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Modeling of CO_2 capture by using monoethanolamine (MEA) in rotating packed bed (RPB)

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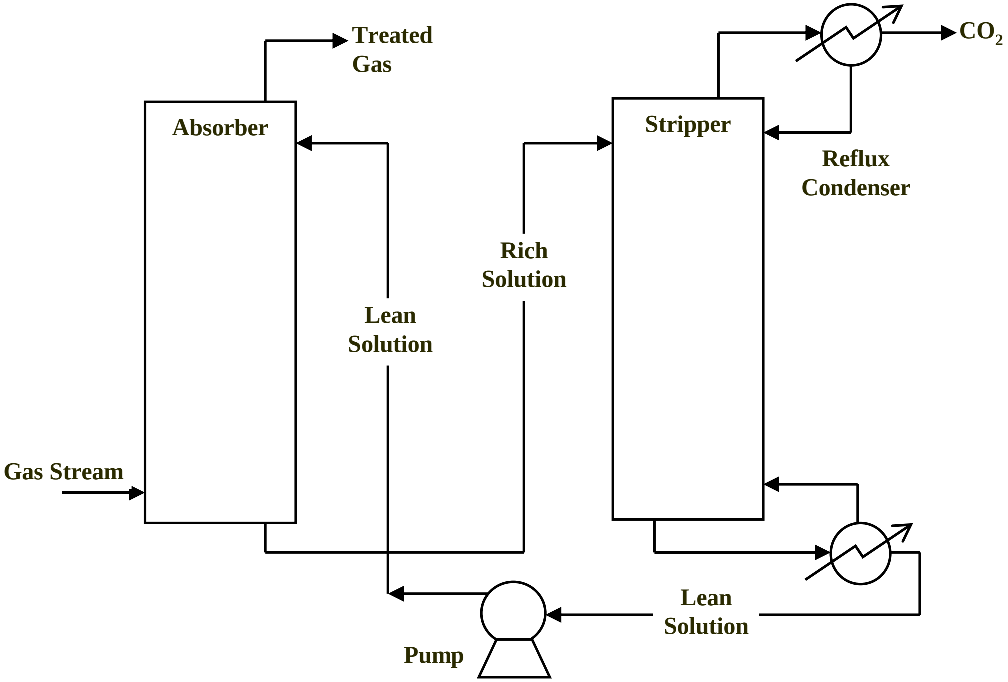
1. Introduction

1.1 Background

- Flowsheet of solvent-based capture Process



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1. Introduction

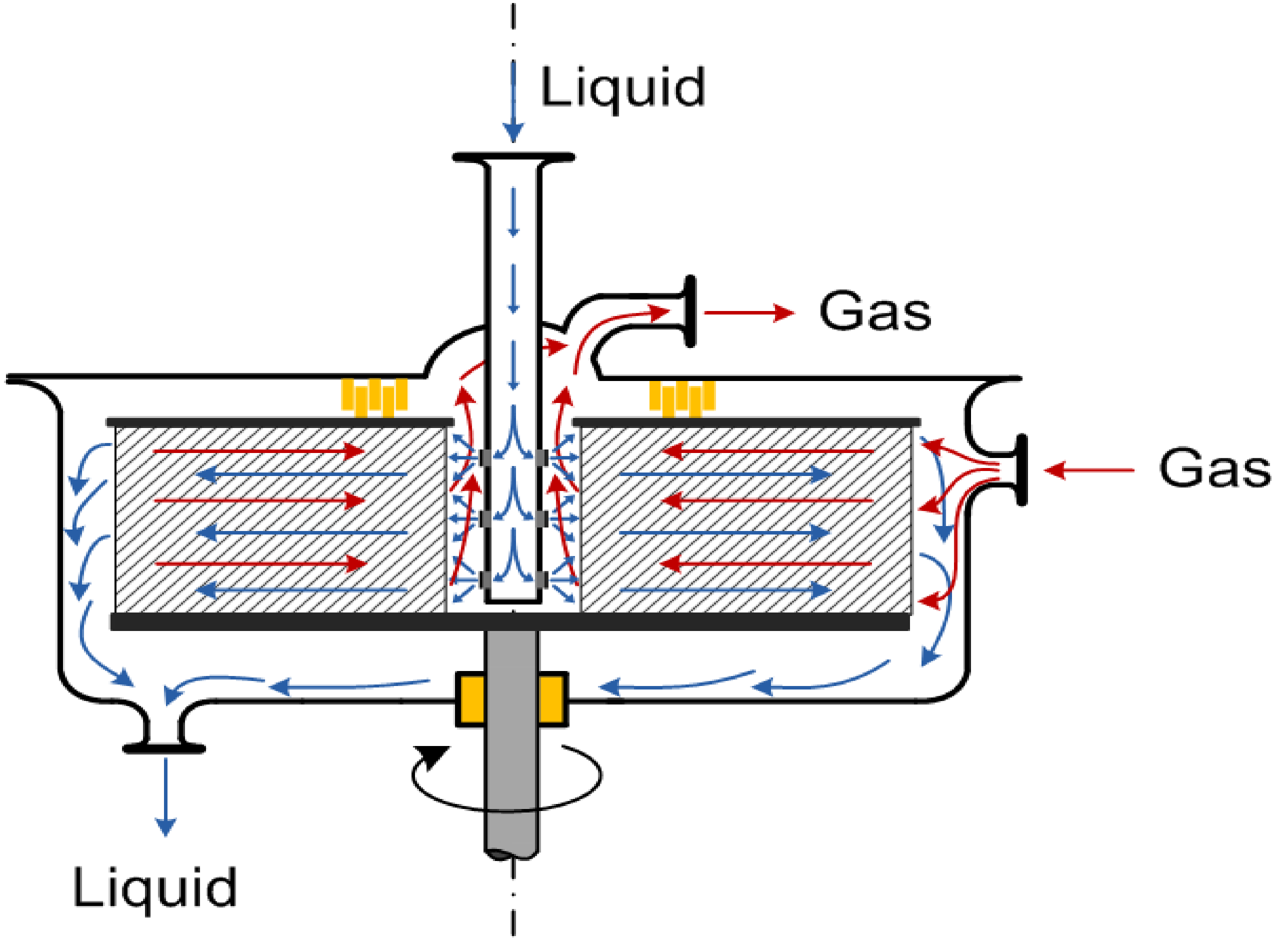
1.2 Motivation

- Large volume of CO_2 to capture (E.g. a 500 MWe coal-fired power plant with about 600 kg/s flue gas flowrate emits over 8000 tons of CO_2 daily) and poor mass transfer performance in the packed beds
- Packed columns inevitably large (E.g. for 90% capture from 500 MWe coal-fired power plant, absorber column of up to 25 m in diameter and over 27 m in height will be needed)
- Ferrybridge CCS, UK:
  - 100 tons/day
  - Absorber (2.3 m x 39 m)
  - Stripper (1.1 m x 30.5 m)
  - Total cost: £21 million
- Improved mass transfer

Ferrybridge capture facility

1. Introduction

1.3 Process intensification



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1. Introduction

1.3 Process intensification

- Rotating packed bed (RPB) is the most suitable PI tool for application in solvent-based capture process [1].

- Intensified mass transfer by centrifugal acceleration equivalent to several gravitational acceleration (HiGee)

  - Considerable increase in the mass transfer rate leading to significant reduction in size and weight of the rigs (12 times smaller than PBs for CO_2 absorber [2])

  - Reduction in energy consumption

  - Wider flooding limit

  - Due to the short residence time in RPB, this system is proper for cases that require short contact time

1. Introduction

1.4 Aim and objectives

- Rate-base mass transfer with enhancement factor was considered to model the RPB absorber using MEA in gPROMS
- Impact of using eight different kinetic models on the prediction of CCL is evaluated.
- Five different enhancement factor relations are utilized to evaluate the effect of these kinetic models.
- Process analysis is performed to find the effect of different operating factors on the CCL.
- The orthogonal array design (OAD) method is applied to perform multivariable sensitivity analysis

2. Model development

2.1 Governing equations

- Mass balance for liquid and gas phases

$$\frac{\partial(F_g y_i)}{\partial r} = a_{gl} N_i\, A_c \qquad B.C.:\begin{cases} \text{at } r = R_o : \; y_i = y_0 \\ at\ r = R_i \; : \; \dfrac{\partial(F_g y_i)}{\partial \mathrm{r}} = 0 \end{cases}$$

$$\frac{\partial(F_l x_i)}{\partial r} = a_{gl} N_i A_c \qquad B.C.:\begin{cases} \text{at } r = R_i \; : \; x_i = x_0 \\ at\ r = R_o \; : \; \dfrac{\partial(F_l x_i)}{\partial \mathrm{r}} = 0 \end{cases}$$

- Energy balance for liquid and gas phases

$$\frac{\partial(F_g C_{pg} T_g)}{\partial r} = a_{gl} q_g A_c \quad B.C.:\begin{cases} \text{at } r = R_o \; : \; T_g = T_{g,0} \\ \text{at } r = R_i \; : \; \dfrac{\partial(F_g C_{pg} T_g)}{\partial \mathrm{r}} = 0 \end{cases}$$

$$\frac{\partial(F_l C_{pl} T_l)}{\partial r} = a_{gl} q_l A_c \quad B.C.:\begin{cases} \text{at } r = R_i \; : \; T_l = T_{l,0} \\ at\ r = R_o \; : \; \dfrac{\partial(F_l C_{pl} T_l)}{\partial \mathrm{r}} = 0 \end{cases}$$

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2. Model development

2.1 Governing equations

- Mass transfer rate

$$N_i = K_{g,i}(P_i - P_i^*)$$

$$\frac{1}{K_{g,i}} = \frac{R_g T_g}{k_{g,i}} + \frac{He_{l,i}}{E_i k_{l,i}}$$

- Heat transfer rate for liquid and gas phases

$$q_g = h_{gl}(T_l - T_g)$$

$$q_l = h_{gl}(T_l - T_g) - \Delta H_{CO_2} N_{CO_2} - \Delta H_{vap} N_{H_2O}$$

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2. Model development

2.2 Chemical reactions and their effects

- Main reaction between CO2 and MEA [3]

$$CO_2 + 2MEA \rightleftarrows MEACOO^- + MEAH^+$$

- Mechanisms
  - Zwitterion [4]:

$$\begin{cases} CO_2 + MEA \underset{k_{-r}}{\overset{k_r}{\rightleftharpoons}} MEAH^+COO^- \\ MEAH^+COO^- + MEA \overset{k_B}{\rightarrow} MEACOO^- + BH^+ \end{cases}$$

  - Termolecular [5]: $CO_2 + MEA \ldots MEA \rightleftharpoons MEACOO^- \ldots MEAH^+$

- Reaction rates of CO2 with MEA [6]

$$r^Z_{CO_2} = k^Z_{obs} C_{l,CO_2} = k_r C_{l,MEA} C_{l,CO_2}$$

$$r^T_{CO_2} = k^T_{obs} C_{l,CO_2} = (k^T_{MEA} C_{l,MEA} + k^T_{H_2O} C_{l,H_2O}) C_{l,MEA} C_{l,CO_2}$$

2. Model development

2.2 Chemical reactions and their effects

- Kinetic models

No	Mechanism	Formula	Valid condition		Reference
(1)	Zwitterion	$k_r = 4.14 \times 10^{11} \exp\left(-\frac{5399}{T_l}\right)$	MEA conc. Temp CO_2 loading	: 0.5-12 M : 298-323 K : NA	(Ying and Eimer, 2013)
(2)	Zwitterion	$k_r = 4.4 \times 10^{11} \exp\left(-\frac{5400}{T_l}\right)$	MEA conc. Temp CO_2 loading	: 0-3.2 M : 313 K : NA	(Versteeg et al., 1996)
(3)	Termolecular	$k_{MEA} = 4.61 \times 10^{9} \exp\left(-\frac{4412}{T_l}\right)$ $k_{H_2O} = 4.55 \times 10^{6} \exp\left(-\frac{3287}{T_l}\right)$	MEA conc. Temp CO_2 loading	: 3-9 M : 293-333 K : 0.1-0.49 mol/mol	(Aboudheir et al., 2003)
(4)	Zwitterion	$k_r = 3.376 \times 10^{12} \exp\left(-\frac{6018}{T_l}\right)$	MEA conc. Temp CO_2 loading	: 0.5-5 M : 293-343 K : unloaded liquid	(Luo et al., 2012)
(5)	Termolecular	$k_{MEA} = 8.07 \times 10^{12} \exp\left(-\frac{4503}{T_l}\right)$ $k_{H_2O} = 3.51 \times 10^{9} \exp\left(-\frac{3055}{T_l}\right)$	MEA conc. Temp CO_2 loading	: 0.5-5 M : 293-343 K : unloaded liquid	(Luo et al., 2012)
(6)	Zwitterion	$k_r = 4.396 \times 10^{9} \exp\left(-\frac{3693}{T_l}\right)$	MEA conc. Temp CO_2 loading	: 1-5 M : 298-343 K : 0-0.4 mol/mol	(Luo et al., 2015)
(7)	Termolecular	$k_{MEA} = 1.844 \times 10^{10} \exp\left(-\frac{4112}{T_l}\right)$ $k_{H_2O} = 2.064 \times 10^{5} \exp\left(-\frac{1766}{T_l}\right)$	MEA conc. Temp CO_2 loading	: 1-5 M : 298-343 K : 0-0.4 mol/mol	(Luo et al., 2015)
(8)	Termolecular	$k_{MEA} = 2.003 \times 10^{10} \exp\left(-\frac{4742}{T_l}\right)$ $k_{H_2O} = 4.147 \times 10^{6} \exp\left(-\frac{3110}{T_l}\right)$	MEA conc. Temp CO_2 loading	: 1-5 M : 298-343 K : 0-0.4 mol/mol	(Luo et al., 2015)

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2. Model development

2.2 Chemical reactions and their effects

- Enhancement factor

No	Formula	Description	Reference
1	$E_{CO_2} = Ha = \frac{\sqrt{k_{obs} D_{l,CO_2}}}{k_{l,CO_2}}$	The pseudo first order reaction regime enhancement factor	(Danckwerts, 1970)
2	$E_{CO_2} = 1 + \frac{1}{\left[\left(\frac{1}{E_i - 1}\right)^{1.35} + \left(\frac{1}{E_1 - 1}\right)^{1.35}\right]^{\frac{1}{1.35}}}$	Explicit form second order reactions	(Wellek et al., 1978)
3	$E_{CO_2} = 1 + (E_2 - 1)\left[1 - \exp\left[-\frac{Ha - 1}{E_2 - 1}\right]\right]$	Explicit form second order reactions	(Porter, 1966)
4	$E_{CO_2} = \frac{\sqrt{(Ha)^2 \frac{E_i - E_{CO_2}}{E_i - 1}}}{\tanh\left(\sqrt{(Ha)^2 \frac{E_i - E_{CO_2}}{E_i - 1}}\right)},$	Implicit form second order reactions	(van Krevelen and Hoftijzer, 1948)
5	$E_{CO_2} = \frac{E_1^2}{2(E_i - 1)}\left(\sqrt{1 + \frac{4(E_i - 1)E_i}{E_1^2}} - 1\right)$	Explicit form second order reactions	(Yeramian et al., 1970)

$$Ha = \frac{\sqrt{k_{obs} D_{l,CO_2}}}{k_{l,CO_2}}, E_i = 1 + \frac{D_{l,MEA} C_{l,MEA}}{2 D_{l,CO_2} C_{l,CO_2}^I}, \qquad E_1 = \frac{Ha}{\tanh(Ha)}, E_2 = \sqrt{\frac{D_{l,CO_2}}{D_{l,MEA}}} + \sqrt{\frac{D_{l,MEA}}{D_{l,CO_2}}}\left(\frac{C_{l,MEA}}{2 C_{l,CO_2}^I}\right)$$

2. Model development

2.3 Equilibrium calculations

- Chemical equilibrium

The well-known non-iterative and simple method, originally presented by Danckwert (1970), revisited by Gabrielsen et al. (2005),

- Physical equilibrium

$$P_i^* = \gamma_i x_i P_i^v \quad i = \text{MEA and } H_2O$$

$$P_{CO_2}^* = \gamma_{CO_2} C_{l,CO_2} He_{l,CO_2}$$

2. Model development

2.4 Physical properties and other parameters

Property	Symbol	Reference
Gas Viscosity	μ_g	Multiflash package in gPROMS
Liquid Viscosity	μ_l	(Weiland et al., 1998)
Gas density	ρ_g	Multiflash package in gPROMS
Liquid density	ρ_l	(Weiland et al., 1998)
Gas heat capacity	C_{pg}	(Harun, 2012)
Liquid heat capacity	C_{pl}	(Agbonghae et al., 2014)
Gas side mass transfer	$k_{g,i}$	(Onda et al., 1968)
Liquid side mass transfer	$k_{l,i}$	(Tung and Mah, 1985), (Hanley and Chen, 2012), (Billet and Schultes, 1999)
Interfacial area	a_{gl}	(Onda et al., 1968)
Henry's constant	He_{l,CO_2}	(Ying et al., 2012)
Liquid diffusivity	D_{l,CO_2}	(Ying and Eimer, 2012)
Gas diffusivity	$D_{g,i}$	(Fairbanks and Wilke, 1950)
Thermal conductivity	λ_g	Multiflash package in gPROMS
Pressure drop	ΔP	(Llerena-Chavez and Larachi, 2009)
Heat transfer coefficient	h_{gl}	(Chilton and Colburn, 1934)
Vapor pressure	P_i^v	(Harun, 2012)
Activity coefficient	γ_i	Multiflash package in gPROMS/(Prausnitz et al., 1998)

3. Results and discussions

3.1 Model results and validation

- The RPB absorber characteristics [7]

Parameter	Values
Rotor speed (rpm)	600, 1000
The diameter of RPB (m)	0.398 (OD), 0.156 (ID)
The porosity of packing (m^3/m^3)	0.76
Packing type	Expanded stainless steel small mesh
Packing height (m)	0.025
Total surface area (a_t) (m^2/m^3)	2132

- CO_2 capture level (CCL) $$CCL\% = \left(\frac{y_{CO_2}^{in} - y_{CO_2}^{out}}{y_{CO_2}^{in}}\right) \times 100$$

- Absolute relative deviation $$ARD\% = \left|\frac{CCL^{Exp} - CCL^{Pre}}{CCL^{Exp}}\right| \times 100$$

- Absolute deviation $$AD\% = \left|y_{CO_2}^{Exp} - y_{CO_2}^{Pre}\right| \times 100$$

3. Results and discussions

3.1 Model results and validation

- Process conditions as input to the RPB absorber (Jassim, 2002)

MEA	Case-Run	Rotor Speed	Pressure	Flow rate		Temperature		Liquid mole fraction			Gas mole fraction		
wt.%		rpm	atm	liquid (l/min)	gas (kmol/h)	gas in (˚C)	liquid in (˚C)	H_2O	CO_2	MEA	H_2O	CO_2	N_2
56.0	1-1	600	1	39.3	2.87	47	39.6	0.6970	0.0216	0.2814	0.1679	0.0471	0.7850
53.2	1-2	600	1	39.3	2.87	47	20.7	0.7171	0.0234	0.2595	0.1690	0.0460	0.7850
56.0	1-3	1000	1	39.3	2.87	47	40.1	0.6970	0.0216	0.2814	0.1702	0.0448	0.7850
55.0	1-5	600	1	21.1	2.87	47	39.5	0.6967	0.0277	0.2756	0.1707	0.0443	0.7850
56.0	1-6	600	1	21.1	2.87	47	22.3	0.6890	0.0274	0.2836	0.1703	0.0447	0.7850
55.0	1-7	1000	1	21.1	2.87	47	39.6	0.6969	0.0276	0.2755	0.1715	0.0435	0.7850
77.0	2-2	600	1	39.3	2.87	47	21.4	0.4688	0.0200	0.5112	0.1714	0.0436	0.7850
74.0	2-3	1000	1	39.3	2.87	47	40.2	0.5057	0.0229	0.4714	0.1714	0.0436	0.7850
75.1	2-4	1000	1	39.3	2.87	47	20.7	0.5008	0.0169	0.4823	0.1721	0.0429	0.7850
76.0	2-6	600	1	21.1	2.87	47	22.1	0.4795	0.0221	0.4984	0.1712	0.0438	0.7850
75.0	2-7	1000	1	21.1	2.87	47	39.4	0.4876	0.0256	0.4868	0.1712	0.0438	0.7850
78	2-8	1000	1	21.1	2.87	47	20.6	0.4515	0.0215	0.5270	0.1697	0.0453	0.7850

3. Results and discussions

3.1 Model results and validation

- Model prediction results compared to the experimental values

Case	Run	Exp. CO_2 capture level %	Pre. CO_2 capture level %	ARD% between Exp. & Pre. CCL	AD% between Exp. & Pre. y_{CO_2}
1	1	94.9	90.98	4.13	0.18
1	2	83	86.86	4.65	0.18
1	3	95.4	97.58	2.28	0.10
1	5	87	88.77	2.03	0.08
1	6	84.1	84.95	1.01	0.04
1	7	89.9	93.41	3.90	0.15
2	2	84.2	90.06	6.97	0.26
2	3	97.5	98.54	1.07	0.05
2	4	91.2	97.05	6.41	0.25
2	6	84.3	87.20	3.45	0.13
2	7	98.1	97.32	0.79	0.03
2	8	91	95.88	5.36	0.22

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3. Results and discussions

3.2 Effects of kinetic reaction and enhancement factor

MEA wt. %	k_{obs1}	k_{obs2}	k_{obs3}	k_{obs4}	k_{obs5}	k_{obs6}	k_{obs7}	k_{obs8}
55 (case 1 run 5)	74506	78928	168008	80864	219718	205574	195957	249800
74 (case 2 run 3)	110908	117491	346078	121167	452343	300530	391575	515844
CCL% (case 1 run 5)	73.61	74.49	84.21	74.54	87.44	88.09	86.45	88.77
CCL% (case 2 run 3)	87.27	87.97	97.19	88.27	98.17	96.55	97.70	98.54

E_{18}	E_{28}	E_{38}	E_{48}	E_{58}
27.97	28.82	27.86	27.65	27.67

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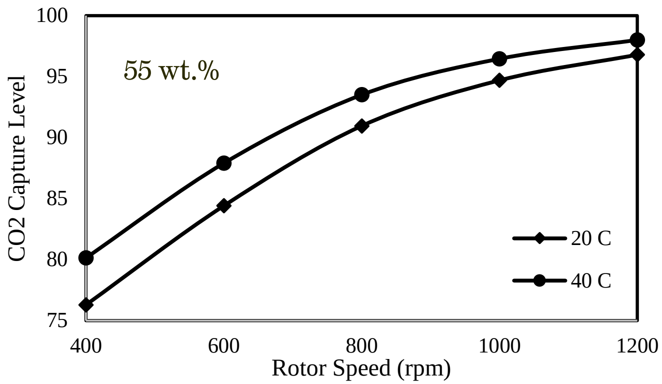
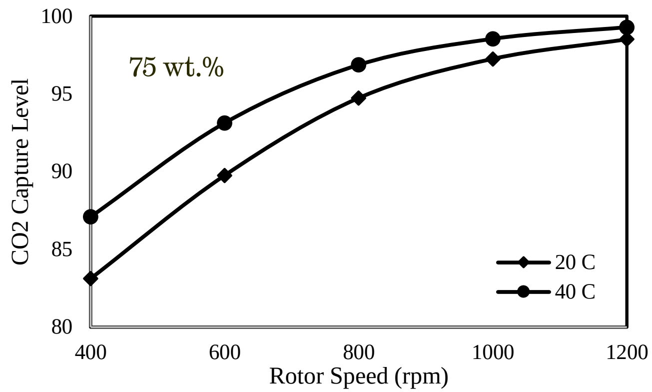
3. Results and discussions

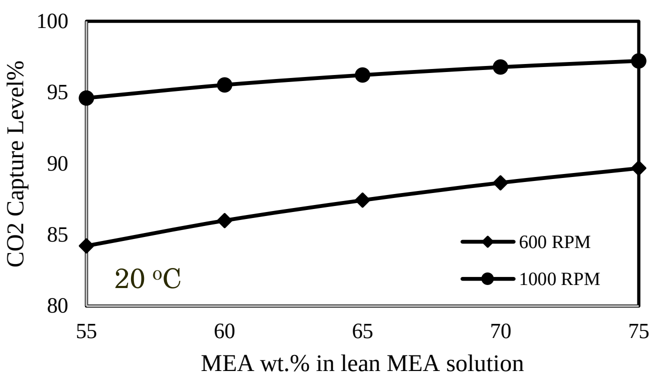
3.3 Process analysis

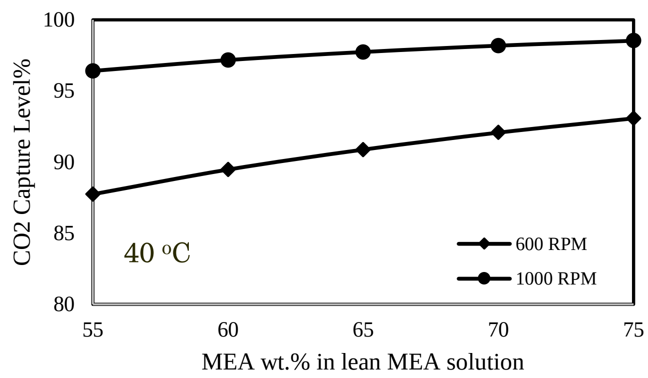
- Effect of rotor speed





- Effect of MEA concentration in lean MEA solution

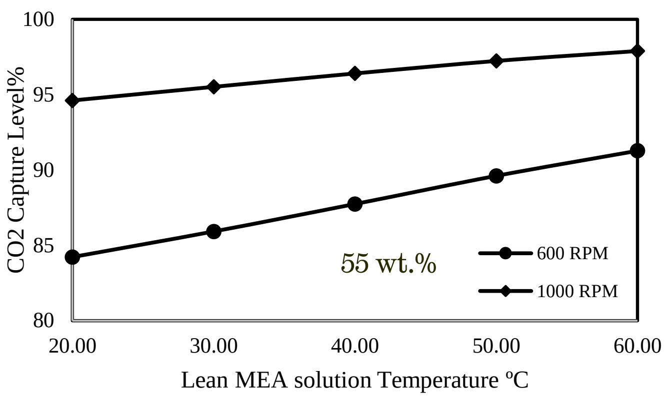


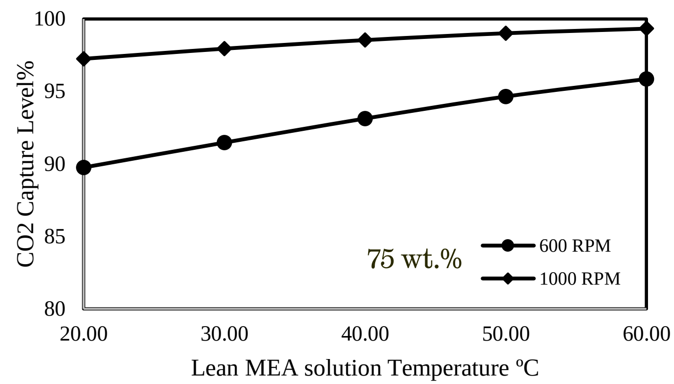


3. Results and discussions

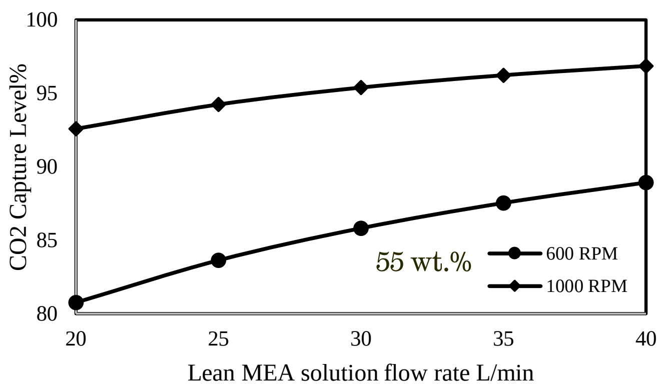
3.3 Process analysis

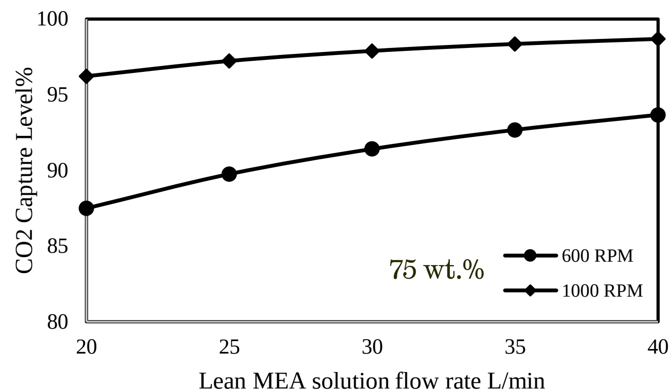
- Effect lean MEA solution temperature





- Effect of lean MEA solution flow rate





3. Results and discussions

3.3 Multivariable sensitivity analysis

- The OAD method (Taguchi et al., 1987) is a statistical method that can be used to find the desired operating condition of a system with respect to different input conditions

- The selected factors and their levels of CCL% and motor power.

Factors	Level 1	Level 2	Level 3	Level 4	Level 5
Rotor Speed (RPM)	400	600	800	1000	1200
MEA Concentration (wt.%)	55	60	65	70	75
Liquid temperature (^{o}C)	20	30	40	50	60
Liquid flow rate (L/min)	20	25	30	35	40

3. Results and discussions

3.3 Multivariable sensitivity analysis

- The amount of power that consumed by the motor of RPB absorber (Singh et al., 1992):

$$P_{motor} = 1.2 + 0.1833 \times 10^{-7} \rho_l R_o^2 \omega^2 Q_l'$$

- P_{motor} is motor power (kW),
- ρ_l is the density of liquid phase (kg/m3),
- R_o is the outer radius of RPB (m),
- ω is angular velocity (rad/s),
- Q_l' is the volumetric flow rate of lean MEA solution (L/min)

3. Results and discussions

3.3 Multivariable sensitivity analysis

	Inputs to the gPROMS model				Outputs of the gPROMS model		
Run	Rotor Speed (rpm)	$C_{l,\ MEA}$ (wt.%)	T_l (ºC)	Q'_l (L/min)	P_{motor} (kW)	CCL%	SNR
1	400	55	20	20	145.595	65.94	36.38
2	400	60	30	25	180.391	73.77	37.36
3	400	65	40	30	214.668	80.68	38.14
4	400	70	50	35	247.891	86.67	38.76
5	400	75	60	40	280.154	91.39	39.22
6	600	60	20	30	486.449	85.88	38.68
7	600	65	30	35	563.418	90.47	39.13
8	600	70	40	40	637.896	94.09	39.47
9	600	75	50	20	318.285	91.46	39.22
10	600	55	60	25	401.214	89.40	39.03
11	800	65	20	40	1146.863	95.10	39.56
12	800	70	30	20	573.305	92.26	39.30
13	800	75	40	25	707.737	95.92	39.64
14	800	55	50	30	857.805	93.36	39.40
15	800	60	60	35	988.983	97.30	39.76
16	1000	70	20	25	1120.574	95.78	39.63
17	1000	75	30	30	1330.073	97.86	39.81
18	1000	55	40	35	1562.720	97.01	39.74
19	1000	60	50	40	1770.769	98.63	39.88
20	1000	65	60	20	885.988	97.63	39.79
21	1200	75	20	35	2240.795	98.84	39.90
22	1200	55	30	40	2580.760	98.32	39.85
23	1200	60	40	20	1291.131	97.08	39.74
24	1200	65	50	25	1596.318	98.85	39.90
25	1200	70	60	30	1894.319	99.59	39.96

4. Conclusion

- ARD% between the experimental and the predicted CCL% value is changing between 0.79 and 6.97 and the AARD% for them is 3.50

- AD% between the experimental and the predicted fractions of CO_2 in the gas phase is changing between 0.03 and 0.26, and the AAD% for them is 0.14.

- The kinetic model has a significant effect on the model results but the enhancement factor relation is not much influential

- The OAD method can provide different scenario and combination of factors affecting on CCL% and motor power and help to find the proper combination of four factors that resulted in the low motor power

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