B.

Between partners the calculated pressures are very compareably. It has a low variability, and presuably a lower impact on the final SRD predictions.

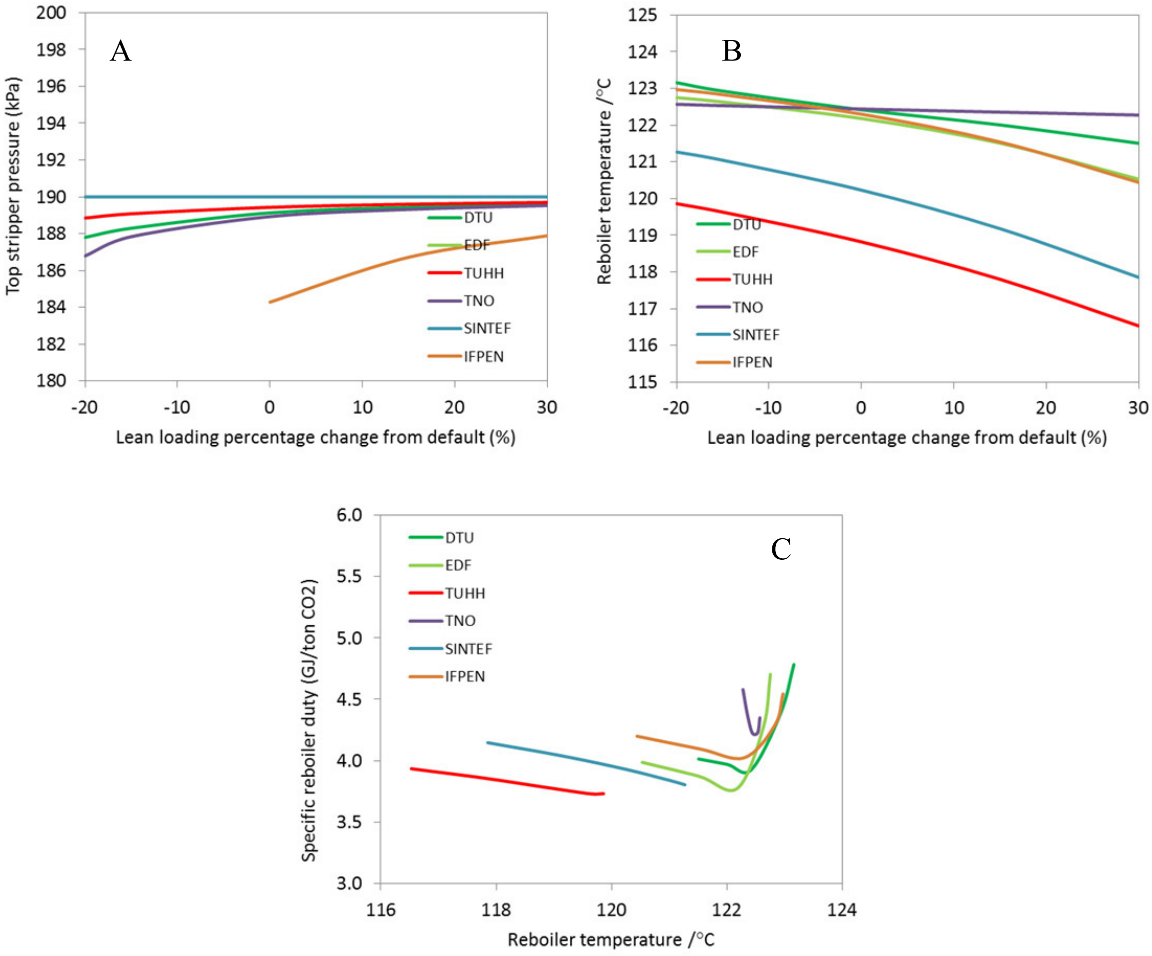

Fig. 7. (A) Pressure in stripper top (reboiler pressure is 190 kPa); (B) Reboiler temperature; (C) a combination of Fig. 6A and 7B

The reboiler temperature shown in figure 7B is a direct consequence of the pressure specification in the reboiler, 190 kPa. There is a slight correlation with the SRD shown in figure 6A: A lower temperature gives a lower SRD. The majority of partners obtain the same temperature. SINTEF and TUHH calculate a noticeable lower temperature. Naturally the same picture is seen for the stream coming into the reboiler, is has a lower temperature as shown in figure 8A, but is gives no explanation for the temperature differences. A reason could be the thermodynamic model used. Table 4 gives no indication of this difference. TUHH applies the same model as three other partners. Even DTU applies a completely different model but calculates the same as the electrolyte NRTL users.

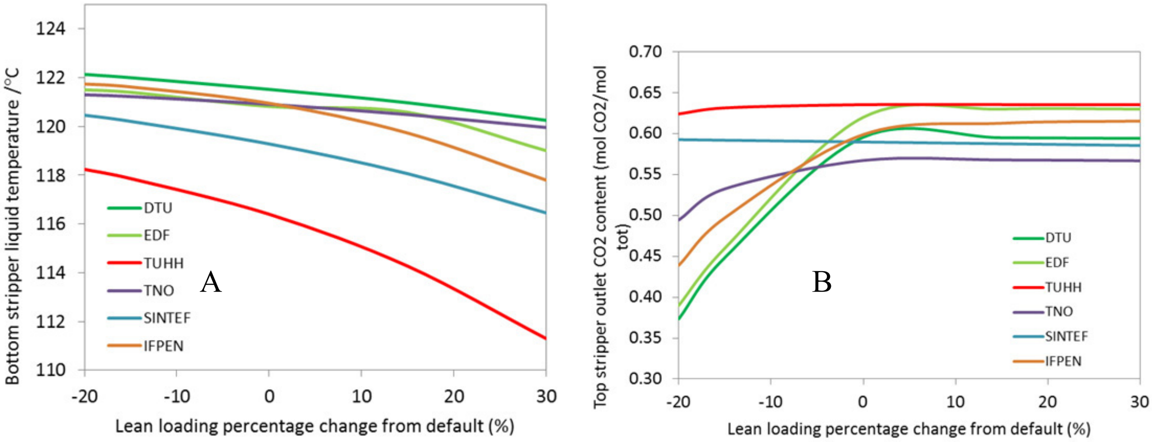

Fig. 8. (A) Outlet liquid temperature of the desorber bottom; (B) mole fraction of CO_2 in the stripped top gas.

It should be said that the reboiler temperature is sensitive to the composition of the fluids in the reboiler. Based on the methodology described above, the lean loading should be identically the same for all the calculations. The water/MEA concentration differences must be the only explanation. There is indication in the results which supports this: Figure 8B shows the top exiting gas. It mainly contains CO_2 and water. TUHH calculate values in the higher end, indicating a low water content. From mass balance conservation we know that the reboiler has more water. This would lower the boiling temperature and this would be the explanation for the observations. It is also supported by the SRD results which shows a lower energy consumption by TUHH. Most likely because they have less water evaporation.

The sensitivity of SRD to the reboiler temperature is obtained by combining figure 6A and 7B. Figure 7C shows the spread of the SRDs. There are no particular outliers, even though the results of TNO has a different shape compared to the other partners.

It can be concluded that accuracy of the calculated reboiler temperature is most likely ±1-5 °C. Very accurate benchmarking for this property can not be expected. This is important for comparisons to experimental data. Blindly picking up measured reboiler temperatures and using it for design specifications is not adviceable. On the other hand it is not important that the desorber bottom temperature is well-known it has the same accuracy, ±1-5 °C, which for this stream is acceptable.

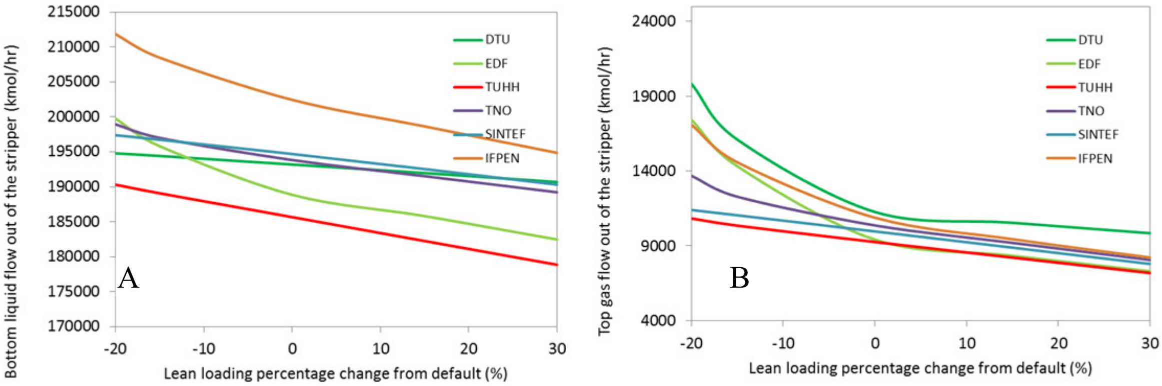

Fig. 9. (A) Desorber bottom liquid flow; (B) Desorber top gas flow.

Accuracy of mass balance is illustrated in figure 9. Bottom flow have a high expected accuracy, variability in the order of 10%. The trends of all the simulations are identical. The top gas flow is not as accurately determined. For the mentioned high flooding cases variability is significant. DTU seem to give values which are higher than other simulations. The observation is also visible in the clean CO_2 flow, figure 10A. Expected variability in the produced CO_2 flow is 10%. Many simulations give noticeable identical results as seen in figure 10A.

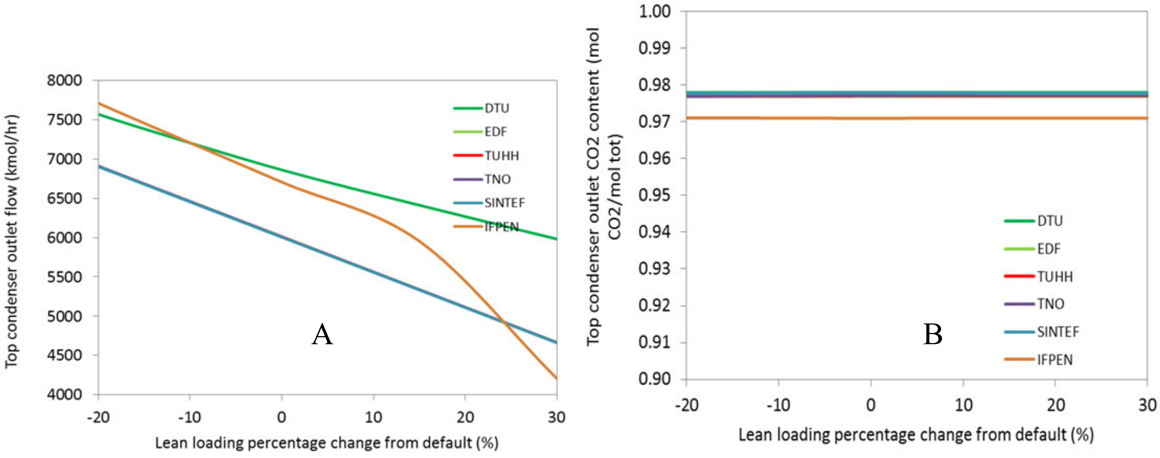

Fig. 10. (A) Clean CO_2 flow; (B) CO_2 flow purity

The purity of the produced CO_2 is shown in figure 10B. This property only depends on temperature for ideal gas systems. A very accurate value is expected since the condenser has a specified temperature of 30 °C. IFPEN shows a slightly different value compared to the other calculations due to an applied conservative pressure loss of 30 to 40 kPa.

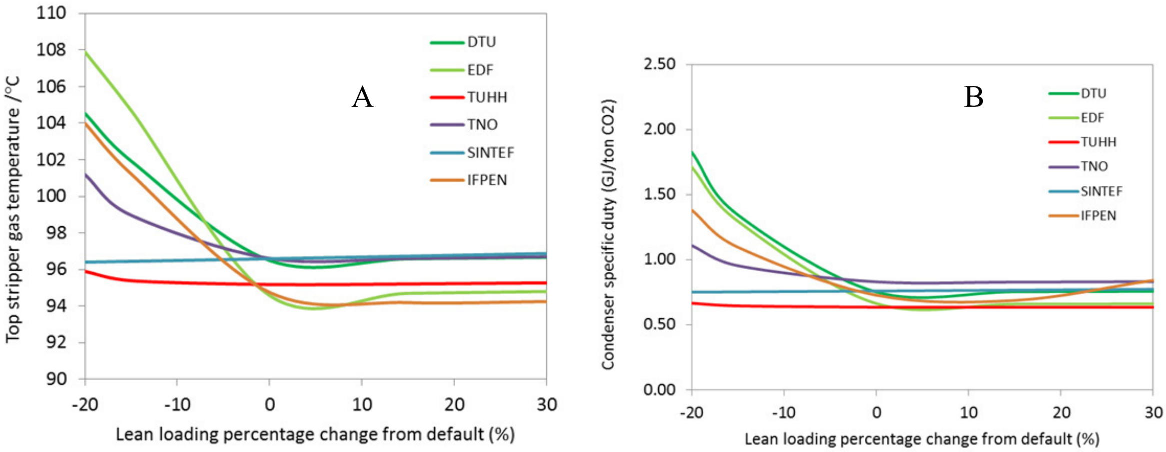

Fig. 11. (A) Desorber top outlet gas temperature; (B) Condenser specific heat duty.

The desorber top temperature and the condenser specific duty is shown in figure 11. The variation is identical to the observations in figure 6, 8B, and 9B - due to flooding. Accurate values are expected for desorber top temperature, ±2 °C, and condenser specific heat duty within 15%.

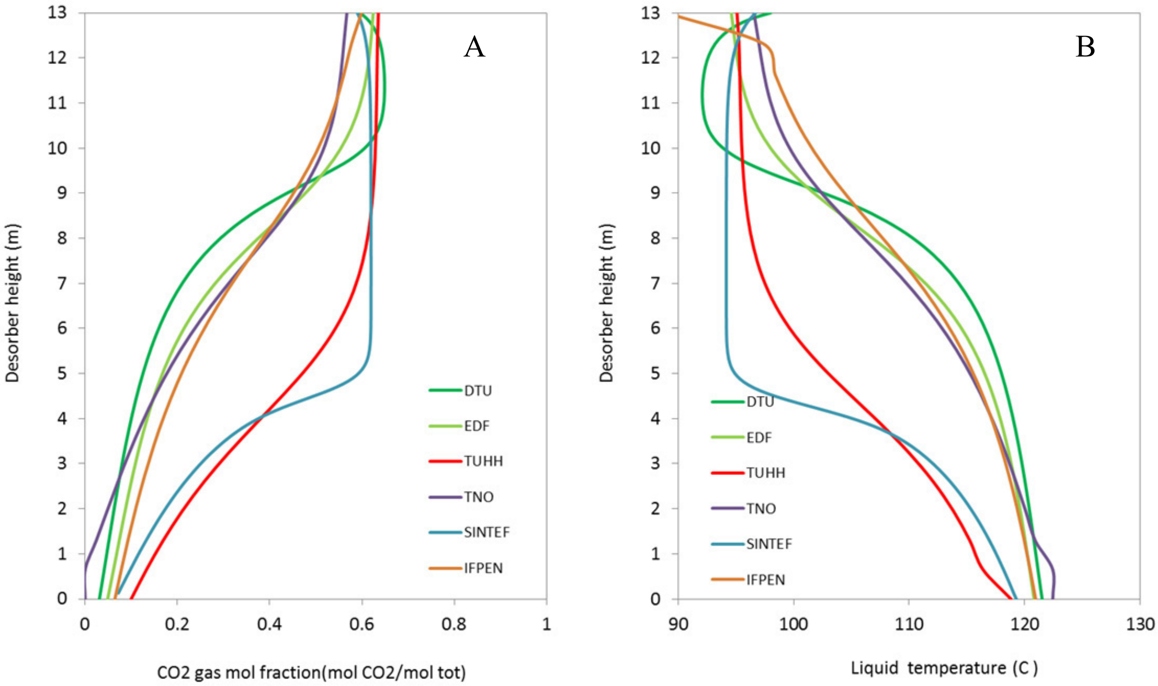

Fig. 12. Desorber CO_2 concentration profile (A) and liquid temperature profile for the case mentioned in table 3.

The desorber efficiency is illustrated in figure 12A, or more specifically the CO_2 gas concentration as function of height. The predictions by TUHH and SINTEF, show that the desorption is complete in the height of 5-7 m. Other partners show that the column is desorbing CO_2 more along the complete height. DTU specifically indicate absorption of CO_2 in the top part of the column. The explanation is found in figure 12B which show a temperature decrease in this section. The observed phenomenon is most likely due to flashing and therby evaporation and cooling – resulting in absorption. The same is observed by SINTEF though not to the same extent.

A great variability is predited for the conditions in the desorber. Carefulness should be taken while comparing profiles of model and pilot data. The accuracy very much depends on the accuracy of the mass transfer correlation. Figure 12 illustrates how desorption predictions by some partners can exstimate feasible height of the column in the order of anything from 5-13 m, conclusions which in practise would have a significant impact on the dicisions of economic investments.

The general conclusions on the desorber profiles is a reasonable accuracy of the top properties, but an unreasonable high scatter in the mid seciton. A number of the partners give consistent and similar results but few do have significantly different results. The reason is probably the applied mass transfer correlation. Within the partners that give reasonably the same results, there is an expected accuracy of 0.1 mol CO_2/mol total and 2 °C. It is noteworthy that Aspen Plus calculations obviously give very different results even though partners apply the same mass transfer model. The profiles obtained from experimental work should be carefuilly compared to the simulation data. There could be deep pitfalls in the prediction of these properties in some of the models used. The benefit is though, that properties in the top of the column are well estimated. Information which is most vital to the conclusions.

4. Main conclusions and summary

The aim of this study is two-fold: to outline the expected accuracy and variability of typical simulation tools for CO_2 capture and secondly to secure that partners in the Octavius project are synchronized with respect to modeling principles and calculations.

The work was initialized by letting people compare their calculations to a known case. The experience has shown that people will try by all efforts to match it. This is not beneficial to the comparison, since assumption and interpretations play a bigger role. Basically any result can be matched with the right kind of tuning. The only way to perform a benchmarking is to make sure all inputs are well defined and there is little room for interpretation.

In this work 6 simulation tools are summarized and modeling basis with assumptions described. Results are compared for absorption and desorption type conditions. A sensitivity study is carried out for each column, varying the lean flow rate in the absorber and the lean loading in the desorber.

Table 6. Expected predictability and variation of the calculated simulation properties

	Expected accuracy	**Variability**
Absorber results		
Capture %	Intermediate. Model scatter observed.	±10%
Top CO_2 molefraction	Intermediate. Model scatter observed.	±10%
Rich Loading	High. Deviation can be caused by inaccurate T meas.	±4%
Outlet temperature (top+bottom)	High, depends on accuracy of meas.	±5 °C
Pressure	High	±1kPa
Flooding	High reproducibility. Little scatter in model results.	±10%
CO_2 gas conc. profiles vs. height	Top + bottom conc. high accuracy. Mid column, less accurate	±6%
CO_2 temp. profiles vs. height	Top + bottom T high accuracy (1-5 °C). Mid column less accurate than meas.	±10 °C
Desorber results		
Specific reboiler duty	High, but low at >70-80% flooding.	5%
Flooding	Reasonable, but low at >70-80% flooding.	±10 %
Pressure	High	±1kPa
Reboiler temperature	Low	±1-5 °C
Bottom temperature	Reasonable	±1-5 °C
Column top CO2 mole fraction	Reasonable, but low at >70-80% flooding.	±10 %
Bottom liq. Flow	High	±10%
Column top gas flow	Low, lower at >70-80% flooding	20%
CO_2 outlet flow	High	10%
CO_2 purity	High	1%
Column top gas temperature	High	±2 °C
Condenser specific heat duty	High	±15%
CO_2 gas conc. profiles vs. height	Top conc. reasonable accuracy. Mid column, less accurate	NA
CO_2 temp. profiles vs. height	Top conc. reasonable accuracy. Mid column, less accurate	>2 °C

The findings of the sensitivity study are found in table 6. It outlines the expected accuracy of the predictions and the general variability among the 6 simulations.

There is a remarkable good agreement between the models. The majority of properties predictions vary between 5-10%, it indicates that approximately this order of accuracy should be expected for a comparison to experimental data. In a benchmarking study a 5-10% difference in calculation is therefore within the typical variability of the models. Note that experimental measurement may be more accurate than the 10% accuracy in the simulations.

A few properties can be picked out which should be treated with care if they are to be used for comparison. This is the CO_2 concentration and temperature profiles as function of height, plus the reboiler temperature. Especially the reboiler temperature is critical. It is a property often used for design specification. The profiles are less accurate in the mid sections of the column which is not critical to the simulation or comparison.

At high flooding, >70-80%, the following properties vary noticeably between simulation results: desorber SRD, flooding per cent, top CO_2 mole fraction, and the desorber top gas flow. The most important of these is the SRD which can not be reliably compared to experimental data at high flooding %.

The results have shown that the models predict the specific reboiler duty within 5-10% which is 0.2-0.4 GJ/ton CO_2 for the calculations performed. This is a significant contribution, and important to bear in mind, while doing a comparison to experimental data.

A good practice in process simulation and pilot experiments would be to meticulously define all inputs and process variables, even the packing type, insulation thickness, etc. Neglecting this would open up for future interpretation and tuning which is not beneficial to accurate model development. The minimum requirement for information is outlined in table 1 to 3.

The work presented creates a basis for future rate based model developers to characterize and compare their results to it may act as a baseline for modeling.

Acknowledgements

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