



Study of Process Intensification for Post-combustion Carbon Capture Through Modelling and Simulation

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Process and Energy Systems Engineering Group at University of Hull, UK

- Technical tools: process modeling, simulation, control and optimization
- \bullet Application areas: conventional power generation, $\rm CO_2$ capture, $\rm CO_2$ transport, energy storage, biomass steam gasification
- Currently 3 Research staff & 9 PhD students
- For more details, please refer to http://www2.hull.ac.uk/science/engineering/our%20staff/acad emic/meihong%20wang.aspx

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Outline



- Background and Motivations for the Research
- Modelling of Post-combustion Carbon Capture (PCC) with Chemical Absorption
- Integration between Coal-fired Power Plant and PCC
- Why is Process Intensifications necessary for PCC?
 - Key Findings from Biliyok et al. (2012), Lawal et al. (2012) and Lawal et al. (2010)
 - Introduction to Process Intensification
 - Current status of PI for PCC worldwide
- Steady state modelling of Intensified Absorber
 - Methodology
 - Correlation Sets used
 - Model Validation & Process Analysis



1.1 Energy Demand

- Energy demand expected to rise with increasing population and the emergence of the Brazil, Russia, India, China and South Africa (BRICS) countries.
- Power generation is the single largest contributor of anthropogenic CO₂ emissions.
- Coal releases twice as much CO₂ as natural gas; but offers economic advantages.









1. Motivations for the Research

1.1 Energy Demand

UK electricity generation by fuel source (DECC, 2010)

- In 2009, about 32% of UK electricity generation is from coal-fired power station
- This is projected to fall to 22% by 2020.
- NGCC power plant has a share of 45% in 2009, which will fall to 29% in 2020.



UK Electricity Generation





1. Motivations for the Research

1.1 Energy Demand

- For UK National Grid status <u>http://www.gridwatch.templar.co.uk/</u>
 - On 12/11/2014, 35% electricity generated from Coal & 37.5% electricity generated from Natural Gas.







1. Motivations for the Research

- 1.2 CO₂ Emissions
 - Carbon dioxide is the main greenhouse gas.
 - Global concentration of CO₂ in the atmosphere was about 280 parts per million by volume (ppmv) in around 1860 (pre-industrialisation levels).
 - In 1958, it was approximately 316 ppmv.
 - It is approximately 369 ppmv in 2005 (UNEP, 2005).
 - CO₂ concentration is around 400 ppm and is increasing by 2-3 ppm every year.
 - Atmospheric CO₂ must remain 450 ppm to ensure that global warming stays below 2°C.



1. Motivations for the Research

1.2 CO₂ Emissions

Main sources

- \circ Fuel combustion activities
- Industrial processes
- Natural gas processing

Sectors

- Power generation (coal, natural gas)
- o Transportation
- Industrial (Manufacturing)

Types of Emitters

- \circ Large emitters of CO₂ (emitting more than 0.1 MtCO₂ per year)
- \circ Small emitters of CO₂ (emitting less than 0.1 MtCO₂ per year)



1. Motivations for the Research

1.2 CO₂ Emissions

• UK CO₂ Emissions clusters (DECC, 2010)



Department of Energy and Climate Change (DECC), (2010), Updated energy and emissions projections, UK Government, Report number URN10D/510

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1. Motivations for the Research

1.3 Climate Change

- Average global temperature increased by 0.74°C in the 20th century.
- Sea levels have risen by 17cm due to thermal expansion of the ocean and melting of ice.
- Dramatic increase in the frequency, intensity and duration of floods, droughts and heat waves.
- Global warming potential (IPCC, 2007)



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1. Motivations for the Research

- 1.4 CO₂ Reduction Target
 - IPCC recommends that CO₂ emissions be cut by 50% by 2050 compared 1990 levels.
 - Trajectory for target CO₂ emissions reduction in the UK (DECC, 2010)
 - The first target requires UK to cut its carbon emissions to achieve reduction of 34% below 1990 levels by year 2020.
 - \checkmark (a) Reduction of 23% for the period 2008-2012;
 - \checkmark (b) 29% for period 2013-2017
 - $\checkmark\,$ (c) to 34% for period to 2018-2022





2. Modelling of PCC using Solvents

- 2.1 CO₂ Separation Technologies
 - PCC: Process Options for CO₂ Capture (Rao and Rubin, 2002)





2. Modelling of PCC using Solvents

2.2 Modelling of PCC with MEA process

Post-combustion Carbon Capture (PCC): Chemical Absorption





2. Modelling of PCC using Solvents

2.2 Modelling of PCC with MEA process

Model Complexity



Kenig, E. Y., Schneider, R. and Górak, A. (2001), "Reactive absorption: Optimal process design via optimal modelling", *Chemical Engineering Science*, vol. 56, no. 2, pp. 343-350.



2. Modelling of PCC using Solvents

2.2 Modelling of PCC with MEA process

Rate-based dynamic modelling based on Two-film Theory





2. Modelling of PCC using Solvents

- 2.2 Modelling of PCC with MEA process
 - Absorber and Stripper model in gPROMS



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2. Modelling of PCC using Solvents

- 2.2 Modelling of PCC with MEA process
 - Chemical Equilibrium is defined by ElecNRTL Activity Coefficient Model in Aspen Properties[®].
 - Maxwell-Stefan Formulation used to determine fluxes across films.
 - Vapour diffusivity calculated by the Fuller method.
 - Liquid diffusivity determined by a method provided by Veersteeg and van Swaaij.
 - Onda correlation used to determine the mass transfer coefficients in the films and the wetted area.
 - Heat of Absorption determined via formulations derived from tests at the University of Texas in Austin.





2. Modelling of PCC using Solvents

2.3 Pilot plants for CO₂ Capture with Chemical Absorption



RWE nPower, Didcot CTF





Univ. Texas at Austin, SRP Pilot Plant

4Ton CO_2 / day



SaskPower Boundary Dam

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2. Modelling of PCC using Solvents

2.3 Pilot plants for CO₂ Capture with Chemical Absorption

- The biggest test facility in the UK Ferrybridge (100 Ton CO₂ / day) – commissioned on 30/11/2012.
- The project worth more than £20million
- A partnership between industry partners Scottish and Southern Energy (SSE), Doosan Power Systems and Vattenfall
- Supported by DECC, the Technology Strategy Board (TSB) and Northern Way



A 500MWe coal-fired subcritical power plant releases over 8000 tonne CO₂/day

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2. Modelling of PCC using Solvents

2.4 Model Validation at pilot scale



 Typical operation would be around 90% CO₂ capture



	Case	L/G ratio (kg/kg)	CO ₂ removal (%)
Steady state validation	32	6.6	95
	47	3.4	69
Dynamic validation	25/26	8.5	93

^a Dugas, R.E. (2006). Pilot Plant Study of Carbon Dioxide Capture by Aqueous Monoethanolamine. Master thesis, Chemical Engineering, University of Texas at Austin.

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2. Modelling of PCC using Solvents



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2. Modelling of PCC using Solvents

- 2.4 Model Validation at pilot scale
 - Dynamic Validation flowsheet for conventional process



^a Lawal, A. (2010), Study of a Post-Combustion CO₂ Capture Plant for Coal-Fired Power Plant through Modelling and Simulation, PhD thesis, Cranfield University, Bedford, UK.



2. Modelling of PCC using Solvents

- 2.4 Model Validation at pilot scale
 - Dynamic Validation Process Inputs and Disturbances
- Slow decrease in lean solvent flow rate into the absorber.
- Fluctuating CO₂
 Composition of flue gas into the absorber.
- Increase in the temperature of flue gas into the absorber.











3.1 Scale-up of the Absorber and Stripper for 500 MWe Coal-fired Subcritical Plant







3.1 Scale-up of the Absorber and Stripper for 500 MWe Coal-fired Subcritical Plant

Absorber and Regenerator Diameters



Required diameter for Regenerator = 8.39m



3. Integration between Coal-fired subcritical power plant and PCC Plant

3.1 Scale-up of the Absorber and Stripper for 500 MWe Coal-fired Subcritical Plant

Absorber and Regenerator Height

• The volume of packing required for mass transfer is estimated using methods suggested by [3].

$$Volume of packing required = \frac{Surface Area of packing required}{Specific area of packing} Accounting for$$

$$Surface Area of packing required = \frac{molar flow of CO_2}{mass transfer flux \times wetted area ratio} maldistribution$$

mass transfer flux = overall mass transfer coefficient \times driving force (ΔC)

overall mass transfer coefficient =
$$\frac{1}{\left(\frac{1}{K_{G}} + \frac{1}{mEK_{L}}\right)}$$

[3] Abu-Zahra, M.R.M. et al. (2007) CO_2 capture from power plants: Part I. A parametric study of the technical performance based on monoethanolamine. *International Journal of Greenhouse Gas Control*, 1:37-46.



3. Integration between Coal-fired subcritical power plant and PCC Plant

3.1 Scale-up of the Absorber and Stripper for 500 MWe Coal-fired Subcritical Plant Summary of preliminary design parameters

Description	Value
Design flue gas mass flow rate (kg/s)	600
CO ₂ capture level (%)	90
Absorber column number	2
Absorber diameter (m)	9
Regenerator column number	1
Regenerator column diameter (m)	9
Absorber operating pressure (10 ⁵ Pa)	1.01
Regenerator operating pressure (10 ⁵ Pa)	1.62
Lean solvent mass fraction (MEA)	0.3048
Lean solvent CO ₂ loading (mol CO ₂ /mol MEA)	0.29





3.2 Integration between Power Plant & PCC Plant







3.2 Integration between Power Plant & PCC Plant







3.3 Flowsheet for Power Plant with PCC Plant



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3. Integration between Coal-fired subcritical power plant and PCC Plant

3.4 Thermal Performance Analysis

Net power output drops to 453MWe
Power plant efficiency drops 6%
42% of steam is drawn off at the IP/LP crossover for solvent regeneration

Note: CO₂ compression and CO₂ capture plant auxiliary electricity requirements were not considered

3. Integration between Coal-fired subcritical power plant and PCC Plant

Vet Power Output (MWe)

3.5 Dynamic Analysis

Dynamic case study: The response of the integrated plant with a step reduction in target power output.

Identified possible interaction between control loops

Response of CO₂ capture plant is slower than that of the power plant



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- 4. Why is Process Intensification necessary for PCC?
- 4.1 Key Findings from Biliyok et al. (2012)
 - Publication in International Journal of Greenhouse Gas Control on Dynamic Modelling, Validation and Analysis of PCC (with MEA) Process



Dynamic modelling, validation and analysis of post-combustion chemical absorption CO₂ capture plant

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4. Why is Process Intensification necessary for PCC?

4.1 Key Findings from Biliyok et al. (2012)

In PCC using MEA process

- Development of dynamic models for PCC using MEA (considering rate-based mass transfer and reactions assumed to be at equilibrium)
- In addition to steady state validation, dynamic model validation performed (in collaboration with University of Texas at Austin).
- Through Case Study (i.e. model-based process analysis), it provides evidence that PCC process is mass transfer limited (while the reaction between MEA and CO₂ is fast enough).
- Further analysis indicates the slow mass transfer is caused by the flow pattern inside packed column (i.e. laminar flow).

 \sim 3Ton CO₂ / day



Univ. Texas at Austin, SRP Pilot plant

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4. Why is Process Intensification necessary for PCC?

4.2 Key Findings from Lawal et al. (2012)

 Publication in Fuel on Integration of full scale Coal-fired subcritical Power Plant with PCC (using MEA) Process



power plants through dynamic modelling and simulation

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4. Why is Process Intensification necessary for PCC?

4.2 Key Findings from Lawal et al. (2012)

- Study of 500 MWe subcritical coalfired power plant integrated with PCC using MEA process through Dynamic Modelling and Simulation
 - The main challenge of PCC for 500 MWe subcritical coal-fired power plant (such as Didcot A) is its large flue gas flowrate (around 600 kg/s).
 - Study of scale-up for PCC plant to match the requirement of full scale coal-fired power plant (to capture over 8,000 tons CO₂/day).
 - Size of Packed Columns required is huge, which translates to high capital cost

Summary of preliminary design parameters for capture plant

Description	Value
Design flue gas mass flow rate (kg/s)	600
CO ₂ mass fraction in flue gas	0.21
CO ₂ capture level (%)	90
Absorber Column Number	2
Absorber Diameter (m)	9
Absorber Height (m)	17
Regenerator Column Number	1
Regenerator Column Diameter (m)	9
Absorber operating pressure (10 ⁵ Pa)	1.01
Regenerator operating pressure (10 ⁵ Pa)	1.62
Lean solvent mass fraction (MEA)	0.3048
Lean solvent CO ₂ loading (mol CO ₂ /mol MEA)	0.29



4. Why is Process Intensification necessary for PCC?

4.3 Key Findings from Lawal et al. (2010)

 Publication in Fuel on Dynamic Modelling and Analysis of pilot scale PCC (using MEA) Process



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Engineering and Physical Sciences Research Council

4. Why is Process Intensification necessary for PCC?

4.3 Key Findings from Lawal et al. (2010)

- Study of Dynamics and Operation of PCC using MEA process at Pilot Scale through dynamic modelling and simulation
 - The dynamics of the PCC using MEA process Ο is very slow (time constant around 57 minutes).
 - The main reason is high L/G ratio required \cap (generally around 6.0 mass/mass for flue gas from typical coal-fired power plants) to achieve the capture level
 - This large flowrate of MEA (at 30.48 wt%) 0 contributes to **high energy consumption**.
 - This also poses considerable challenges in Ο process operation when integrated with power plants.



Reboil

96 94

92

90 88 Capture

Level (%)

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4. Why is Process Intensification necessary for PCC?

4.4 Introduction to Process Intensification (PI)

- Process Intensification (PI) is a strategy for making major reductions in the volume of processing plant without compromising its production rate.
- Rotating packed bed (RPB) is one of the PI technologies proposed by Prof Ramshaw in 1979.
- RPB takes advantages of centrifugal forces to generate high gravity and consequently boost the mass transfer performance.



Rotating Packed Bed used for REACTIVE STRIPPING –40 times smaller plant (Dow Chemical, HOCI process)



4. Why is Process Intensification necessary for PCC?

4.4 Introduction to Process Intensification (PI)



Schematic diagram of a rotating packed bed setup and corresponding segmentation (Llerena-Chavez and Larachi, 2009)



- 4. Why is Process Intensification necessary for PCC?
- 4.5 Current status of PI for PCC worldwide
 - Experimental study on intensified Absorber
 - Newcastle
 - Carried out experimental study of intensified absorber using MEA solvent as absorbent.
 - ✓ The experimental rig has been upgraded (Lee et al., 2012)
 - Beijing University of Chemical Technology (BUCT)
 - Iiquid side volumetric mass transfer coefficient (k_Lα) in RPB shows at least one order of magnitude improvement than conventional packed column (Zhang *et al.*, 2011)
 - o India
 - ✓ Compared RPB with split packing RPB (Rajan *et al.*, 2006; Agarwal *et al.*, 2010; Reddy *et al.*, 2011).
 - ✓ Improvement in both gas and liquid phase mass transfer
 - o Taiwan
 - Used mixed alkanolamines solvent which results in improved CO₂ capture level
 - ✓ Counter-current flow arrangement and cross flow arrangement



- 4. Why is Process Intensification necessary for PCC?
- 4.5 Current status of PI for PCC worldwide
 - Study on intensified Absorber through modelling
 - o **Taiwan**
 - Cheng and Tan (2011) used continuous stirred tank model in series to model/simulate intensified absorber.
 - o University of Hull
 - ✓ Aspen Plus and visual FORTRAN used to model and simulate intensified absorber (Joel *et al.*, 2014a,b)
 - Model validation with two sets of mass transfer correlations (Joel *et al.,* 2014b)
 - ✓ Compared conventional and intensified absorber, and found a volume reduction factor of 12 times (Joel *et al.*, 2014b)
 - o BUCT
 - ✓ End effect problem along the radial direction (Yi et al., 2009)
 - Mechanism of gas–liquid mass transfer with reactions in RPB at higher gravity level was illustrated (Yi *et al.*, 2009)



4. Why is Process Intensification necessary for PCC?

4.5 Current status of PI for PCC worldwide

- Experimental and Modelling study on intensified Stripper
 - o Newcastle
 - ✓ Jassim *et al.* (2007) reported RPB stripper for desorption runs for 30 wt%, 54 wt% and 60 wt% MEA solution
 - ✓ Reduction factor in stripper height of 8.4 and stripper diameter of 11.3 (Jassim *et al.*, 2007)
 - \circ Taiwan
 - ✓ Cheng *et al.* (2013) setup was an improvement to what was reported in Jassim *et al.* (2007)
 - ✓ They introduced a back pressure regulator in order to operate the regenerator at higher temperature and pressure (Cheng *et al.*, 2013)
 - $\circ~$ In both studies, reboiler is not intensified

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- 4. Why is Process Intensification necessary for PCC?
- 4.5 Current status of PI for PCC worldwide
 - Summary
 - There are good number of studies on intensified Absorber through experiments and/or modelling
 - Few studies on pressure drop across column validated with experimental data
 - ✓ No experimental data on electricity consumption for driving the motor.
 - There are very limited studies on intensified Stripper/Regenerator through experiments and/or modelling
 - ✓ The size of intensified stripper reduced significantly, but the reboiler is still huge.
 - There is merely no study on intensified heat exchangers for PCC application
 - There is no study of whole intensified PCC process
 - ✓ There is no pilot plant for whole intensified PCC process
 - There is no study of the whole intensified carbon capture process through experiments or modelling



5. Steady state modelling of Intensification Absorber

5.1 Methodology







5. Steady state modelling of Intensification Absorber

Correlation sets used for the modelling and simulations

Correlations	Set 1	Set 2			
Liquid-phase mass transfer coefficient	Tung and Mah (1985)	Chen <i>et al.,</i> (2006)			
Gas-phase mass transfer coefficient	Onda <i>et al.,</i> (1968)	Chen, (2011)			
Interfacial area	Onda <i>et al.,</i> (1968)	Luo <i>et al.</i> (2012)			
Liquid hold-up	Burns <i>et al.,</i> (2000)	Burns <i>et al.</i> , (2000)			
Dry pressure drop	Llerena-Chavez and Larachi (2009)	Llerena-Chavez and Larachi (2009)			

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5. Steady state modelling of Intensification Absorber

5.3 Model Validation

Input process conditions for Run 1 to Run 4 (Jassim et al., 2007)

Variable	Runs					
	Run 1	Run 2	Run 3	Run 4		
Rotor speed (RPM)	600	1000	600	1000		
Lean MEA temperature (°C)	39.6	40.1	41	40.2		
Lean MEA pressure (atm.)	1	1	1	1		
Flue gas flow rate (kmol/hr)	2.87	2.87	2.87	2.87		
CO ₂ composition in Flue gas (vol %)	4.71	4.48	4.40	4.29		
Lean-MEA flow rate (kg/s)	0.66	0.66	0.66	0.66		
Lean-MEA composition (wt %)						
H ₂ O	40.91	40.91	22.32	23.41		
	3.09	3.09	2.68	2.59		
MEA	56.00	56.00	75.00	74.00		

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5. Steady state modelling of Intensification Absorber

5.3 Model Validation

Simulation results with 2 different sets of correlations compared to the experimental data for Run 1 and Run 2

Variable	Run 1				Run 2					
	Expt.	Set 1	Error 1	Set 2	Error 2	Expt.	Set 1	Error 1	Set 2	Error 2
CO ₂ loading of Lean MEA, (mol CO ₂ /mol MEA)	0.0772	0.0772		0.0772		0.0772	0.0772		0.0772	
CO_2 loading of Rich MEA, (mol CO_2 /mol MEA)	0.0828	0.0827	0.1208	0.0829	0.1208	0.0828	0.0825	0.3623	0.0827	0.1208
Average Lean MEA/Rich MEA, (mol CO ₂ /mol MEA)	0.0800	0.0800	0.0000	0.0800	0.0000	0.0800	0.0799	0.1250	0.0801	0.1250
CO ₂ capture level (%)	94.9	92.9	2.1075	96.72	1.9178	95.4	93.26	2.2432	96.95	1.6247

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5. Steady state modelling of Intensification Absorber 5.3 Model Validation

Simulation results with 2 different sets of correlations compared to the experimental data for Run 3 and Run 4

Variable	Run 3					Run 4				
	Expt.	Set 1	Error 1	Set 2	Error 2	Expt.	Set 1	Error 1	Set 2	Error 2
CO ₂ loading of Lean–MEA (mol CO ₂ /mol MEA)	0.0492	0.0492		0.0492		0.0483	0.0483		0.0483	
CO_2 loading of Rich-MEA (mol CO_2 /mol MEA)	0.0531	0.0530	0.1883	0.0531	0.0000	0.0510	0.0521	2.1569	0.0524	2.7451
Average Lean-MEA/Rich- MEA (mol CO ₂ /mol MEA)	0.0512	0.0511	0.1953	0.0512	0.0000	0.0497	0.0502	1.0060	0.0503	1.2072
CO ₂ capture level (%)	98.20	93.28	5.0102	97.36	0.8554	97.50	93.57	4.0308	98.66	1.1897

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- **5.** Steady state modelling of Intensification Absorber 5.3 Model Validation - Summary
 - Set 2 correlations gives a better error prediction compared to Set 1.
 - □ The difference in error prediction at 56 wt% MEA concentration between Set 1 and Set 2 is not large
 - There is wide error prediction at 74 wt% MEA concentration between Set 1 and Set 2
 - Set 2 correlations account for the effect of viscosity and packing geometry while Set 1 correlations do not.



5. Steady state modelling of Intensification Absorber

5.4 Process Analysis – Key findings

- With RPB Absorber, there is no temperature bulge observed. Potential Reasons:
 - Because of the high gravity, most of the flow in RPB is droplet and thin film flow. This makes it difficult for liquid build-up in the packing which may result in energy build-up.
 - ✓ High degree of mixing and little residence time of the solvent in column makes it difficult to have energy build-up.
- With RPB Absorber, the Absorber can reduce 12 times in volume.





□If you have interest in this work, please refer to the following two recent publications:

✓ Joel, A. S., Wang, M. and Ramshaw, C. (2014), Process analysis of intensified absorber for post-combustion CO₂ capture through modelling and simulation, *Int. Journal of Greenhouse Gas Control,* Vol. 21, p91-100.

✓ Joel. A, S., Wang, M., Ramshaw, C. (2015), Modelling and simulation of intensified absorber for post-combustion CO_2 capture using different mass transfer correlations, *Applied Thermal Engineering*, doi: 10.1016/j.applthermaleng.2014.02.064.

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Key Publications

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Thanks for your attentions!