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Optimization of post combustion carbon capture process-solvent selection

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Abstract
The reduction of the main energy requirements in the CO_2 capture process that is re-boiler duty in stripper section is important. Present study was focused on selection of better solvent concentration and CO_2 lean loading for CO_2 capture process. Both coal and gas fired power plant flue gases were considered to develop the capture plant with different efficiencies. Solvent concentration was varied from 25 to 40 (w/w %) and CO_2 lean loading was varied from 0.15 to 0.30 (mol CO_2/mol MEA) for 70-95 (mol %) CO_2 removal efficiencies. The optimum specifications for coal and gas processes such as MEA concentration, CO_2 lean loading, and solvent inlet flow rate were obtained.

Keywords: Carbon dioxide capture; Coal and gas power plant; Lean loading; Solvent concentration.

1. Introduction
The atmospheric concentration of green house gases (GHG) has mainly increased due to human activities. The emissions of different green house gases have been studied and measured all around the world. Carbon dioxide (CO_2) is considered as the most important GHG and annual percentage emission from different sectors are seen in Figure 1 [1].
Fossil fuel (especially coal) still plays the most important role in the energy sector. On the other hand, that is leading the percentage of CO_2 emissions to the atmosphere. Therefore, carbon dioxide capture and storage (CCS) technologies are important to continue fossil fuel fired power plants. However, CCS is still having several challenges in large scale, which will significantly reduce the overall efficiency of a power plant. The reduction of the main energy requirements in the CO_2 capture process that is re-boiler duty in stripper section is important to implement. The overall re-boiler energy requirement consists of three major parts, which are the energy needed for liberating attached CO_2 from amines, the heat required to increase the solvent temperature, and energy use for water evaporation process. Post combustion chemical absorption process is considered as preferred option. Main reason behind that is, it is easy to apply in already available coal and gas power plants with small modifications. Post combustion chemical absorption processes use a solvent to chemically react with CO_2 from the flue gas and liberated that absorbed CO_2 in the stripper. There are several solvents available and selections of best solvent and properties of the solvent stream are important to optimize. Present study was focused on selection of the best solvent concentration and CO_2 lean loading for CO_2 capture process. Both coal and gas-fired power plant flue gases are considered to develop the capture plant with different efficiencies. Number of simulations was performed in Aspen Plus with different solvent conditions to check the lowest re-boiler

duty and lowest solvent inlet flow rate. Finally, most suitable solvent concentration and lean loading are selected for three different CO_2 capture processes.

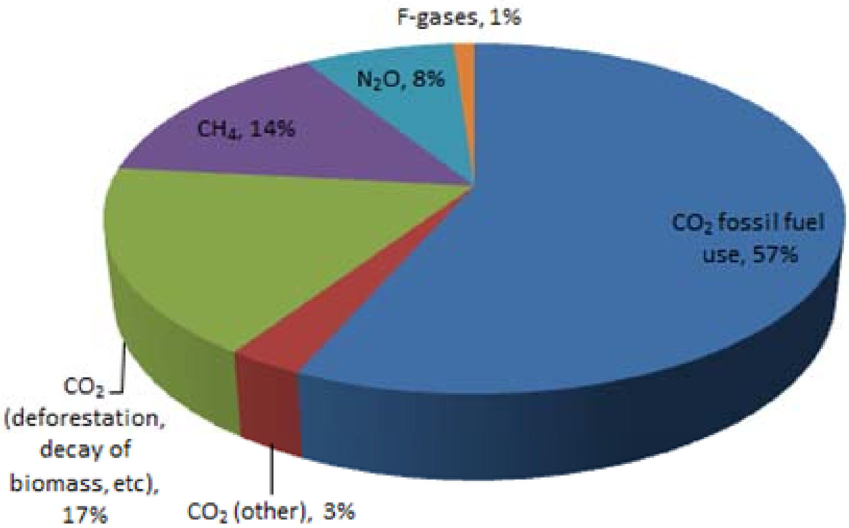

Figure 1. Percentage of CO_2 emissions from different sources [1]

2. Model development

The Electrolyte Non Random Two Liquid (NRTL) property method in Aspen Plus is used to implement the CO_2 capture model. The 500 MW coal and gas fired power plant flue gas data are taken from the literature [2, 3]. The composition of the flue gas inlet stream is tabulated in Table 1.

Table 1. Flue gas composition and parameters [2, 3]

Parameter	Coal Fired	Gas Fired
Flow rate [kg/s]	673.4	793.9
Temperature [K]	313	313
Pressure [bar]	1.1	1.1
Major Composition	Mol%	Mol%
H_2O	8.18	8.00
N_2	72.86	76.00
CO_2	13.58	4.00
O_2	3.54	12.00
H_2S	0.05	0.00

The implemented process flow diagram for the carbon capture process is given in the Figure 2. The main chemical reactions between MEA and CO_2 are taken into consideration [4] with available thermodynamic and kinetic data [5].

The calculation procedure in rate based electrolyte NRTL model in Aspen Plus consists of material and energy balances, mass and heat transfer, phase equilibrium, and summation equations [6]. According to the packing type, mass transfer correlations are varied. Many of the mass transfer correlations are also provided the interfacial area value. However, interfacial area factor can be specified in the packing section in Aspen Plus model. The required area for actual mass transfer uses in Aspen Plus is the multiplication of area from the correlation with this interfacial area factor [7].Therefore, large number of input data and parameters are important to provide to achieve these complicated calculations. The input conditions and model specifications that have been used for model development in the absorber, and stripper are shown in Table 2. Most of the specifications are recommended specifications for rate based model of the CO_2 capture process by Aspen Tech [7], and some of them are taken from literature [8].

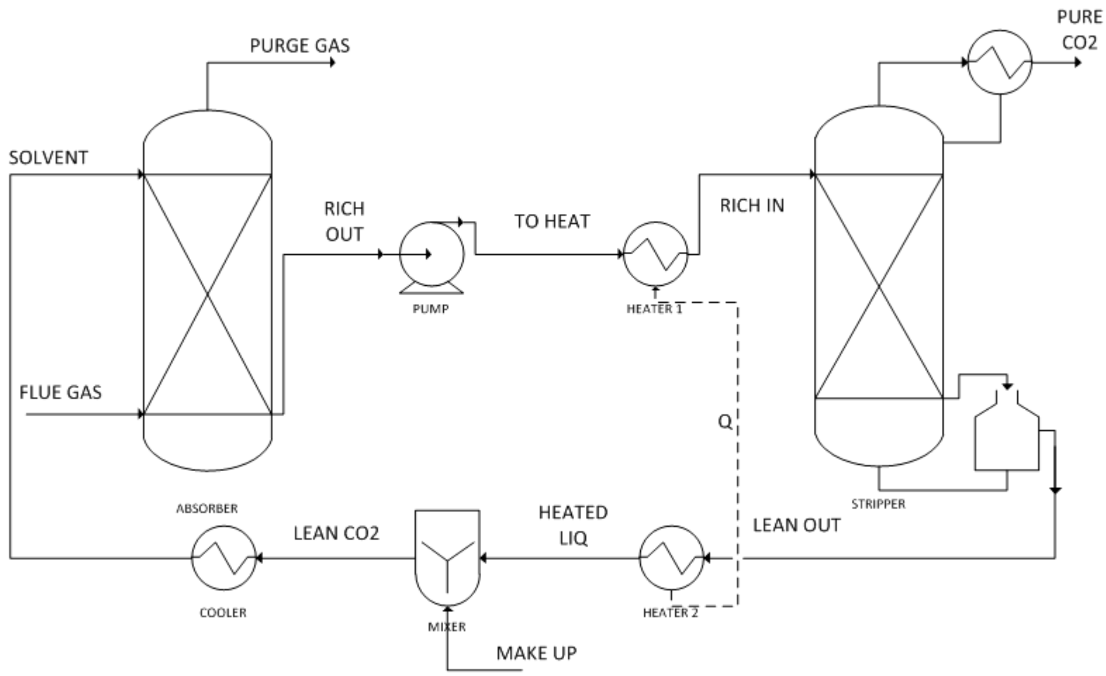

Figure 2. Process flow diagram

Table 2. Absorber and stripper column specifications

Specification	Coal fired flue gas		Gas fired flue gas	
	Absorber	Stripper	Absorber	Stripper
Number of stages	15	15	15	15
Operating pressure	1 bar	2 bar	1 bar	1.6 bar
Re-boiler	None	Kettle	None	Kettle
Condenser	None	Partial-vapour	None	Partial-vapour
Packing type	Mellapak,Sulzer, Standard, 250Y	Flexipac, Koch, metal,1Y	Mellapak, Sulzer, Standard, 250 Y	Flexipac, Koch, metal,1 Y
Packing height	20m	18m	24m	18m
Packing diameter	15m	12m	18m	12m
Mass transfer coefficient method [9]	Bravo et al. (1985) [9]	Bravo et al. (1985) [9]	Bravo et al. (1985) [9]	Bravo et al. (1985) [9]
Interfacial area method [9]	Bravo et al. (1985) [9]	Bravo et al. (1985) [9]	Bravo et al. (1985) [9]	Bravo et al. (1985) [9]
Interfacial area factor	1.5	2	1.2	1.5
Heat transfer coefficient method	Chilton and Colburn	Chilton and Colburn	Chilton and Colburn	Chilton and Colburn
Holdup correlation [10]	Billet and Schultes (1993) [10]	Billet and Schultes (1993) [10]	Billet and Schultes (1993) [10]	Billet and Schultes (1993) [10]
Film resistance	Discrxn for liquid film and Film for vapour film	Discrxn for liquid film and Film for vapour film	Discrxn for liquid film and Film for vapour film	Discrxn for liquid film and Film for vapour film
Flow model	Mixed	Mixed	Mixed	Mixed

In both coal and gas fired capture simulation models, Mixed flow model is selected. There are four different flow models are available in the Aspen Plus rate base model. Due to the high amount of CO_2 composition in flue gas, Mixed flow model is recommended in literature [7].

3. Simulations

Solvent concentration and CO_2 lean loading are considered for simulations with different efficiencies. Solvent concentration is varied from 25 to 40 (w/w %) and lean loading is varied from 0.15 to 0.30 (mole CO_2/mole MEA) for 70-95 (mol %) CO_2 removal efficiency. Exactly similar simulations are performed to analyze both coal and gas fired flue gas removal processes.

3.1 Coal fired power plant flue gas simulations

The simulation results for coal fired system are considered under this section. Figure 3 indicate re-boiler duty variation with CO_2 lean loading when MEA concentration is fixed at 25, 30, 35, and 40 (w/w %) respectively.

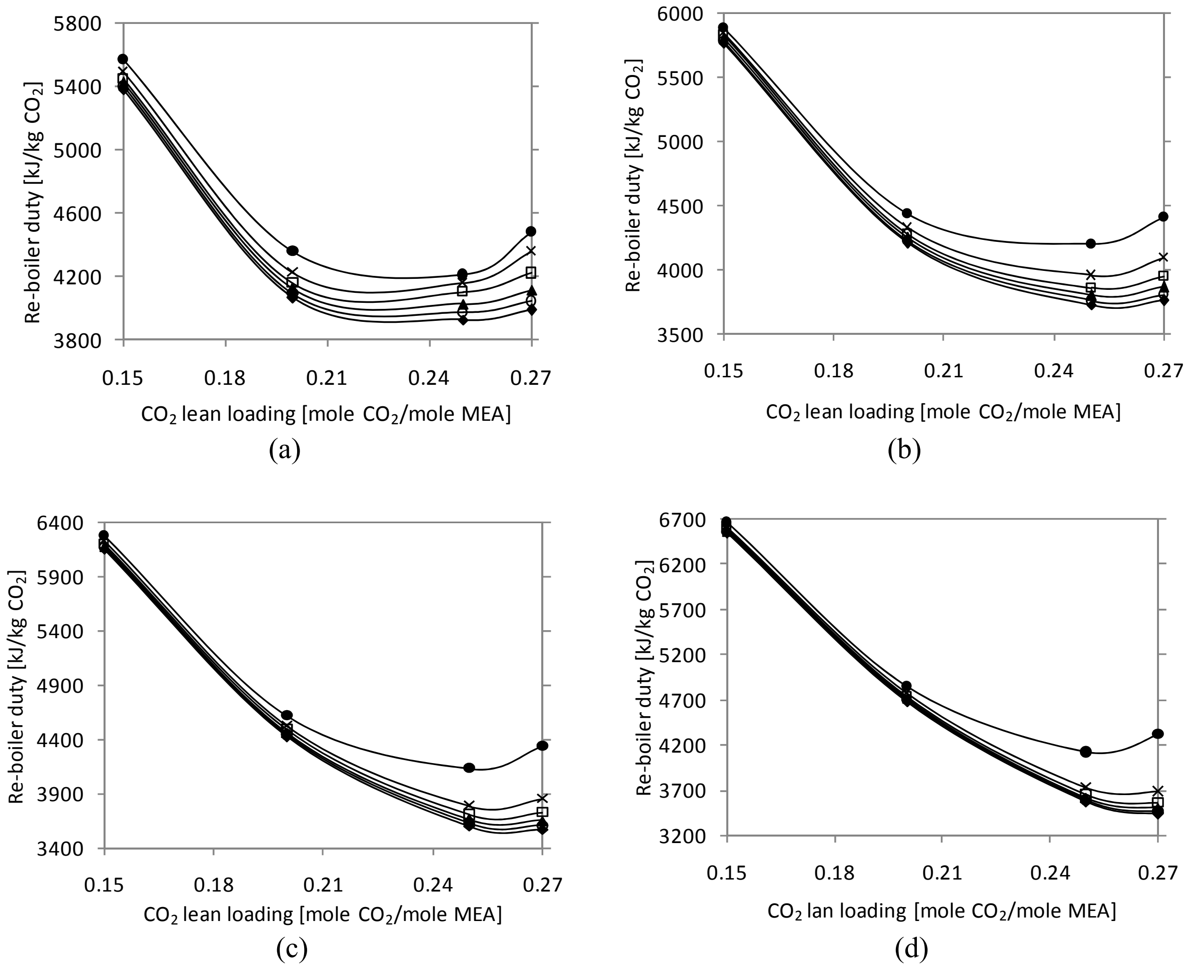

Figure 3. Re-boiler duty variation with CO_2 lean loading with different MEA concentrations, (a) 25w/w%, (b) 30w/w%, (c) 35w/w% and (d) 40w/w%, in coal fired flue gas, symbols refer to efficiencies: ♦, 70%; o, 75%; ▲, 80%; □, 85%; ×, 90%; ●, 95%

From Figure 3 it is clear that the re-boiler energy requirement decreases with the increase of lean solvent loading until the minimum is obtained. However, after a certain limit of the lean loading value, re-boiler duty again started to increase. The point which gives lowest re-boiler energy is defined as the optimum lean solvent loading. At the same time, inlet solvent flow rate is changed to achieve the specified CO_2 removal efficiency. In all four cases (MEA concentration from 25% to 40%), lowest re-boiler duty is shown at 70% efficiency. When CO_2 removal efficiency is increased, re-boiler duty is increased. According to the figures, lowest re-boiler duty is shown in Figure 3(d), which has 40% MEA concentration. The required lowest energy demand in the re-boiler for most important efficiency values have been analyzed separately and given in Figure 4. The efficiencies 85%, 90% and 95% are considered as most considerable and good values for the removal process.

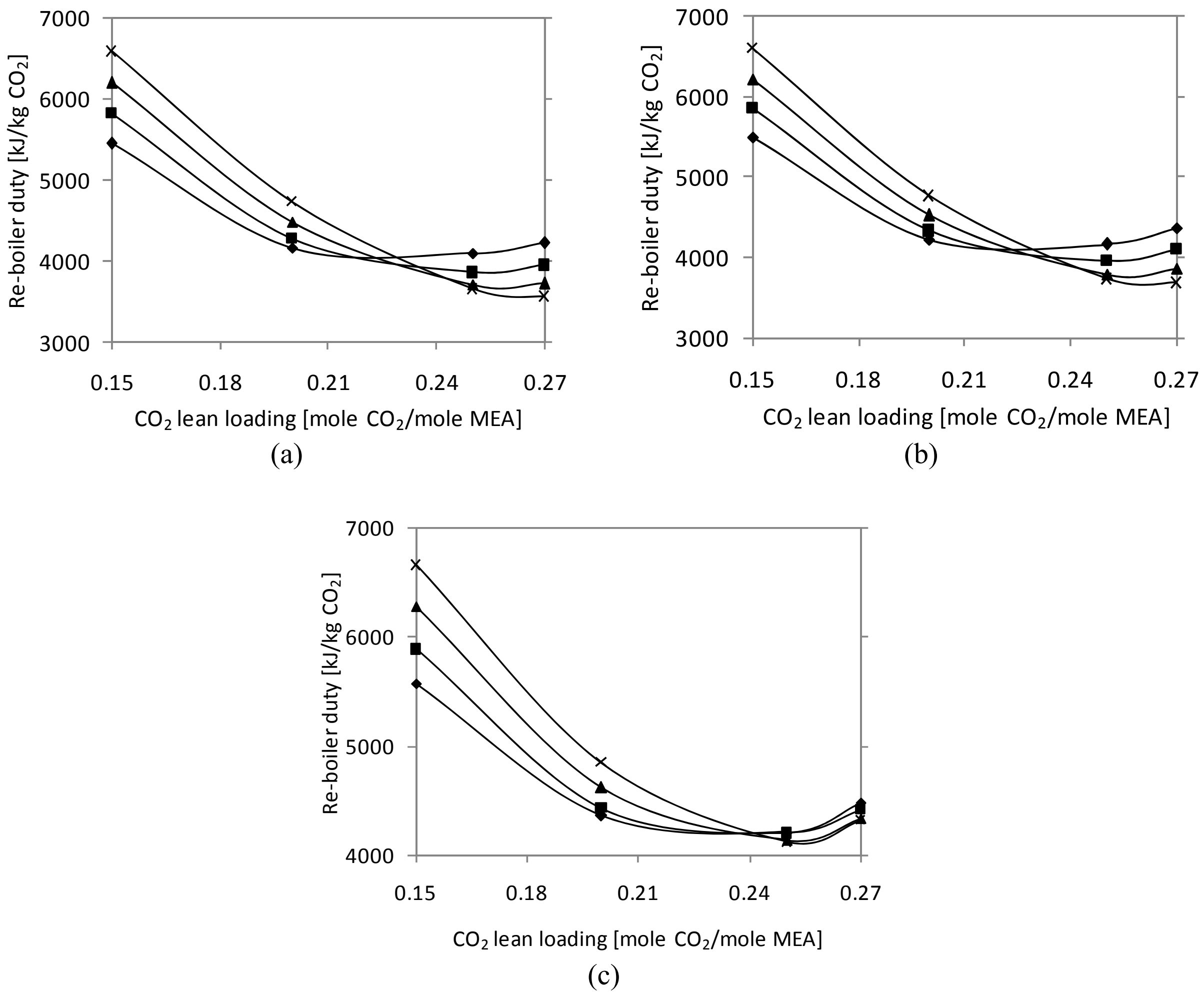

Figure 4. Re-boiler duty variation with CO_2 lean loading when removal efficiency is (a) 85%, (b) 90%, (c) 95% in coal fired flue gas, symbols refers to MEA concentrations: ♦, 25% MEA; ■, 30% MEA; ▲, 35% MEA; ×, 40% MEA.

For 85% CO_2 removal efficiency, lowest re-boiler duty is given at 40% MEA concentration and 0.27 CO_2 lean loading (Figure 4(a)). Similarly from Figure 4(b) and (c), it can be seen that lowest re-boiler duty is given at 40% MEA concentration and 0.27 lean loading for 90% removal efficiency process and 0.25 lean loading for 95% removal efficiency. It is not just re-boiler duty requirement, but also solvent flow rate minimization is important to optimize the process. The solvent flow rate requirement for 0.27 (mole CO_2/mole MEA) CO_2 lean loading model is given in Figure 5.

It can be seen from Figure 5, that the required solvent inlet flow rate is decreasing with the increased of MEA concentration. When the removal efficiency is gradually increased, required solvent flow rate is increasing. For all removal efficiency models, lowest solvent requirement is given for 40% MEA concentration. However, increasing the amine concentration is believed to have corrosive effects in all sections in capture plant. This can be minimized by adding a small amount of corrosive inhibitors to the inlet solvent stream. The presence of these inhibitors is supposed to have negligible effect on the CO_2 removal process.

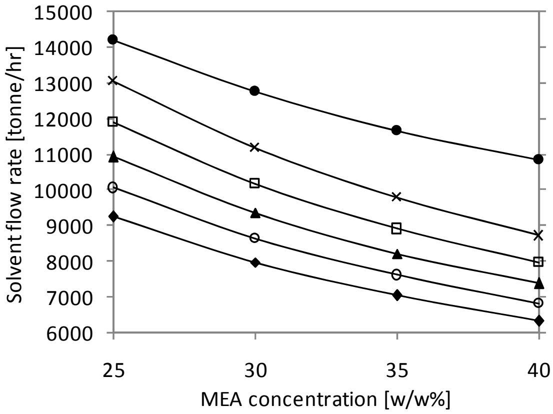

Figure 5. Solvent flow rate variation with MEA concentration when CO_2 lean loading 0.27(mole CO_2/mole MEA) in coal fired flue gas, symbols refer to efficiencies: ♦, 70%; o, 75%; ▲, 80%; □, 85%; ×, 90%; ●, 95%.

3.2 Gas fired power plant flue gas simulations

Figure 6 indicate re-boiler duty variation with CO_2 lean loading when MEA concentration is fixed at 25, 30, 35 and 40% respectively. All simulations were performed exactly similar to coal fired flue gas simulations.

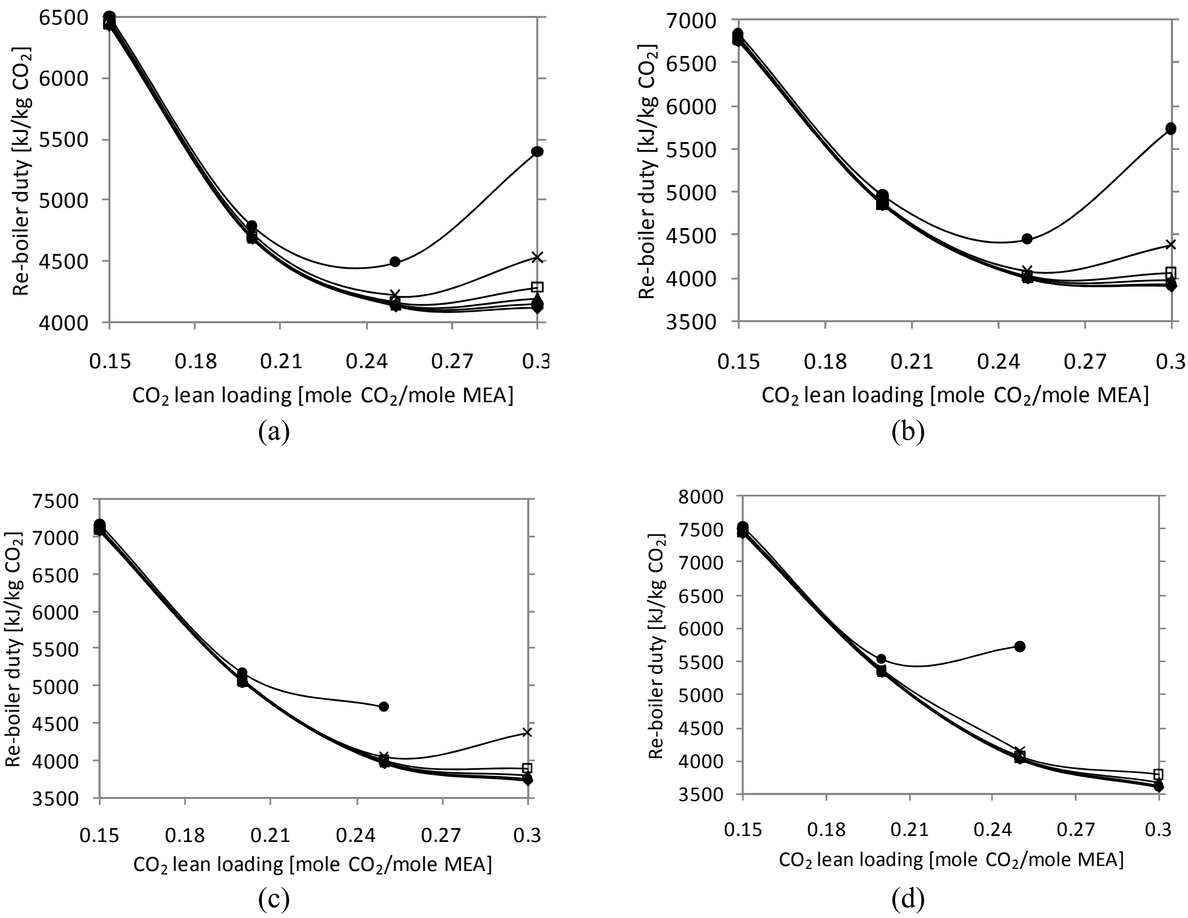

Figure 6. Re-boiler duty variation with CO_2 lean loading when MEA concentration, (a) 25w/w%, (b) 30w/w%, (c) 35w/w% (d) 40w/w%, in gas fired flue gas, symbols refer to efficiencies: ♦, 70%; o, 75%; ▲, 80%; □, 85%; ×, 90%; ●, 95%.

Similar to coal fired system, Figure 6, re-boiler duty is decreasing as lean loading increase. However, after a certain lean loading value, re-boiler duty again starts to increase. In all four cases (MEA concentration from 25% to 40%), lowest re-boiler duty is shown for 70% efficiency simulation plot. The trends of the figures are obtained almost similar to the coal fired cases. The required lowest energy demand in the re-boiler for efficiency values 85%, 90% and 95% have been analyzed separately and given in Figure 7.

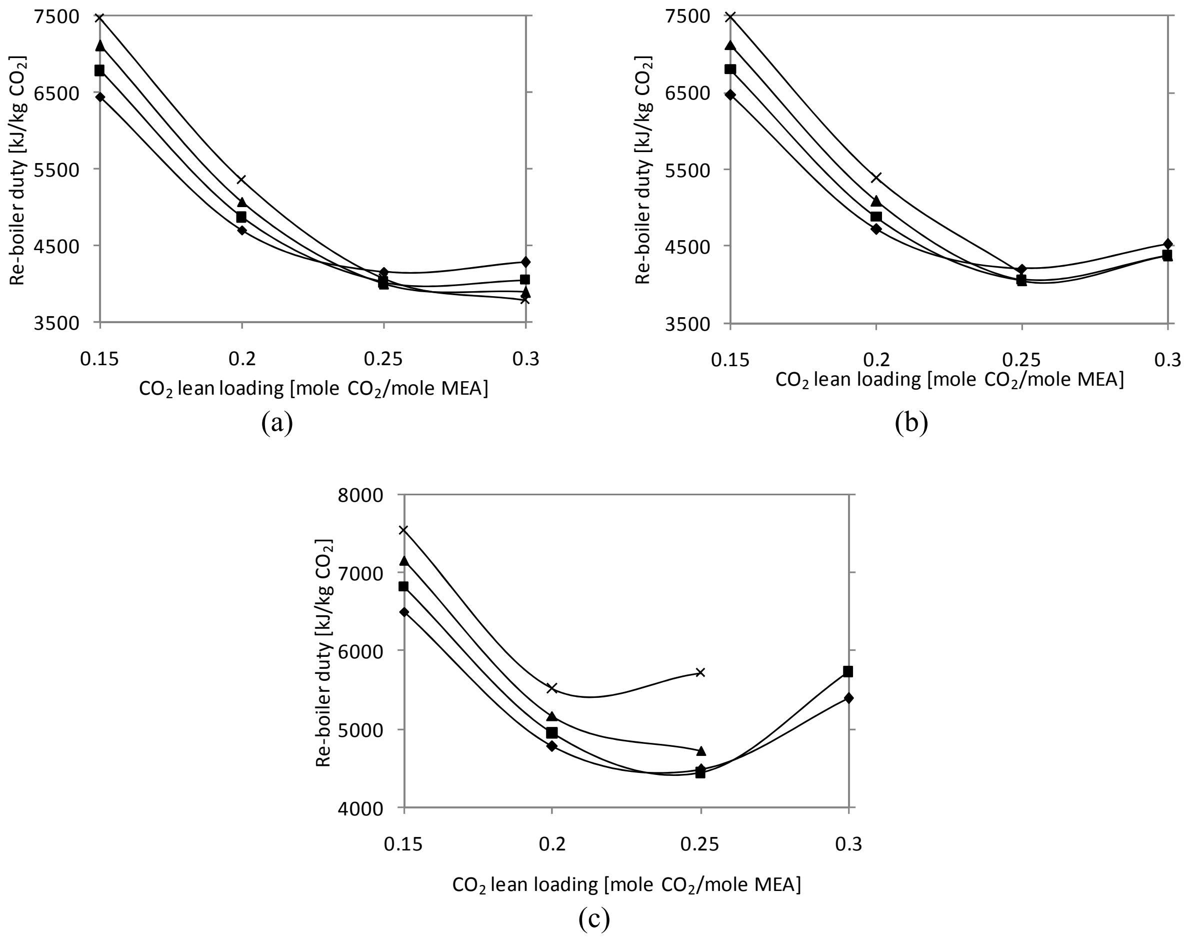

Figure 7. Re-boiler duty variations with CO_2 lean loading when removal efficiency is (a) 85%, (b) 90%, (c) 95% in gas fired flue gas, symbols refer to MEA concentrations: ♦, 25% MEA; ■, 30% MEA; ▲, 35% MEA; ×, 40% MEA

For 85% CO_2 removal efficiency, lowest re-boiler duty is given at 40% MEA concentration and 0.30 CO_2 lean loading (Figure 7(a)). Similar to that from Figure 7(b) and (c), it can be seen that lowest re-boiler duty is given at 35% MEA concentration and 0.25 lean loading for 90% removal efficiency, and 30% MEA concentration and 0.25 lean loading for 95% removal efficiency. Figure 8 is showing the solvent flow rate variation with MEA concentration at 0.25 and 0.30 CO_2 loading, respectively.

As MEA concentration is increased, required solvent flow rate is decreased. For 85% and 90% efficiency, lowest solvent flow rate is given when the lean loading is 0.25 and 40% MEA concentration and for 95% efficiency, lowest solvent flow rate gives when lean loading 0.25 and 35% MEA concentration. When the lean loading is increased to 0.30, once again lowest solvent flow rate is given for 40% MEA concentration.

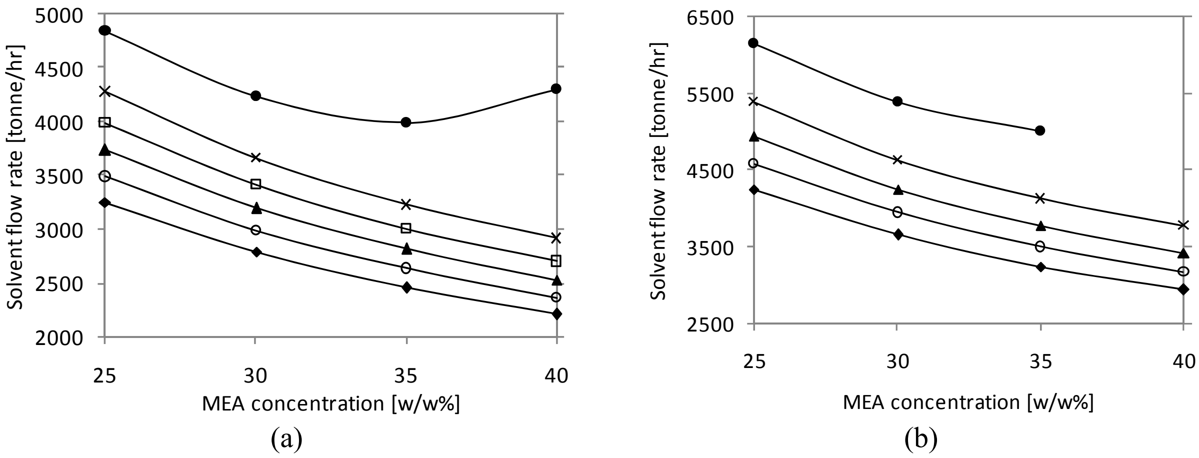

Figure 8. Solvent flow rate variation with MEA concentration when CO_2 lean loading is (a) 0.25 and (b) 0.30 (mole CO_2/mole MEA) in gas fired flue gas, symbols refer to efficiencies: ♦, 70%; o, 75%; ▲, 80%; ×, 85%; ●, 90%

4. Conclusion

The most important factor for process optimization in the capture process is the thermal energy requirement in the regeneration process, as it is responsible for overall thermal efficiency. At the same time, inlet solvent flow rate is also considered. The lowest re-boiler duty with minimum solvent flow rate will give optimal energy requirement and lowest operating cost. The lowest re-boiler duties are calculated as 3634.2, 3736.4, and 4185.5 kJ/kg CO_2 for the 85, 90, and 95% CO_2 removal process for coal fired power plant and 3781, 4050, and 4240 kJ/kg CO_2 for 85%, 90%, and 95% for gas fired power plant. The optimum specifications for the coal and gas processes such as MEA concentration, CO_2 lean loading, and solvent inlet flow rates are summarized in Table 3 for different efficiency values. The re-boiler energy demand is decreasing with increasing amine concentration in the solvent inlet flow stream.

Table 3. Optimum solvent conditions for both coal and gas fired power plant flue gas capture process

Specification	85% Removal Efficiency	90% Removal Efficiency	95% Removal Efficiency
Coal fired power plant CO_2 capture			
MEA concentration [w/w%]	40	40	40
CO_2 lean loading [mole CO_2/mole MEA]	0.27	0.27	0.25
Solvent flow rate [tonne/hr]	7965	8719	8940
Gas fired power plant CO_2 capture			
MEA concentration [w/w%]	40	35	30
CO_2 lean loading [mole CO_2/mole MEA]	0.30	0.25	0.25
Solvent flow rate [tonne/hr]	3775	3224	4240

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