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Solvent-based post-combustion capture: Process simulation, validation and scale-up

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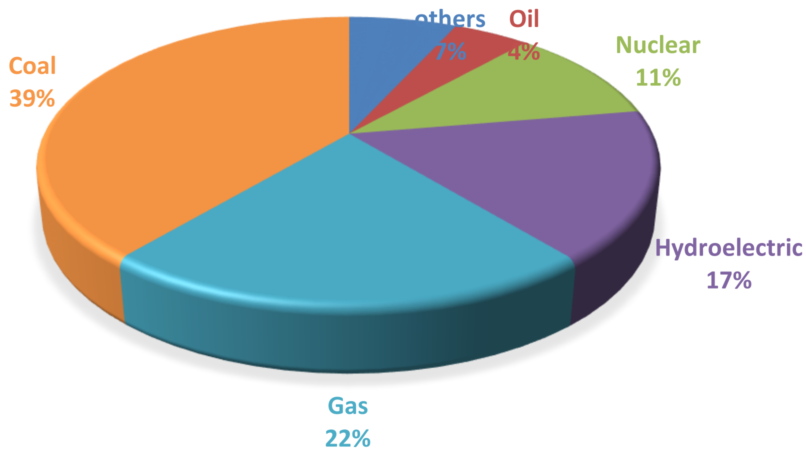
INTRODUCTION

Background

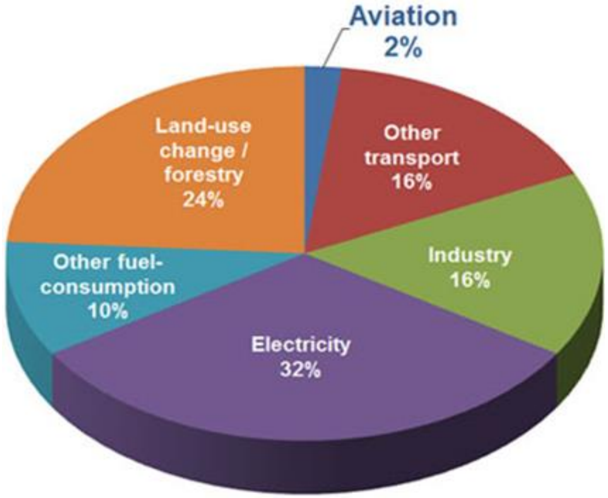
- Fossil fuels play vital roles in meeting the increasing global energy demand.
- Fossil fuel combustion for electricity generation in power plants is responsible for largest emission of CO_2

Global energy generation 2014



Source: The shift project

Global CO_2 Emission by sector

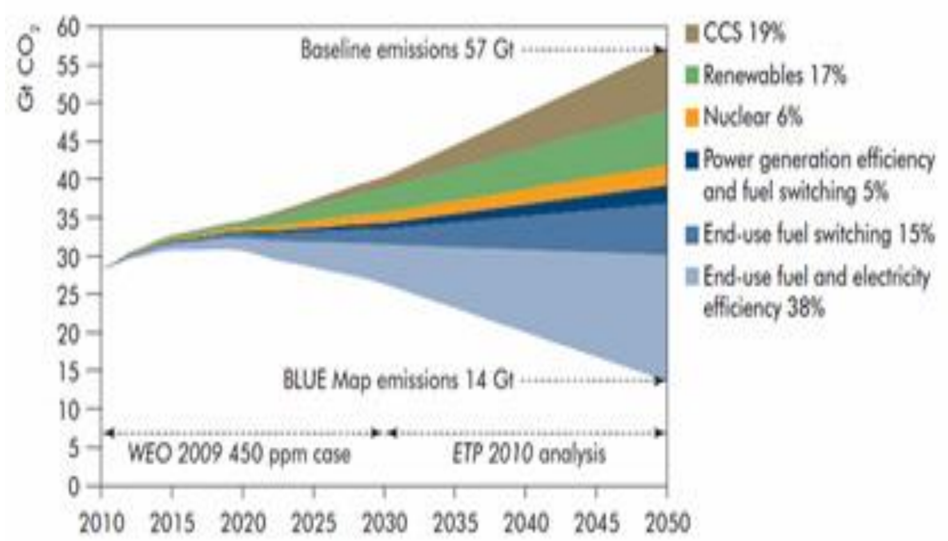


Source: Sustainable aviation CO_2 Roadmap

INTRODUCTION

Background

- Carbon capture and storage (CCS) has been identified as a technology to reduce CO2 emission from the power plant.
  - CCS to be responsible for one-fifth (19%) reduction in global CO_2 emission by 2050.
- Post-combustion Capture plant has the most potential to be commercialized in the power sector.
- Chemical absorption is the most preferred technology to capture carbon from fossil fuel power plant (Lawal et al. 2012)
- Monoethanolamine (MEA) are the most commonly used.



Key technologies for CO_2 emissions reduction 2010—2050 (IEA, 2010)

Motivation

- Solvent-based PCC process have been studied through Process modelling and simulation.
  - Models are validated using pilot plant data
- Validated models are often scaled from pilot plant scale to commercial scale (To enable the study of large scale plants)
- Most of the commercial-scale design are based on assuming a value for the pressure drop in the packed column (to determine the columns diameter)
- However, the accuracy of this scale-up procedure has not been demonstrated
- This research is focussed on developing an alternative method for the scale-up of the solvent-based PCC process using simple empirical correlation.

SOLVENT-BASED PCC PROCESS DESCRIPTION

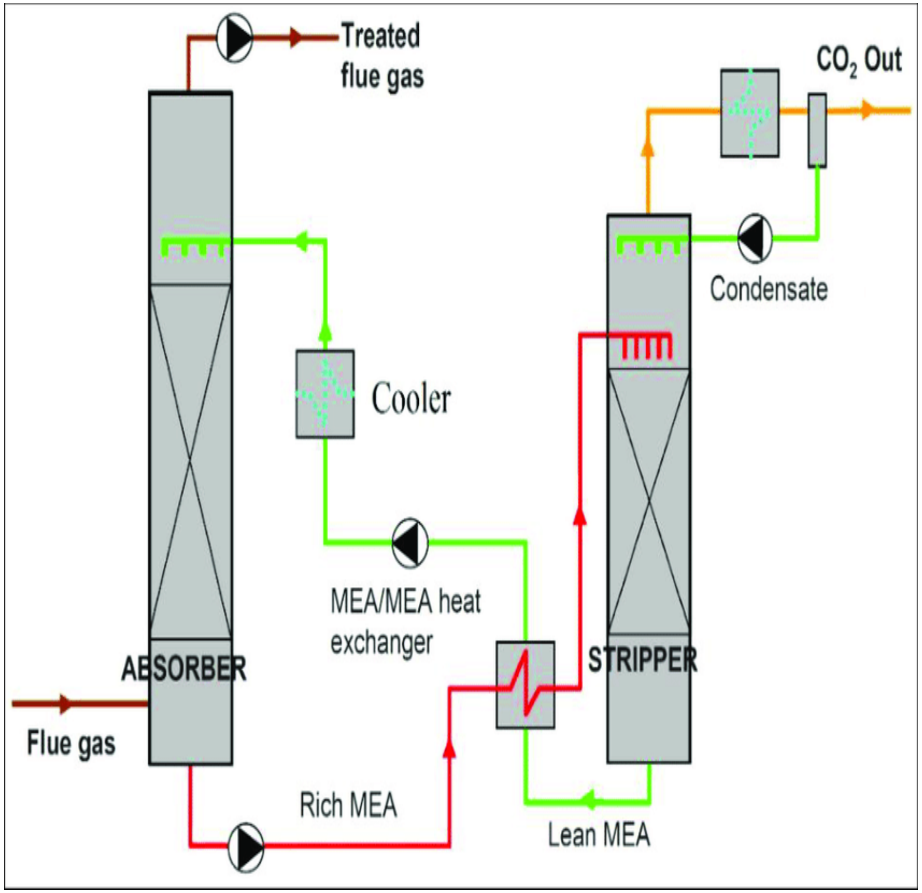
Solvent-based PCC process description

The Absorber

- CO_2 in the flue gas is absorbed by the amine solvent
- Treated gas leaves through the absorber top
- The amine solvent rich in CO_2 leaves through the absorber bottom to the stripper

The stripper

- The rich amine solvent is regenerated in the stripper to produce the original solvent and CO_2.
- The CO2-rich stream leaves through the top of the stripper.
- The lean solvent is returned to the absorber



Schematic of the CO_2 removal process. Gervasi et al. (2014)

AIM, OBJECTIVES AND NOVEL CONTRIBUTIONS

Aim

To carry out simulation, validation and scale-up studies of the solvent-based PCC process. The aim will be achieved with the following objectives.

Objectives

- Model development of the Solvent-based PCC plant.
- model validation with experimental data from the chosen pilot plants.
- Model scale-up of the pilot plant.

Novel Contribution

Application of an alternative scale-up methodology for Solvent-based PCC plant using the flooding velocity as basis for calculation.

- Offers the advantage of estimating the column diameter without the GPDC chart and assumed pressure drop.

LITERATURE REVIEW

Pilot plants

Laboratory of thermodynamics, University of Kaiserslautern

- Experimental studies on effects of operational variables on process behaviour, test of different packing types

Main specifications

	diameter(m)	packing height(m)	packing type
Absorber	0.125	4.25	Mellapak 250Y
Stripper	0.125	0.84 m	Mellapak 250 Y
Water wash column	0.125	0.42	Mellapak 250Y

Pilot-scale Advance Capture Technology (PACT), University of Sheffield

- Impact of different CO2 concentrations on the post-combustion CO2 capture process with MEA

Main specifications

	diameter (m)	packing height (m)	packing type
Absorber and Desorber	0.303	6.0	IMTP 40
Water wash column	0.303	1.2 m	IMTP 40

Separation research programme, University of Texas, Austin

- Separation performance and mass transfer of the absorber and stripper respectively

	diameter(m)	packing height(m)	packing type
Absorber and stripper	0.427	6.1	Flexipac/IMTP 40

No washing section.

LITERATURE REVIEW

Modelling and simulation of the PCC process

- Process modelling and simulation of the solvent-based CO_2 capture process have been carried out by several researchers at different levels of complexity.

- The two approaches commonly used to model the process are:
  - Equilibrium-based model approach
  - Rate-based model approach
    - More appropriate for modelling the PCC process

- The CO_2capture plant has been studied using
  - Dynamic simulation
  - Steady state simulation

LITERATURE REVIEW

Dynamic and steady state modelling of the solvent-based PCC

Reference	Simulation tool	Model complexity	Model validation	Description and model application

Lawal et al. (2010)	gPROMS and Aspen properties	Rate based mass transfer and chemical equilibrium, model scale-up and integration to power plant model	Steady state validation with data from the SRP pilot plant (Dugas, 2006)	Power plant model development integrated with full-scale PCC CO_2 capture model.
				• Investigated plant performance with different
				    • absorber column heights
				    • MEA concentrations

Akesson et al. (2012)	Dymola/Modelica	Rate based mass transfer and chemical equilibrium	Dynamic validation with data from the Esbjerg pilot plant (Faber et al., 2011)	Dynamic model validation and model reduction for demonstration of NMPC.
Nittaya et al. (2014)	gPROMS	Rate based mass transfer and enhancement factor.	Steady state validation using data from the SRP pilot plant (Dugas, 2006)	Process scale-up and investigation of effects of changes in • Absorber height • Flue gas flow rate • CO_2 capture level
Enaasen et al. (2014)	K-Spice	Rate based mass transfer and enhancement factor	Validation with data from the Brindisi CO_2 pilot plant	Dynamic model validation
Canepa et al. (2013)	Aspen Plus	Rate based mass transfer with kinetic reactions	Steady state validation with data from SRP pilot plant	Model scale-up, integration to full scale PCC to investigate effect of EGR on energy penalty.
Agbonghae et al. (2014)	Aspen Plus	Rate based mass transfer with kinetic reactions	Steady state validation with data from the Kaiserslautern pilot plant (Notz et al., 2012)	Model scale-up to commercial scale with techno-economic assessment.

LITERATURE REVIEW

SCALE-UP

Column diameter required for absorption operation at large-scale for the solvent-based PCC has often been estimated using the GPDC chart and following these steps:

- Estimation of the required solvent (F_{lean}) for the absorption operation.

$$F_{lean} = \frac{F_{FG} x_{CO2} \varphi_{CO2}}{100Z(\alpha_{Rich} - \alpha_{Lean})} \left(\frac{M_{Amine}}{44.009} \left\{ 1 + \frac{1-\omega_{Amine}}{\omega_{Amine}} \right\} + z\alpha_{Lean} \right) \text{ ....} \quad (1)$$

(Agbonghae et al, 2014)

F_{lean} = Mass flow rate lean solvent, F_{FG} =mass flow rate of flue gas, M_{Amine}= molar mass of the amine

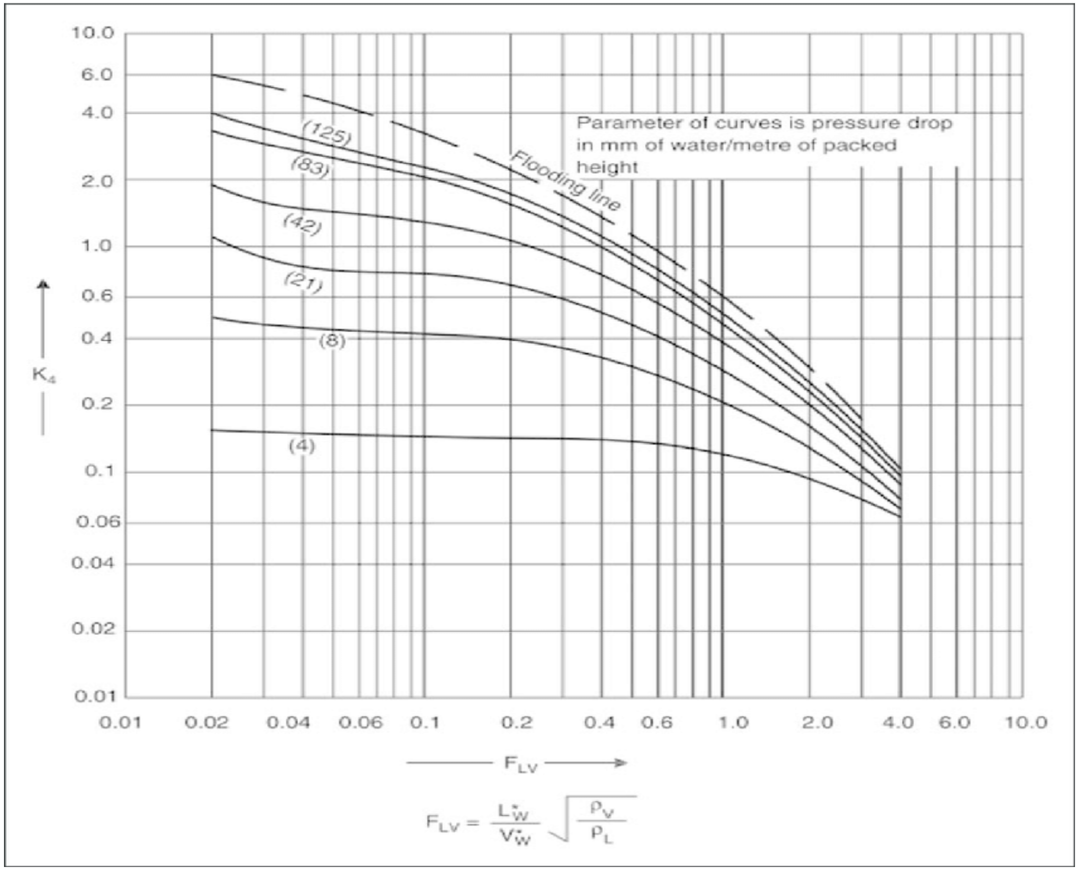
Xco_2= mass fraction of CO2 in flue gas, φ_{CO2}=percentage of CO2 recovered from the flue gas

Z=number of equivalent/mole amine=1 for MEA $\alpha_{Rich} - \alpha_{Lean}$=Rich and lean amine CO2 loading.

- Calculation of the flow parameter (abscissa of the GPDC)
- Estimation of the load parameter from the GPDC chart using the calculated flow parameter and the assumed pressure drop.
- Calculation of the column vapour mass flow rate per unit cross-sectional area
  - from which the total area is obtained.

LITERATURE REVIEW

SCALE-UP



The GPDC chart (Sinnot, 2005)

- For packed column, Pressure drop of 15-50 mmH_2O/m of packing was recommended by Sinnot (2005)
  - For good liquid and gas distribution
  - To avoid flooding
- For most scale-up work available in literature pressure drops of 20.83 and 42 mmH_2O/m packing are mostly adopted.
  - Due to the foaming nature of the amine system
  - Easily read off from the GPDC charts.

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LITERATURE REVIEW

Studies from literature that Adopted the GPDC scale-up approach

	Lawal et al. (2012)	Canepa et al. (2012)	Biliyok and Yeung (2013)	Agbonghae et al. (2014)	Luo and Wang (2016)
CO_2 capture rate (%)	90	90	90	90	90
Power plant size (MW_e)	500	250	440	673	250
Type of power plant	Subcritical coal-fired	Gas-fired CCGT	Gas-fired NGCC	Subcritical coal-fired	Gas-fired CCGT
Lean loading (mol/mol)	0.290	0.303	0.234	0.200	0.300
Rich loading (mol/mol)	0.470	0.472	0.494	0.506	0.456
L/G ratio (kg/kg)	5.300	2.020	1.040	2.930	1.580
Absorber					
Number	2	2	4	2	1
Diameter (m)	9	9.5	10	16.67	14
Packing height (m)	27	30	15	23.04	15
Packing type (m)	IMTP40	IMTP40	Mellapak 250X	Mellapak 250Y	Mellapak250Y
Stripper					
Number	1	1	1	1	1
Diameter (m)	9	8.2	9	14.25	6
Packing height (m)	-	30	15	25.62	9.4
Packing type (m)	Flexipac 1Y	Flexipac 1Y	Mellapak 250X	Mellapak 250Y	Mellapak 250Y
Pressure drop (mmH_2O/m packing)	42	42	42	20.83	20.83

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PROPOSED METHOD FOR ESTIMATING COLUMN DIAMETER

Based on the correlation for predicting flood point and pressure drop in columns presented by Kister and Gill (1991)

- An expression of the form below can be written for the relationship between the abscissa and the ordinate

$$CP = A\log^2(Flv) + B\log(Flv) + c \qquad (1) \qquad \text{(Kister and Gill, 1991)}$$

where

Flv is the flow parameter given by $F_{lv} = \frac{L}{G}\sqrt{\frac{\rho_L}{\rho_G}}$ (2) (Sherwood, et al 1938)

And CP, the capacity parameter is given as;

$$CP = \sqrt{U_{G,fl}^2 \left(\frac{\rho_G}{\rho_L - \rho_G}\right) \left(\frac{\mu_L}{\rho_L}\right)^{0.1} F_P} \qquad (3) \qquad \text{(Piché, 2001)}$$

Where $U_{G,fl}$ is the flooding velocity, ρ_G and ρ_L are the gas and liquid density, μ_L is the liquid viscosity and F_p is the packing factor.

PROPOSED METHOD FOR ESTIMATING COLUMN DIAMETER

The pressure drop at which incipient flooding occurs in the column can be determined using the Kiste Gill equation given as;

$\Delta P_{fl} = 0.115 F_P^{0.7}$ (in-water /ft of packing) (4) (Kister and Gill, 1991)

- Equation (4) is applicable when $10 \leq F_P \leq 100$ (ft^{-1}) (Piché et al, 2001)
- At $F_P > 60$ ft^{-1} pressure drop prediction accuracy decreases (Kister and Gill, 1991 and Perry, 1999).

The constants A, B and C in equation (1) are functions of the flooding pressure drop and are given by following equations.

$A = 0.0665 \ln(\Delta P_{fl}) - 0.1106$ $0.5 \leq \Delta P_{fl} \leq 5.0$ inH20/ft

$B = -0.252 \ln(\Delta P_{fl}) - 0.8918$ $0.5 \leq \Delta P_{fl} \leq 1.0$ inH20/ft

$B = -0.8900$ $1.0 \leq \Delta P_{fl} \leq$ inH20/ft

$C = 0.1221 \ln(\Delta P_{fl}) + 0.714$ $0.5 \leq \Delta P_{fl} \leq 5.0$ inH20/ft

(Piché et al, 2001)

PROPOSED METHOD FOR ESTIMATING COLUMN DIAMETER

Equation 1 can be re-written in the form shown below;

$$CP = \log[\log(F_{lv})^{A}] + \log(F_{lv})^{B} + \mathrm{C} \qquad (5)$$

By combining equations 2, 3, 4 and 5 and re-arranging for the flooding velocity, we arrived at the following equation;

$$U_{G,fl} = \left(\frac{\rho_L - \rho_G}{\rho_G}\right)^{0.5} \left(\frac{\rho_L}{\mu_L}\right)^{0.05} F_P^{-0.5} \log\left[log\left(\frac{L}{G}\sqrt{\frac{\rho_L}{\rho_G}}\right)^{A}\right] + \log\left(\frac{L}{G}\sqrt{\frac{\rho_L}{\rho_G}}\right)^{B} + \mathrm{C} \qquad (6)$$

Equation (6) can be used to estimate the flooding velocity in a packed column once the liquid and gas flowrates as well as the physical properties such as the gas and liquid densities and viscosity are known.

Packed columns are usually designed to operate within 60-80% of the flood point velocity (Perry, 1999).

PROPOSED METHOD FOR ESTIMATING COLUMN DIAMETER

Assuming a value of 70 % of flooding velocity, the operating velocity in the column can be determine by multiplying the flooding velocity by 0.7

$$U_{oprt} = 0.7U_{G.fl} \quad (7)$$

The diameter (D_{oprt}) required by a column operating at 70% of flooding velocity is given as;

$$D_{oprt} = \sqrt{\frac{4G}{\pi U_{oprt}\rho_G}} \quad (8)$$

- To test the accuracy of equations 6-8 above, they were used to estimate the diameter of packed absorber columns for different cases previously reported in the literature.
- The details of the various cases and the results obtained are shown in tables below.

CASES REPORTED FROM LITERATURE

Inlet Flow Parameters

	Liquid			Gas		
	Flow rate	Density	viscosity	Flow rate	Density	Reference
Plants	L (Ib/sec)	ρ_L (Ib/ft³)	μ_L (Ib/ft.s)	G (Ib/sec)	ρ_G (Ib/ft³)	
University of Kaiserslautern pilot plant	0.123	65.84	0.001064	0.044	0.0661	(Notz, et al, 2012)
250 (MW_e) gas-fired NGCC power plant	1352.40	63.4	0.002386	784.80	0.0682	(Canepa et al., 2013)
300 MW_e coal-fired power plant	1301.02	66.80	0.001164	778.89	0.0761	(Khalilpour and Abbas, 2011)
400 MW_e gas-fired NGCC power plant	1316.84	65.35	0.001165	1371.72	0.0795	(Agbonghae et al., 2014)
694 MW_e sub-critical coal-fired power plant	5755.75	67.05	0.001050	1967.78	0.092024	(Agbonghae et al., 2014)
827 MW_e sub-critical coal-fired power plant	5511.14	67.06	0.004210	2055.63	0.089069	(Agbonghae et al., 2014)

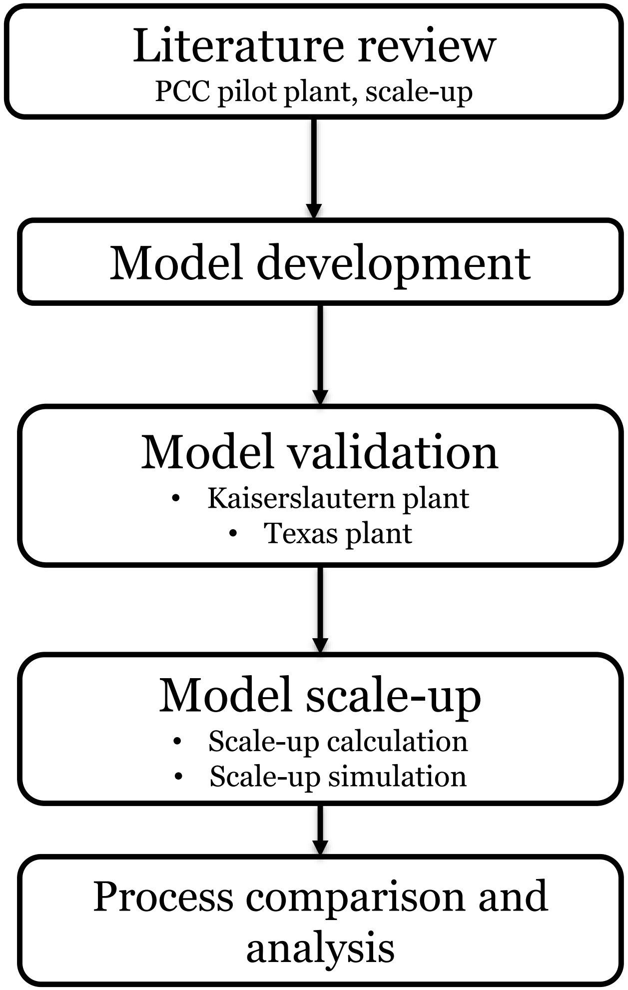
RESULTS

	Packing		Results						
	Type	Factor	Pressure drop at flooding	Flooding velocity	Operating velocity	Estimated diameter	Estimated diameter	Reported diameter	Relative error
Plants		(ft^{-1})	ΔP_{fl} (in-H_2O/ft)	$U_{G,fl}$(ft/s)	U_{oprt} (ft/s)	D_e (ft)	D_e (m)	D_a (m)	%Rel. error
pilot plant	Mellapak 250 Y	28.099	1.1879	7.164	5.015	0.411	0.125	0.125	0.00
250 (MW_e) gas-fired NGCC power plant	IMTP 40	24	1.0638	9.896	6.927	46.00	14.00	14.00	0.00
300 MW_e coal-fired power plant	Ceramic Berl-saddle	45	1.65113	6.65	4.65	52.90	16.12	15.00	7.46
400 MW_e gas-fired NGCC power plant	Mellapak 250 Y	20.11	0.934	13.54	9.48	50.91	15.52	16.92	8.27
694 MW_e sub-critical coal-fired power plant	Mellapak 250 Y	20.11	0.934	6.24	4.36	78.96	24.07	23.08	4.28
827 MW_e sub-critical coal-fired power plant	Mellapak 250 Y	20.11	0.934	6.499	4.54	80.05	24.40	23.91	2.04

MODEL DEVELOPMENT

- The absorber and the stripper columns of the pilot plants were developed using a detailed rate-based (RADFRAC) model in Aspen Plus.
- For the Kaiserslautern pilot plants, the eNRTL is selected for the liquid phase properties and the PC-SAFT equation of state for the vapour phase properties.
- For the Texas pilot plant, eNRTL physical property method was used for the liquid phase and the Redlich-Kwong Equation of state (EOS) was used for the vapour phase.
- Correlations for transport properties are included in the model (such as the mass transfer coefficient, heat transfer coefficient, interfacial area, liquid hold up and pressure drop).

Project execution plan



PILOT PLANTS DATA

Plants main specifications	Kaiserslautern	Texas
CO_2 content in the flue gas (mol%)	3-14	15.2-18.0
Flue gas flow rate	30-100 (kg/h)	395-990 (kg/h)
Solvent flow rate	20-350 (kg/h)	849.6-6692.4 (kg/h)
Absorber		
Diameter (m)	0.125	0.427
Height of packing (m)	4.2	6.1
Packing type	Mellapak 250Y	IMTP 40
Operating pressures (bar)	Atmospheric pressure	Atmospheric pressure
Regenerator		
Diameter (m)	0.125	0.427
Height of packing (m)	2.52	6.1
Packing type	Mellapak 250 Y	Flexipac 1 Y
Operating pressures (bar)	1-2.5	1.6

- For the Kaiserslautern pilot plant, two sets of experiments from Notz et al. (2012) were chosen for model validation purposes. These are:
  - Experiments A15-A19 involving low CO_2 concentration in the flue gas
  - Experiments A28—A33 involving high CO_2 concentrations in the flue gas.
- For the Texas pilot plant, three experiments from Dugas (2006) were chosen for model validation purposes, these are cases 28, 32 and 47.
- Process steady state models were simulated in Aspen plus®.

MODEL VALIDATION

Model validation for the Kaiserslautern pilot plant (A15-A19)

Case	Rich loading (mol CO_2/Mol MEA)			CO_2 Capture (Kg/h)			Specific duty (MJ/kgCO_2)		
	Exp.	Model	Rel. error (%)	Exp.	Model	Rel. error (%)	Exp.	Model	Rel. error (%)
A15	0.359	0.357	0.55	6.34	6.31	0.47	5.81	5.73	1.37
A16	0.414	0.411	0.72	6.37	6.50	2.04	7.38	7.36	0.27
A17	0.371	0.377	1.62	6.38	6.37	0.15	5.47	5.41	1.09
A18	0.387	0.383	1.03	6.43	6.43	0.00	5.35	5.27	1.49
A19	0.354	0.343	3.11	6.43	6.41	0.31	6.27	6.02	3.98

MODEL VALIDATION

Model validation for the Kaiserslautern pilot plant (A28-A33)

Cases	Rich loading (mol CO_2/mol MEA)			CO_2 capture (kg/h)			Specific duty (MJ/kg CO_2)		
	Exp.	Model	Rel. error (%)	Exp.	Model	Rel. error (%)	Exp.	Model	Rel. error (%)
A28	0.470	0.473	0.63	6.63	6.68	0.75	3.68	4.00	8.69
A29	0.465	0.464	0.22	6.64	6.84	3.01	3.92	3.62	7.65
A30	0.459	0.452	1.52	6.67	6.50	2.54	4.38	4.12	5.93
A31	0.454	0.454	0.00	6.71	6.17	8.05	4.30	4.24	1.39
A32	0.449	0.459	2.23	6.61	6.82	3.18	4.57	4.62	1.09
A33	0.441	0.440	0.23	6.60	6.63	0.45	4.35	4.32	0.68

MODEL VALIDATION

Model Validation for pilot plant at the University of Texas (SRP)

Cases	Rich loading (mol CO_2/mol MEA)			CO_2 capture level (%)		
	Exp.	Model	Rel.error (%)	Exp.	Model	Rel. error (%)
28	0.412	0.410	0.49	86	85	1.16
32	0.428	0.436	1.87	95	90	5.26
47	0.539	0.481	10.76	69	69	0.00

•Process steady state models were simulated in Aspen plus to meet the values reported for the rich solvent CO_2 loading and the CO_2 capture in the pilot plant.

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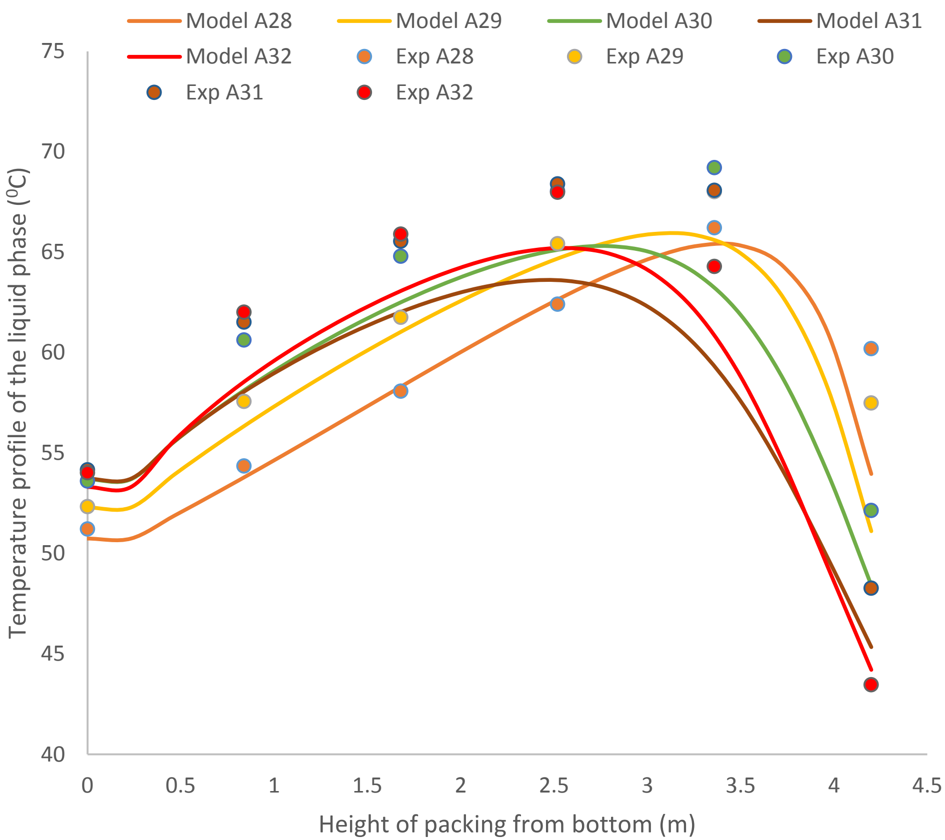
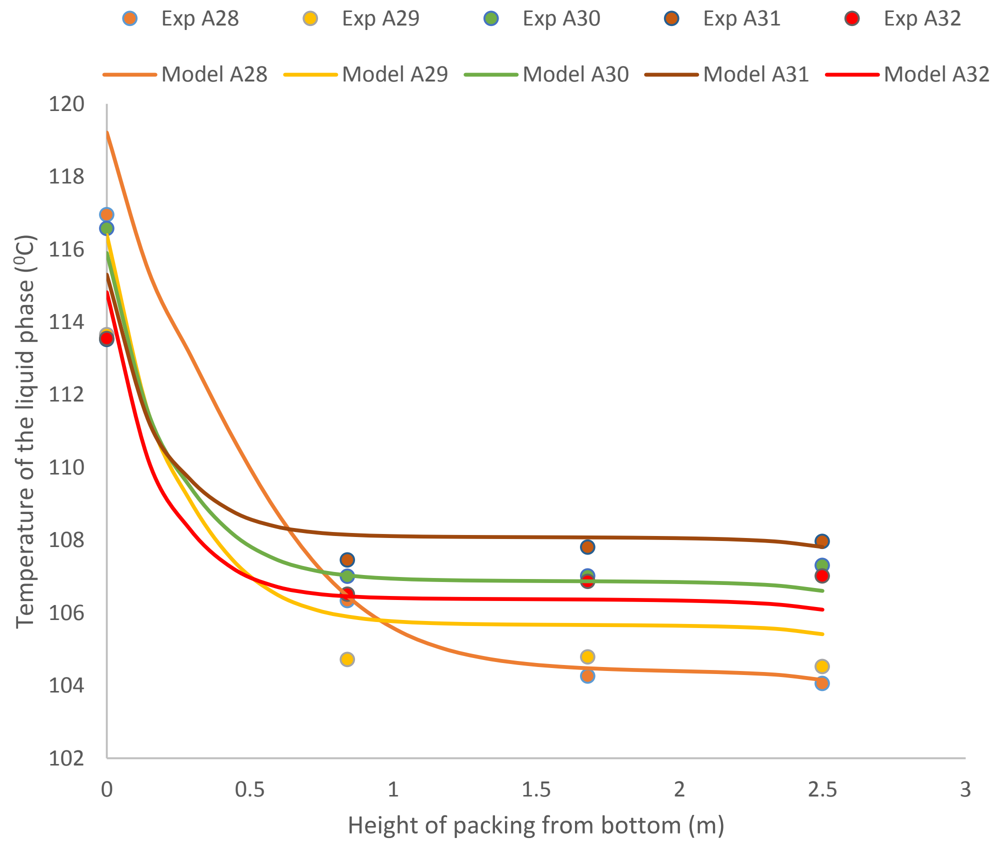
MODEL VALIDATION

Comparison of the absorber and Stripper temperature profiles between the model and pilot plant measurement for experiments A28—A32 in the Kaiserslautern plant





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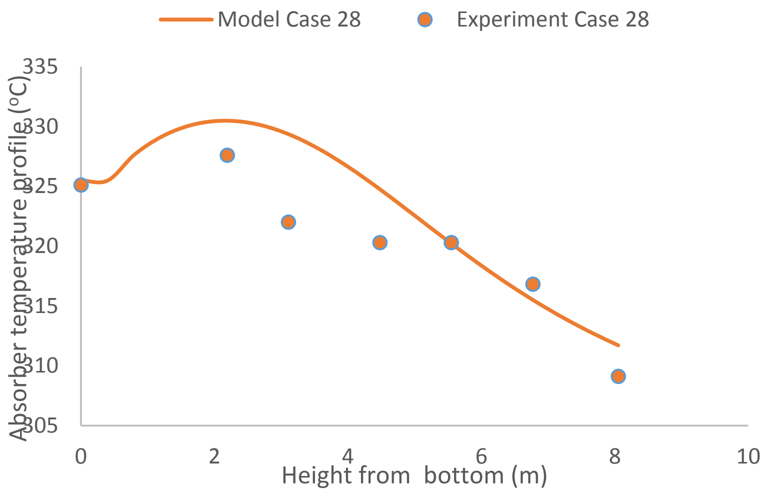
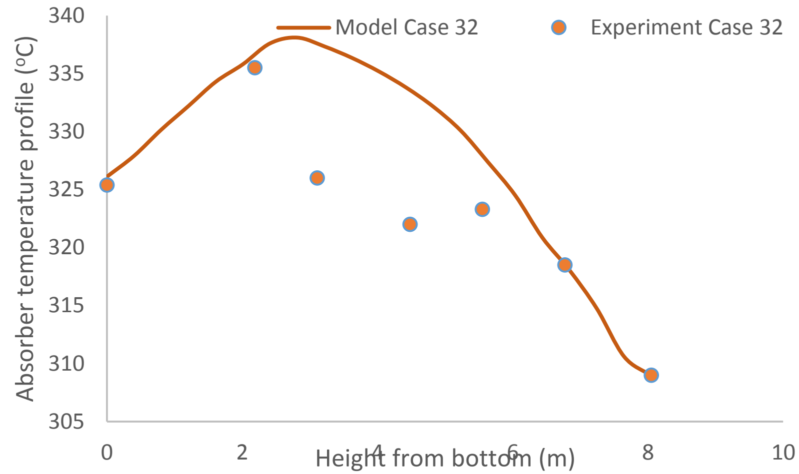
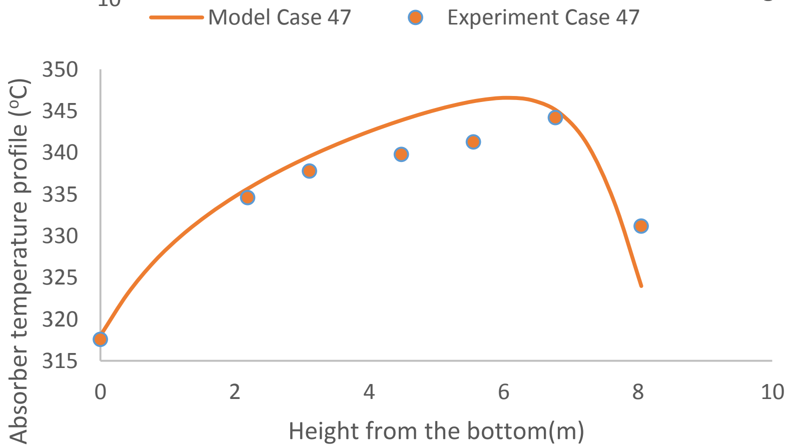
MODEL VALIDATION

Comparison of the absorber temperature profiles of the model and pilot plant measurement for the pilot plant at the University of Texas







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MODEL SCALE-UP

The method proposed in this study was used to estimate the column diameter required to process:

- the flue gas from a 450 MW_e NGCC power plant (Agbonghae et al. 2014)
- The flue gas from a 750 MW_e super-critical coal-fired power plant (Nittaya et al. 2014)
  (these plants have both been scaled from the pilot plant models using the GPDC chart method)

➢ The validated model for the University of Kaiserslautern pilot plant was scaled for the 450MW_e NGCC case
  - Results compared to those obtained in the study by Agbonghae et al. (2014)

➢ The validated model for the University of Texas pilot plant was scaled for the 750 MW_e super-critical coal-fired power plant case.
  - Results compared to those obtained in the study by Nittaya et al. (2014)

- The packed bed height was estimated using similar method in literature (Lawal et al, 2012; Canepa et al, 2014; Nittaya et al, 2014)

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MODEL SCALE-UP

Input Parameters

Description	450 MW_e NGCC (gas-fired)	750 MW_e Super-critical (coal-fired)
Flue gas flow rate (kg/s)	725	700
Composition (mass fraction)	CO_2: 0.0404; H_2O: 0.0867; N_2: 0.7432; O_2: 0.1209; Ar: 0.0089	CO_2: 0.2356; H_2O: 0.0148; N_2: 0.7296; O_2: 0.0199
Flue gas temperature (°C)	40	48
MEA concentration in lean solvent (wt%)	30	30
Lean MEA inlet temp (°C)	40	41
Capture level (%)	90	87
Absorber operating pressure (bar)	1.2	1.03
Stripper operating pressure (bar)	1.62	1.6

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MODEL SCALE-UP

RESULTS: This study Vs Agbonghae et al. (2014) for the 450 MW_e NGCC

	Agbonghae et al (2014)	This Study	Difference (%)
Flue gas flow rate (kg/s)	725	725	0.00
Lean solvent low rate (kg/s)	694.55	671.7	3.4
Lean CO_2 loading (mol CO_2/mol MEA)	0.20	0.22	10
Rich CO_2 loading (mol CO_2/mol MEA)	0.483	0.488	0.83
Absorber diameter (m)	2 x 12.88	2 x 11.95	7.22
Absorber Packing height (m)	19.06	19.02	0.26
Packing type	Mellapak 250Y	Mellapak 250Y	
Pressure drop (mm-H_2O/m packing)	20.83	18.97	8.93
Stripper diameter (m)	7.74	7.74	0.00
Stripper packing height (m)	28.15	27.5	2.31
Packing type	Mellapak 250Y	Mellapak 250Y	
Pressure drop (mm-H_2O/m packing)	5.31	4.96	6.60
Specific reboiler duty	3.96	3.79	4.29
Capture (%)	90	90	0.00

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MODEL SCALE-UP

RESULTS: This study Vs Nittaya et al. (2014) for the 750 MW_e coal-fired

	Nittaya et al. (2014)	This Study	Difference (%)
Flue gas flow rate (kg/s)	700	700	
Lean solvent low rate (kg/s)	3152	3101.7	1.60
Lean CO_2 loading (mol CO_2/mol MEA)	0.3	0.325	8.3
Rich CO_2 loading (mol CO_2/mol MEA)	0.5	0.484	3.2
Absorber diameter (m)	3 x 11.8	3x 10.78	
Absorber Packing height (m)	16.5	16.01	3.03
Packing type	IMTP 50	IMTP50	
Pressure drop (mm-H_2O/m packing)	42.0	36.02	14.00
Stripper diameter (m)	10.4	10.45	0.48
Stripper packing height (m)	16.0	16.00	0.00
Packing type	IMTP50	IMTP50	
Pressure drop (mm-H_2O/m packing)	-	5.45	
Specific reboiler duty (GJ/tCO2)	4.4	4.27	2.95
Capture (%)	87	87	0.00

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CONCLUSION

- A new approach proposed for packed bed scale-up without the need for assuming pressure drop
- Model development and validation with data from the two pilot plants (Kaiserslautern and Texas) have been carried out
  - Model prediction matched well with pilot plant measurements for the two pilot plants
  - Model captures temperature profiles in the absorber and stripper of the two pilot plants.
  - better predictions for coal fired conditions than gas-fired condition for the Kaiserslautern pilot plant.
- Scale-up of the validated model based on this method was carried out
  - The design was based on 70% flooding
  - Results compared with scale-up methods using GPDC chart (a 450MW$_e$ NGCC and a 750 MW$_e$ super-critical coal-fired)
  - Results shows that it can predict the column diameter to within less than 10% error.

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