Simulation of CO_2 capture from an aluminium production plant

S. Dayarathna[1], A. Weerasooriya[1], S. Hussain[1], M. Zarsav[1],
A. Mathisen[2], H. Sørensen[2] & M. C. Melaaen[1]
[1]*Telemark University College, Norway*
[2]*Tel-Tek, Norway*

Abstract

Effective capture of CO_2 from different industrial processes is considered as an important strategy with the growing concern over the greenhouse gas emission issue all around the world. The aluminium industry accounts for a large amount of CO_2 emissions into the atmosphere during its operations annually, generally at low CO_2 concentrations below 1 vol% which eventually makes the CO_2 capture process more difficult and costly. Therefore, the CO_2 capture process at different alternative flue gas streams having CO_2 concentrations of 3, 4, 7 and 10 vol% were simulated to analyze the effect of CO_2 concentration and other process parameters on re-boiler energy demand and the capture efficiency of the plant.

Post combustion capture together with chemical absorption has been selected for this study and monoethanolamine (MEA) has been selected as the CO_2 capture solvent. An open loop CO_2 capture process was modeled and simulated using rate based electrolyte NRTL property method in Aspen Plus in order to observe the variation of specific re-boiler heat duty and the capture efficiency with the different process parameters. The capture efficiency of the process was kept at 85% and 90% to observe the effect of main process parameters including absorber height, absorber diameter and stripper height on the specific re-boiler heat duty at the stripper.

The results from the simulations indicated that the optimum specific re-boiler heat duty for the flue gas CO_2 concentrations from 3 to 10 vol% lies within the range of 3.56 to 3.60 MJ/kg of CO_2 captured for 85% efficiency and 3.59 to 3.61 MJ/kg of CO_2 captured for 90% efficiency respectively. Optimum specific re-boiler heat duty shows a small difference, between 3 and 10 vol% CO_2 concentrations for a given capture efficiency and between 85% and 90% capture

WIT Transactions on Ecology and The Environment, Vol 181, © 2014 WIT Press
www.witpress.com, ISSN 1743-3541 (on-line)
doi:10.2495/EID140621

efficiencies for a given CO_2 concentration. Hence 90% capture efficiency is preferred for this process.
Keywords: aluminium production plant, flue gas, post combustion, carbon dioxide capture, aspen plus, simulation, process optimization.

1 Introduction

Global warming is considered as one of the major aspects of the climate change issue which will make changes that can affect the water supply systems, power and transportation systems, natural environment and the health and safety of human beings. Global warming refers to the rise in average temperature near earth's surface due to the entrapment of energy in the atmosphere by greenhouse gases. Global climate data shows that the earth's average temperature has risen by 0.8ºC over the past century and is estimated to rise 1.1 to 6.4ºC over the next hundred years [1].

Carbon dioxide is the primary greenhouse gas released to the environment by various human activities. The major sources of the CO_2 emissions are electricity generation, transportation and industrial activities. Considering about the industrial activities, most industrial processes produce CO_2 through fossil fuel combustion. But several other industries including mineral production and metal production produce CO_2 through chemical reactions [2]. Among the non-ferrous metal production processes, aluminium industry accounts for a significant amount of global CO_2 emissions per annum [3].

With the increasing concern over the greenhouse gas emission issue, governments and relevant authorities around the world have come up with several solutions to tackle the problem. Even though the most effective way to reduce CO_2 emissions is to reduce fossil fuel consumption through energy efficiency, energy conservation and fuel switching, carbon capture and sequestration (CCS) also plays an important role in reducing CO_2 emissions from different production processes [2].

During the aluminium production process, large amount of CO_2 is produced at the electrolysis stage where alumina (Al_2O_3) is converted in to aluminium (Al). This particular process requires a temperature of around 1000ºC and therefore a cooling system is required to prevent production cells from structural damages. An air flow is used to cool down the process and the flue gas formed when cooling air mixed with CO_2, SO_2 and other compounds, released from the aluminium cells [4]. This outlet gas stream is then sent through a flue gas treatment facility before releasing into the environment. Due to the extensive amount of air used in the cooling process, the CO_2 concentration of the flue gas eventually falls below 1 vol% which increases the cost of capture. Therefore, the main objective of this study is to evaluate the possibility of having higher CO_2 concentrations in the flue gas and minimize the energy demand of the process based on the optimization of different process parameters in order to reduce the cost of capture.

Post combustion capture together with chemical absorption has been selected for this study and aqueous MEA has been selected as the CO_2 capture solvent.

Post combustion capture is the most well established capture technology in the industry and generally used for the flue gas streams with high volumetric flow rate and considerably low CO_2 volume percentage [5]. In addition, post combustion capture systems are rather easy to incorporate into an existing process without major modifications to the plant. The primary amine, MEA has been widely used in practice as CO_2 capture solvents because of its higher reactivity towards carbon than other secondary and tertiary amines, suitability for low CO_2 partial pressure gas streams and yielding higher purity with quick reaction rates [6, 7].

2 Model development

In this study, CO_2 capture process of the flue gas from aluminium production plant is simulated using Aspen Plus. The process flow diagram of a typical Aspen plus model is shown in the Figure 1. Flue gas with four different CO_2 concentrations was studied and the operating parameters were set to achieve fixed CO_2 capture efficiencies of 85% and 90% in the system depending on the case.

Flue gas leaving from the general scrubbing facilities at the aluminium plant is entering the absorber column from the bottom section while the solvent (i.e. aqueous MEA in this study) stream entering the column from the top section. During the upward flow of flue gas inside the absorber, most of the CO_2 in the gas stream reacts with the MEA solution to produce a CO_2 rich MEA stream which flows to the bottom of the column. The flue gas leaving the top of the absorber column called as purge gas contains small amount of non-reacted CO_2,

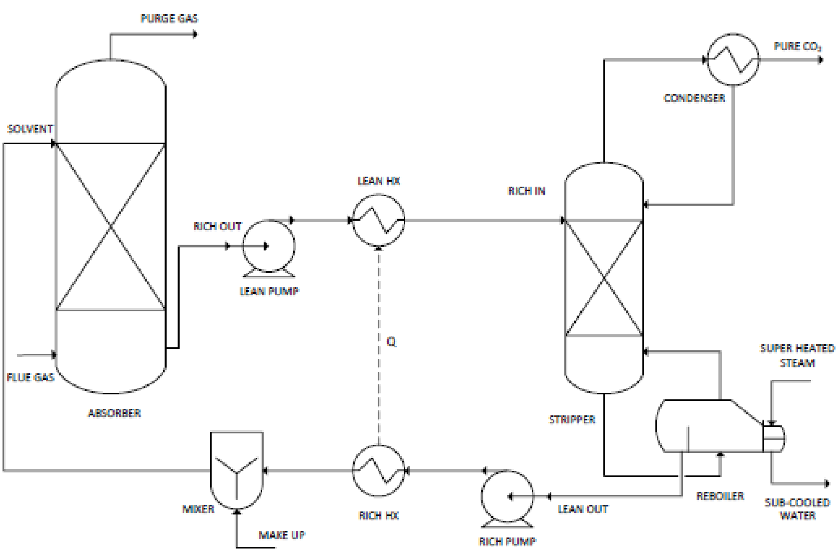

Figure 1: Process flow diagram of the CO_2 capture process.

nitrogen, oxygen, water vapor and trace amount of MEA. The CO_2 rich MEA solution at the bottom of the absorber column is then pumped into the stripping column. The temperature of the rich MEA stream should be increased up to around 107ºC before feeding into the stripping column.

The heated rich MEA solution is then fed into the stripping column from the top and flows downwards through the packing section where the captured CO_2 in the MEA solution is stripped off using the steam which is produced in the re-boiler section at the bottom of the column [8]. The re-boiler is the most energy intensive element of the entire CO_2 capture process and also the main focus of this study is to minimize the re-boiler duty by varying different parameters. The stripped gas stream containing mostly pure CO_2 (around 95–98%) and a small amount of water leaves from the top of the column and sent through a condenser to remove the moisture and then compressed and sent to the storage facility.

The MEA solution leaving from the bottom of the stripping column contains low amount of CO_2 and hence called lean MEA. The typical temperature of this lean MEA solution is around 120ºC and it should be cooled down to around 40ºC before recycling into the absorber column again. The cooling effect is mainly achieved by a cross heat exchanger (also called the lean-rich heat exchanger) that transfers the heat from the lean MEA stream to the rich MEA. A makeup stream of H_2O and MEA is also connected to the lean MEA stream in order to adjust for the component losses during the process.

2.1 Aspen plus model parameters

There are several chemical reactions take place in a system involving aqueous MEA and CO_2. The solution chemistry involved in the absorption and desorption of CO_2 into the MEA solution and the relevant thermodynamic and kinetic data which are available in the literature [9, 10] have been considered during setting the appropriate model parameters.

Electrolyte Non Random Two Liquid (NRTL) property method has been used in the simulations as it is considered to be the best property method in Aspen Plus for CO_2 capture systems.

2.1.1 Absorber and stripper column parameters

The absorber and stripper are the most important blocks or unit operation models in this flow sheet. "RadFrac" unit operation model (block) together with the "Rate-Based" calculation type has been used for absorber and stripper column modelling. In addition, "counter-current" flow model has been used for the simulations as it provides more accurate results for packed columns [11].

The simulations were run to evaluate the effect of flue gas compositions of 3%, 4%, 7% and 10% to achieve selected efficiencies of 85% and 90%. Throughout the simulation process, several absorber and stripper parameters were kept constant for all the above mentioned cases. Those parameters were selected from the literature [12] available for CO_2 capture systems involving aqueous MEA as the solvent and listed in Table 1 below.

Table 1: Absorber and stripper column specifications.

Specification	Value	
	Absorber	**Stripper**
Number of stages	15	24
Operating pressure (top stage)	1 bar	1.75 bar
Pressure drop	0.1 bar	0.1 bar
Packing type	Structured	Structured
Packing specifications	MELLAPAK, Sulzer, Standard, 250Y	FLEXIPAC, Koch, Metal, 1Y
Mass transfer coefficient method	Bravo *et al.* (1985)	Bravo *et al.* (1985)
Interfacial area method	Bravo *et al.* (1985)	Bravo *et al.* (1985)
Heat transfer coefficient method	Chilton and Colburn	Chilton and Colburn
Holdup correlation	Bravo *et al.* (1985)	Billet and Schultes (1993)
Film resistance	Liquid phase – Discrxn Vapor phase – Film	Liquid phase – Discrxn Vapor phase – Film
Re-boiler	None	Kettle
Condenser	None	Partial-vapor

2.2 Flue gas data

Flue gas data from a typical aluminium production plant which has been used during the simulation process is listed in Table 2 and the data marked with * are estimated values.

Table 2: Compositions, total flow rates and temperatures of the flue gas.

Process gas composition [vol%]				**Flow rate from one cell [Nm³/h]**	**Flow rate from 116 cells [Nm³/h]**	**Temperature [°C]**
CO_2	O_2	H_2O	N_2			
3	20.7	1.0	75.3	2667	309372*	225
4	20.0*	0.9*	75.1*	2000	232000*	265
7	19.4*	0.6*	73.0*	1143*	132588*	329*
10	18.8*	0.3*	70.9*	800	92800*	365

3 Simulations and optimization

CO_2 capture from the flue gas streams having 3, 4, 7 and 10 vol% of CO_2 has been simulated using an open loop model in Aspen Plus while achieving the specified efficiencies of 85% and 90% in the stripper column. The main objective of the optimization process was to minimize the specific re-boiler heat duty (MJ/kg CO_2 captured) at the stripper column which can be achieved by varying several process parameters in the CO_2 capture process. This study has focused mainly on the parameters such as absorber diameter, absorber height, stripper height and solvent flow rate for the optimization process while keeping the other parameter such as MEA concentration, lean loading and inlet temperature of the solvent and the packing specifications as constants. Table 3 lists the parameters which were kept as constants throughout the whole simulation process. The specified capture efficiencies were achieved by varying solvent flow rate.

Table 3: Constant parameters during the simulation.

Parameter	Value
MEA concentration	0.25 W/W
Lean loading	0.25 mol CO_2/mol MEA
Solvent inlet temperature	40ºC
Flue gas inlet temperature	9.5ºC
Packing Specifications	See Table 1

3.1 Optimization on absorber diameter

Optimization of the absorber is restricted by flooding and superficial gas velocity inside the column. Flooding can occur in smaller diameter columns while superficial gas velocity is decreasing with increasing column diameters. Low superficial gas velocities are not desirable for the mass and heat transfer inside the packed columns. Therefore, the superficial gas velocities were kept between 2–3.5 ms^{-1} during the optimization process and the results obtained for different cases were presented in Table 4. Optimum absorber diameter for both 85% and 90% capture efficiencies of each case were same. For the 7 and 10 vol% CO_2 cases where flue gas flow rates were relatively lower, it was required to keep the absorber diameter at a minimum value in order to achieve a solution without flooding. Therefore, the superficial velocities were kept below the desired limit of 2 m/s.

3.2 Optimization on absorber packing height

After achieving an optimized value for absorber diameter, the specific heat duty of the capture process was further decreased with increasing absorber packing height. Figure 2 shows the variation of specific heat duty with absorber height for both 85% and 90% capture efficiencies for all the cases of this study.

Table 4: Optimum absorber diameters and superficial velocities.

Case	Absorber diameter [m]	Superficial velocity [ms^{-1}]
3% CO_2	7.2	2.01
4% CO_2	6.25	2.00
7% CO_2	5.1	1.72
10% CO_2	4.6	1.48

It can be observed from the figures that the specific re-boiler heat duty decreases with the increasing packing height. Furthermore, larger variations observed at the smaller heights while a little variation at the larger heights. Also it can be noted that the specific heat duty is below 3.7 MJ/kg of CO_2 captured

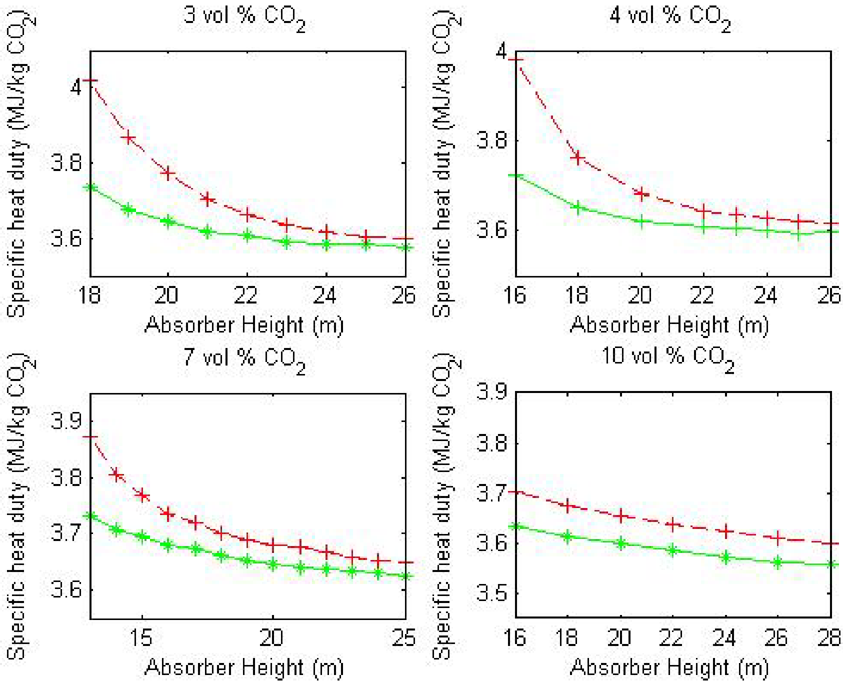

Figure 2: Variation of specific re-boiler heat duty with absorber height for 3, 4, 7, 10 vol% CO_2 concentrations in the flue gas, symbols refer to efficiencies: *, 85%; +, 90%.

when the absorber packing height exceeds 21 meters. Therefore, taking into the account of the fact that the increment of capital cost with the packing height, it is decided to keep the packing height in the range of 20–24m depending on the case considered.

3.3 Optimization on stripper packing height

Changing the stripper height showed a similar effect as the absorber height on the specific re-boiler heat duty. With the increase of stripper height, the specific re-boiler heat duty decreased continuously but for the larger heights, the variation was too small. Absorber and stripper parameters which were kept constant during the simulations are listed in Table 5.

Table 5: Constant parameters for absorber and stripper height optimization.

Case	Efficiency	Absorber optimization			Stripper optimization		
		Absorber diameter [m]	Stripper height [m]	Stripper diameter [m]	Absorber diameter [m]	Absorber height [m]	Stripper diameter [m]
3% CO_2	85%	7.2	7.0	3.0	7.2	24.0	3.0
	90%	7.2	8.0	3.0	7.2	24.0	3.0
4% CO_2	85%	6.25	7.0	3.0	6.25	23.0	3.0
	90%	6.25	7.0	3.0	6.25	24.0	3.0
7% CO_2	85%	5.1	6.0	3.0	5.1	18.0	3.0
	90%	5.1	6.0	3.0	5.1	14.0	3.0
10% CO_2	85%	4.6	7.0	3.0	4.6	18.0	3.0
	90%	4.6	7.0	3.0	4.6	18.0	3.0

Also it can be observed that the CO_2 purity of the gas leaving the stripper also increased with the stripper height. For the open-loop simulations, the CO_2 quality was around 93% to 94%. Figure 3 shows the variation of specific heat duty with the stripper height for the four different cases studied.

As it can be observed from the above figures, the variation of specific re-boiler heat duty with the stripper height is less significant after 10m, it is decided to keep the stripper height around 10–11m for all of the cases studied.

3.4 Optimum results summary

A summary of the optimum results obtained from the simulations are presented in Table 6.

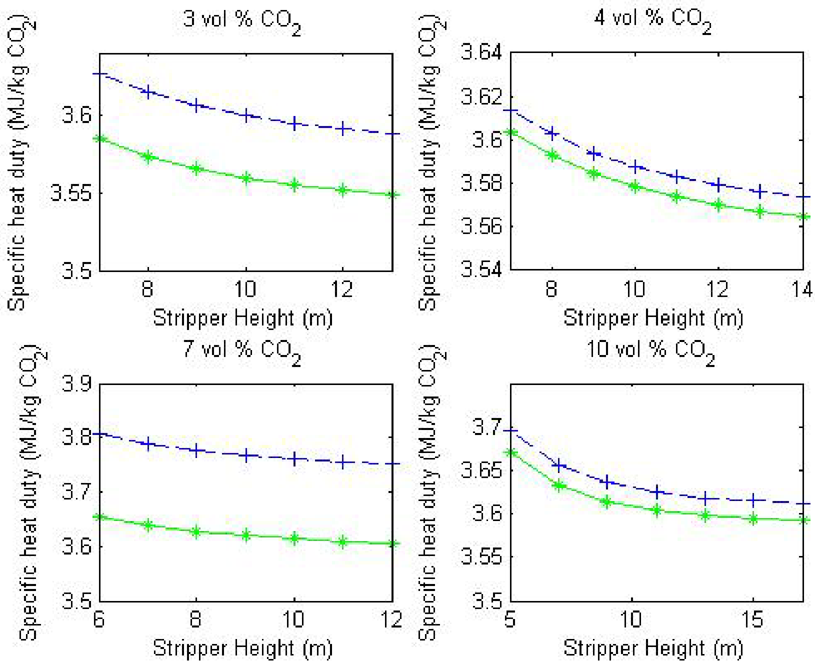

Figure 3: Variation of specific re-boiler heat duty with stripper height for 3, 4, 7, 10 vol% CO_2 concentrations in the flue gas, symbols refer to efficiencies: *, 85%; +, 90%.

Table 6: Summary of the optimum results.

CO_2 concentration	3 vol% CO_2		4 vol% CO_2		7 vol% CO_2		10 vol% CO_2	
Capture efficiency	85%	90%	85%	90%	85%	90%	85%	90%
Absorber diameter [m]	7.2	7.2	6.25	6.25	5.1	5.1	4.6	4.6
Absorber height [m]	24	24	22	23	20	22	20	22
Stripper diameter [m]	3	3	3	3	3	3	3	3
Stripper height [m]	11	11	10	10	10	11	9	9
MEA flow rate [tonne/hr]	313	335	315	334	316	336	314	334
Reboiler heat duty [MW]	15.3	16.4	15.4	16.4	15.5	16.5	15.5	16.5
Specific heat duty [MJ/kg CO_2]	3.56	3.59	3.58	3.61	3.61	3.62	3.60	3.61
Purity of CO_2 [%]	93.9	93.7	93.7	93.6	93.7	93.7	93.6	93.6

4 Conclusions

The aluminium industry accounts for a large amount of CO_2 emissions into the atmosphere during its operations and the low CO_2 concentration of the flue gas makes the capture process difficult and costly. Different flue gas streams from the aluminium production plant having absorber inlet temperature of 9.5ºC and CO_2 concentrations of 3, 4, 7 and 10 vol% were successfully simulated using Aspen Plus during this study. Then the effect of different process parameters on the specific re-boiler heat duty of the stripper and the capture efficiency of the plant were analysed.

It is investigated from the simulation results that the increase of absorber and stripper packing height results in a decrease of the specific re-boiler heat duty (i.e. higher the packing section, lower the specific heat duty). But after a certain point, specific re-boiler heat duty declines insignificantly and lay within 3.56–3.62 MJ/kg CO_2 captured for all cases. Therefore, it can be concluded that the optimum height of the absorber and stripper will be in the range of 20–24 m and 10–11 m respectively for all the cases in order to have a minimum re-boiler heat duty.

Specific re-boiler duty also shows a decreasing trend with increasing absorber diameter. But the optimization possibilities of the absorber diameter is quite restricted due to the fact that the superficial gas velocity inside the column must be within 2–3.5 ms^{-1} in order to maintain the efficient mass and heat transfer.

From all the final optimization results, it is evident that the specific re-boiler heat duty does not vary a lot between 3 vol% to 10 vol% CO_2 concentration cases for a given capture efficiency. Furthermore, for a given CO_2 concentration in the flue gas, it is observed that an increased specific re-boiler heat duty for the 90% efficiency than the 85% efficiency, even though the difference was not very large. Therefore, it is preferred to operate the capture process at 90% efficiency as it doesn't demand too much re-boiler energy compared to the 85% efficiency cases.

References

[1] United States Environmental Protection Agency. *Climate Change: Basic Information*. Available:http://www.epa.gov/climatechange/basics/

[2] United States Environmental Protection Agency. *Carbon Dioxide Emissions*.Available:http://www.epa.gov/climatechange/ghgemissions/gases/CO2.html

[3] Intergovernmental Panel on Climate Change. *IPCC Fourth Assessment Report: Climate Change 2007*. Available: http://www.ipcc.ch/publications_and_data/ar4/wg3/en/ch7s7-4-2.html

[4] H. Björk and J. Aronsson, "Process Integration and Performance of Chilled Ammonia CO_2 Capture Technology," M.Sc. Thesis, Department of Energy and Environment, Chalmers University of Technology, 2011.

[5] A. Kothandaraman, "Carbon Dioxide Capture by Chemical Absorption: A Solvent Comparison Study," Ph.D Thesis, Massachusetts Institute of Technology, USA, 2010.
[6] Y. Liu, L. Zhang, and S. Watanasiri, "Representing vapor-liquid equilibrium for an aqueous MEA-CO_2 system using the electrolyte nonrandom-two-liquid model," *Industrial & engineering chemistry research,* vol. 38, pp. 2080-2090, 1999.
[7] E. Blomen, C. Hendriks, and F. Neele, "Capture technologies: Improvements and promising developments," *Energy Procedia,* vol. 1, pp. 1505-1512, 2009.
[8] U. S. P. R. Arachchige, N. Aryal, and M. C. Melaaen, "CO_2-flue gas seperation for a gas-fired power plant," in *Tenth Annual Conference on Carbon Capture and Sequestration*, 2011.
[9] D. M. Austgen, "A model of vapor-liquid equilibria for acid gas-alkanolamine-water systems," Ph.D. Thesis, The University of Texas at Austin, 1989.
[10] S. Freguia, "Modeling of CO_2 removal from flue gases with monoethanolamine," Master Thesis, University of Texas at Austin, 2002.
[11] Aspen Technology Inc., "Flow Models," ed, 2010.
[12] U. S. P. R. Arachchige, M. Mohsin, and M. C. Melaaen, "Optimized Carbon Dioxide Removal Model for Gas Fired Power Plant," *European Journal of Scientific Research,* vol. 86, pp. 348-359, 2012.