DEVELOPMENT OF A COMPACT CO_2 CAPTURE PROCESS TO COMBAT INDUSTRIAL EMISSIONS

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Details of the project

Title: ***Development of a Compact CO_2 Capture Process to Combat Industrial Emissions***

Sponsor: ***EPSRC (EP/N024672/1), £1.22M, from Nov 2016 to Oct 2019***

Investigators

The University of Edinburgh: Prof Xianfeng Fan, Dr Martin Sweatman, Dr Hyungwoong Ahn

Newcastle University: Dr Jonathan Lee

The University of Sheffield: Prof Meihing Wang, Consultant: Colin Ramshaw

Project Partners

- ***Carbon Clean Solutions Limited (Drs Richard Matter, James Hall)***
- ***UK-China CCUS Centre (Drs JiaLi, Xi Liang)***
- ***Ferrite Microwave Technologies LLC***
- ***SK innovation co Ltd***
- ***Tan Delta Microwaves Ltd***

Objectives

Develop a compact, efficient and flexible CO_2 capture process using solvents

Combine a rotating packed bed absorber with microwave assisted regeneration.

WP 1: Rotating packed bed ,
Dr Toluwanimi Kolawole

WP2: Microwave assisted regeneration, amine corrosion and degradation
Dr Francis Bougie

WP3: Molecular modelling of microwave regeneration
Dr Nasser Afify

WP4: Process modelling & Technical and economic performance assessment
Dr Eni Oko

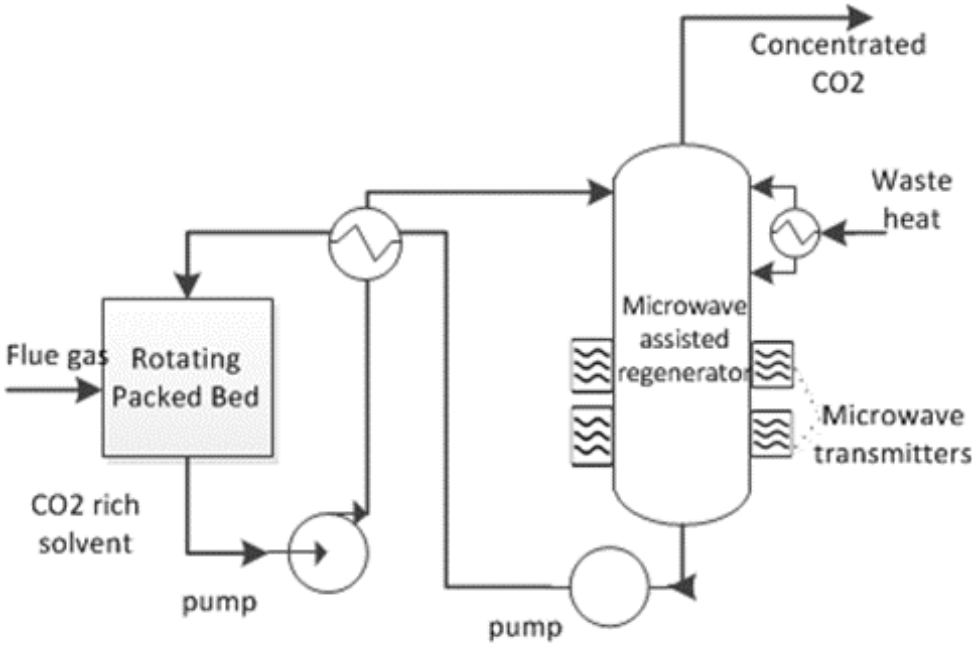


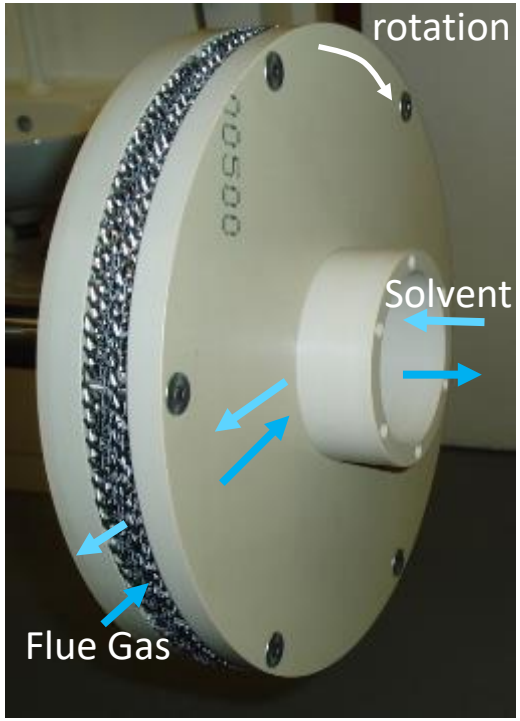
Fig. 1 Illustration of compact CO2 capture system

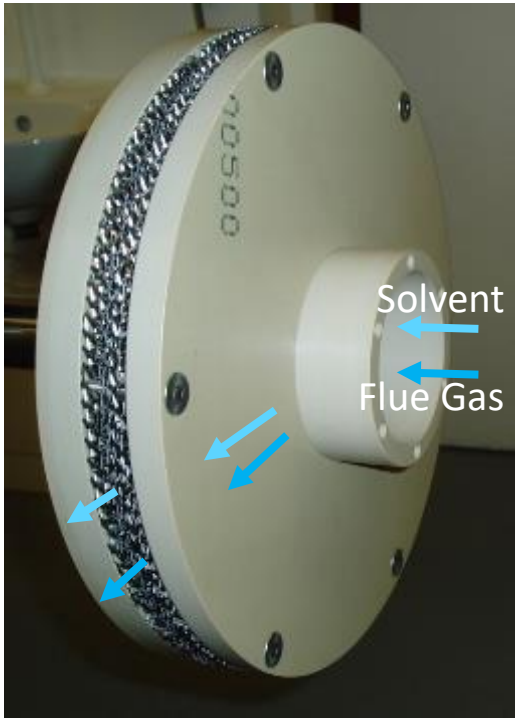
WP1: Rotating Packed Bed

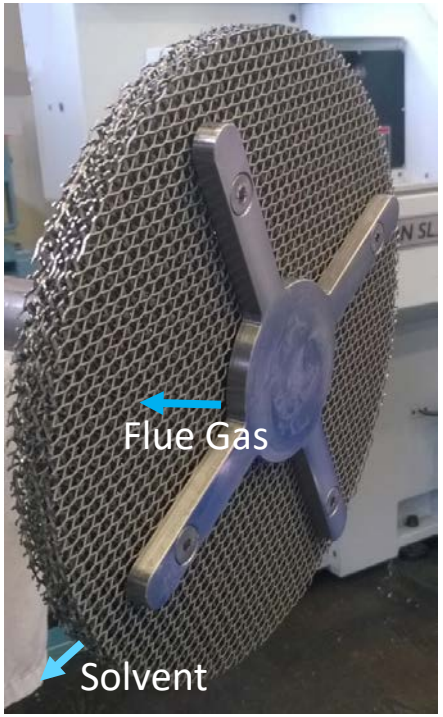
Investigating the effect of flow configuration

Packing is stacked sheets of stainless steel mesh (a_p = 694 m^2/m^3, ε = 0.84)

WP1: Rotating Packed Bed







Counter-current flow

Advantages

High rate of mass transfer

Disadvantages

Throughput limitation

High gas side pressure drop

Co-current flow

Advantages

No throughput limitation.

Potential to act as a fan or very low gas side pressure drop

Disadvantages

Loss in mass transfer performance

Cross flow

Advantages

No throughput limitation.

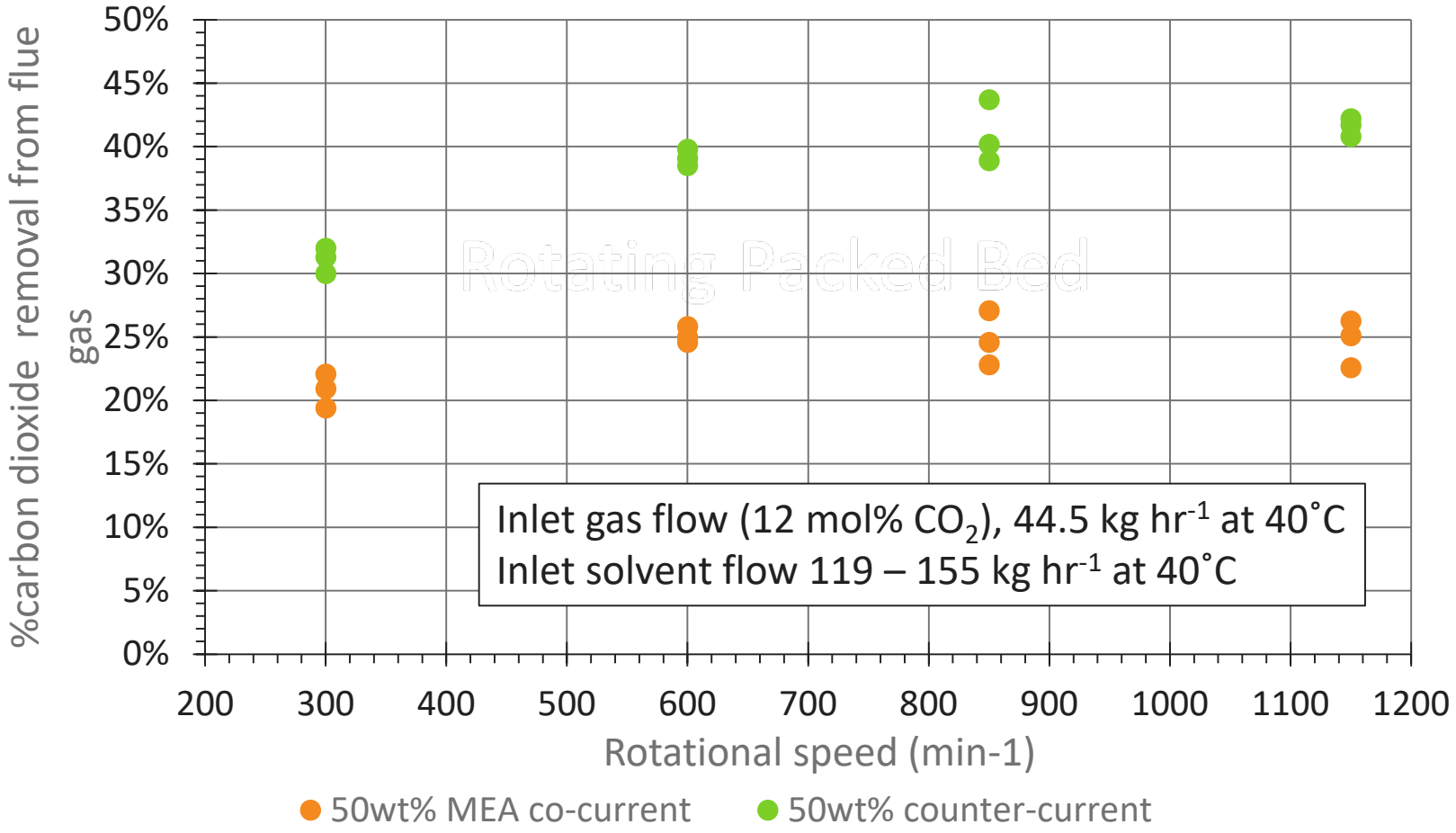
Low gas side pressure drop

Disadvantages

Loss of mass transfer performance

WP1: Rotating Packed Bed

Effect of rotational speed on CO_2 removal



WP1: Rotating Packed Bed

Work delivered

- Initial findings using the data to estimate the size of full scale absorbers:
  - Co-current absorber diameter would be 34% larger than the counter-current absorber.
  - Increasing the diameter leads to an increase in the power required to accelerate the liquid to the tip speed of the rotating packed bed.
  - This power increase outweighs the decrease in gas side pressure drop

- Currently gathering data for the cross flow configuration.

WP2: Microwave Regeneration

Work delivery:

1. **Regeneration** by microwave irradiation **of solutions** with high CO_2 absorption capacity and fast reaction rate.
2. Study the **effect** of the presence **of other gases** on regeneration efficiency by MW.
3. Investigate **degradation** and **corrosion** under MW heating.
4. Compare the energy cost with conventional heating

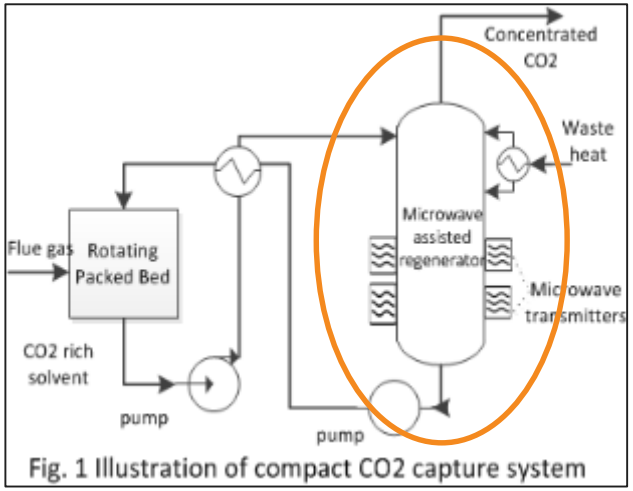


Fig. 1 Illustration of compact CO2 capture system

➢ **Several investigated parameters**

- ✓ Amine type and concentration.
- ✓ Solution composition.
- ✓ Initial content of CO_2, of dissolved gas, of additives.
- ✓ MW power, irradiation time, heating mode.
- ✓ T_{reg} of the solution.

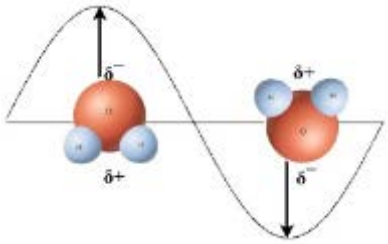
Find the
best amine solution
and
experimental conditions
for CO_2 capture with
MW regeneration

A paper has been published in Applied Energy, 192, 2017

WP2: Microwave Regeneration

- **Principle**

*Microwave, or dielectric, heating is based on the ability of **molecules with** a **dipole moment** to absorb microwave energy and effectively convert it into heat.*



$$\tan\delta = \frac{\varepsilon''}{\varepsilon'}$$

Loss tangent (tan δ)

Dielectric loss factor (ε″)

Dielectric constant (ε′)

f(ω,T)

→ Ability to dissipate microwave energy.

→ Linked to the amount of electric energy that can be stored within the heated material.

Values related to both *chemical structure* and *intermolecular interactions* (solution composition).

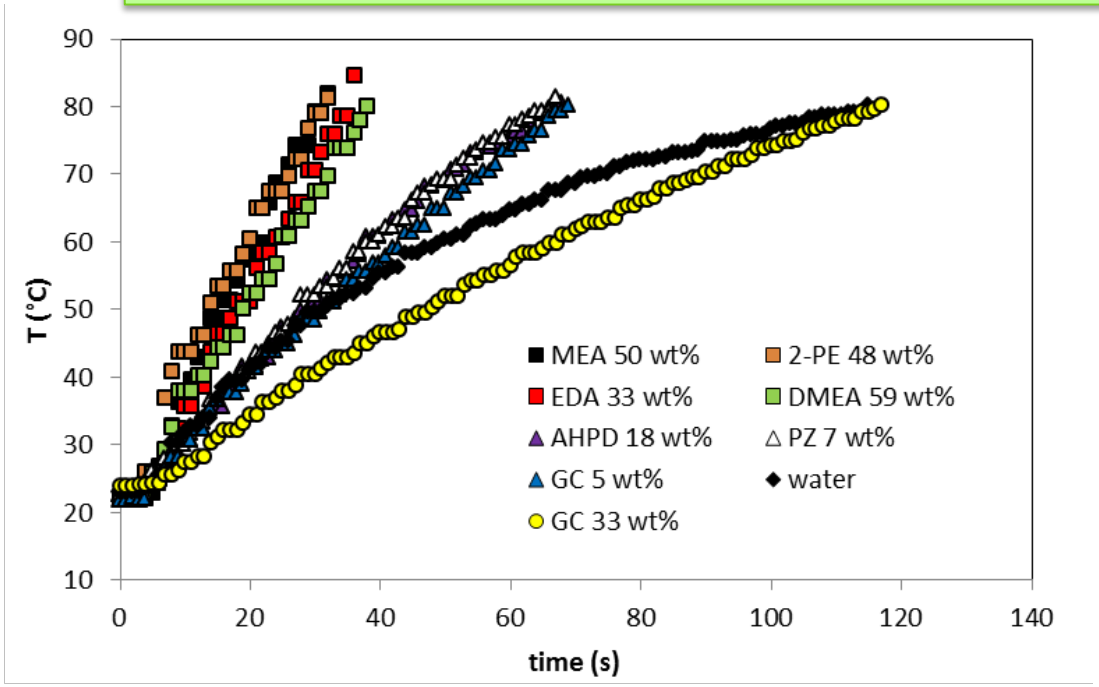
- **Advantages**

✓ **Instantaneous** and **volumetric heating** (without heat transfer restrictions associated with conventional conductive or convective heating).

✓ Specific heating and possible non-thermal effects.

WP2: Microwave Regeneration

Amine screening with **MW heating rate and CO_2 adsorption capacity**



Abbreviation	Name	Polarity (D)
PZ	piperazine	0
DMEA	dimethylmonoethanolamine	0.85
2-PE	2-piperidineethanol	1.41
	water	1.85
EDA	ethylenediamine	2.47
MEA	monoethanolamine	2.75
AHPD	2-amino-2-hydroxymethyl-1,3-propanediol	3.03
GC	guanidine carbonate	4.69

- Various amines
- Various concentration (0-70 wt%)

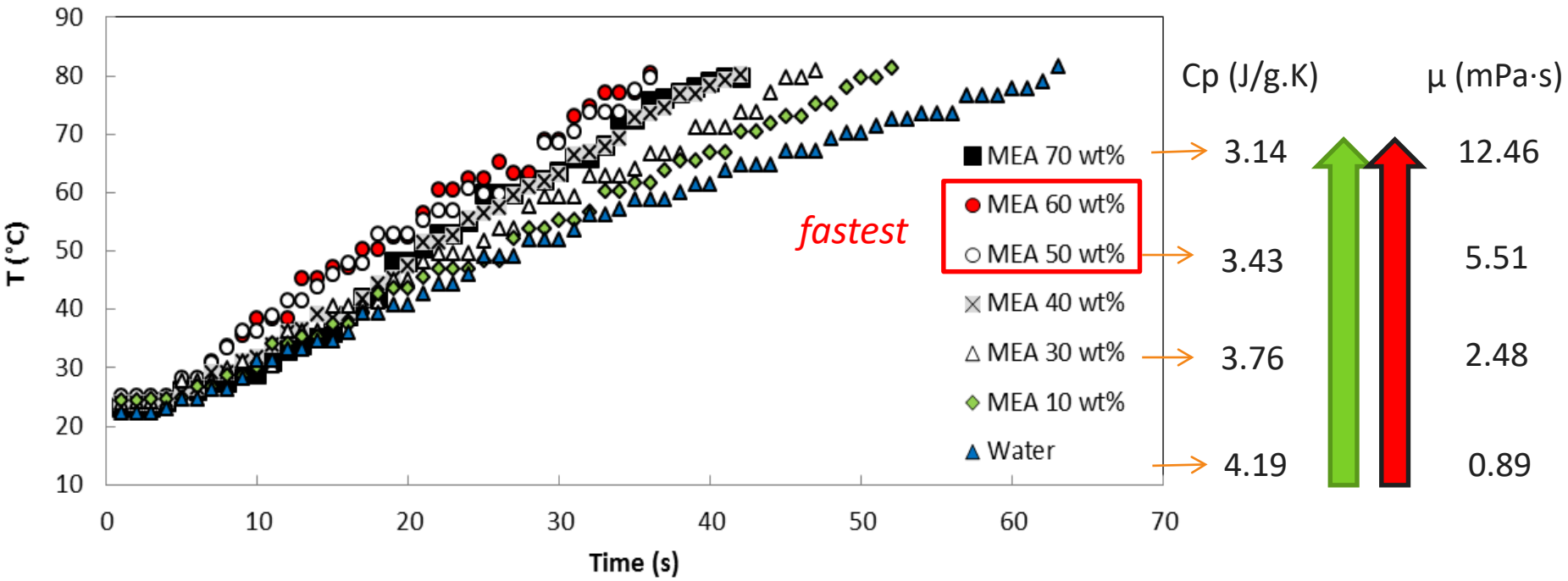
✓ **2-PE (48wt%), MEA (50 wt%)** and **EDA (33wt%) are quite interesting.**

✓ **DMEA (59 wt%)** also but tertiary amine… (will test with **PZ addition**).

But **need MEA (benchmark amine) data/results** as basis for comparison

WP2: Microwave Regeneration

Effect of MEA concentration on **MW heating**



- Maximal heating rate explained by the **opposite effect** of:
  - **Heat capacity:** lower value mean **faster heating** as less energy needed.
  - **Viscosity**: molecules have a **slower response** to the oscillating MW electric field in highly viscous media.

Influence of the heat capacity and viscosity of the solutions

WP2: Microwave Regeneration

Optimal MEA concentration with **CO_2 abs/ MW reg.**

MEA conc.	Rich loading	Cyclic capacity	Desorption energy	Energy/CO_2	Energy/CO_2^2
wt%	-	mol CO_2	J	kJ/mol	kJ/mol^2
10	0.56	0.0019	9086	4782	2516898
30	0.52	0.0030	8242	2747	915778
40	0.49	0.0034	7704	2266	666436
50	0.47	0.0036	6593	1832	508750
60	0.41	0.0026	5510	2119	815089

- Energy / CO_2 cyclic capacity → as low as possible.
- Energy / [CO_2 cyclic capacity]^2 → as low as possible.

Optimization factor: combine a **low Energy/CO_2** ratio and a **high quantity of CO_2**

50 wt% MEA is the optimal concentration with MW regeneration under the tested conditions (20 min abs. + 10 min reg. at 80°C)

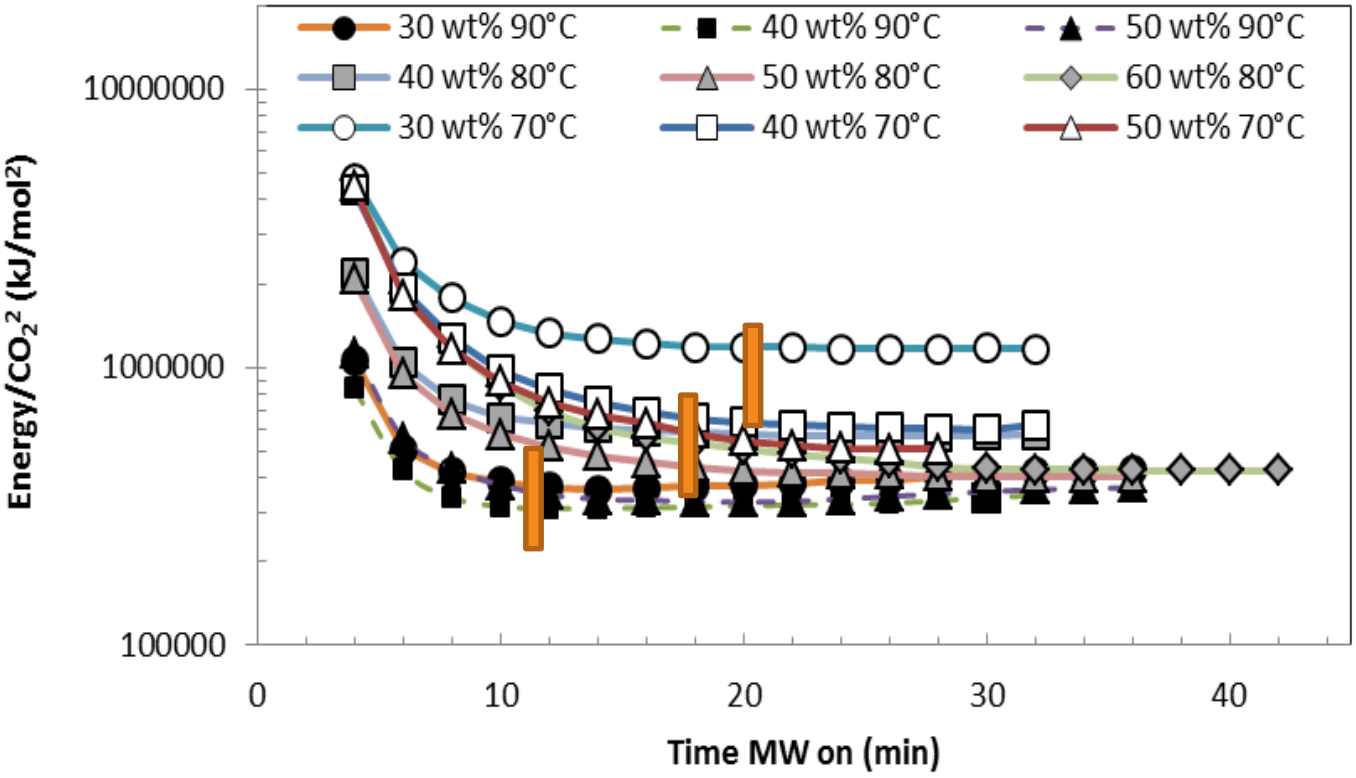
50 wt% vs 30 wt%
Cyclic capacity →+ 20%
Energy consumption → -20%

WP2: Microwave Regeneration

Optimization of the MW regeneration process

- Other parameters like the **regeneration temperature**, the **MW power** intensity or the **CO_2 loading** inside the solution **may influence the MW regeneration efficiency**.

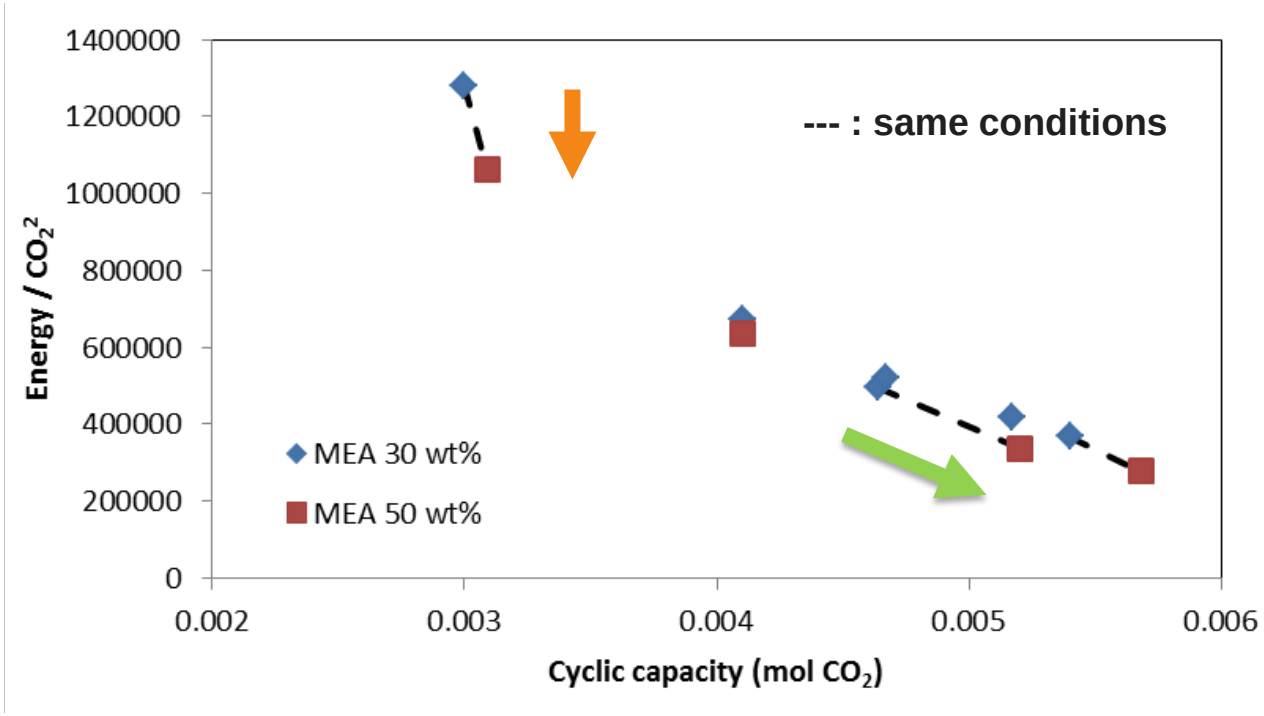
Regeneration temperature and time



WP2: Microwave Regeneration

Optimization of the MW regeneration process

- **CO_2 loading and cyclic capacity**

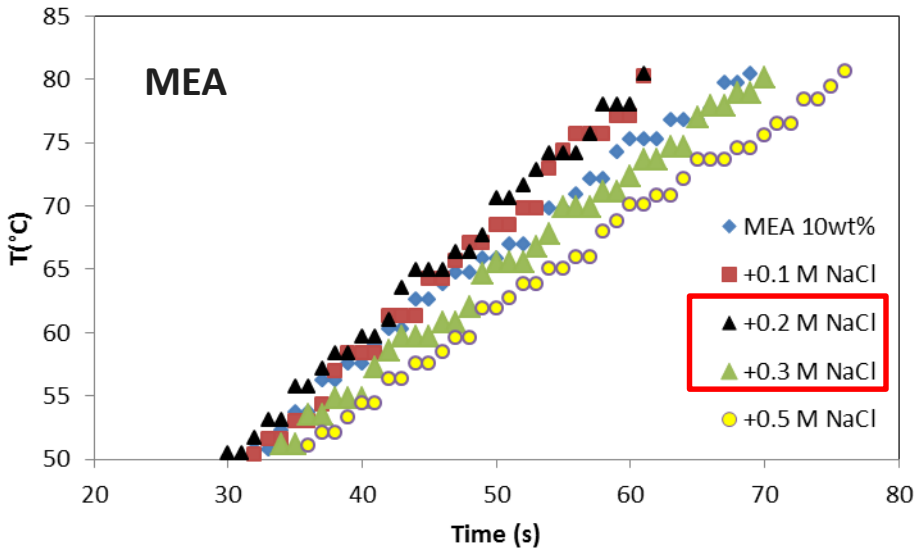


- **For the same cyclic capacity: 50 wt% require less energy.** (see: ↓)
- **Under the same conditions: 50 wt% has higher cyclic capacity or require less energy.** (see: →)

WP2: Microwave Regeneration

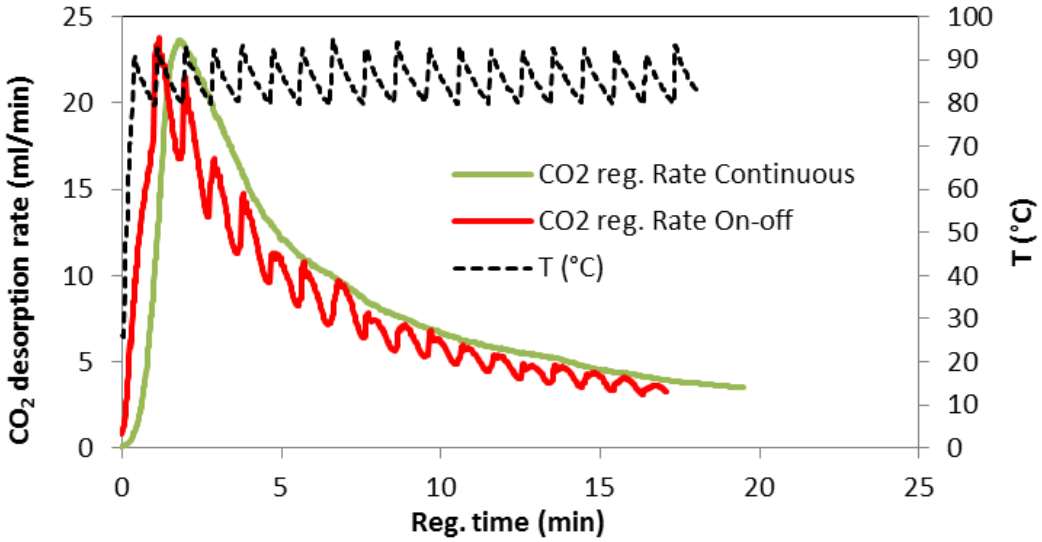
Other parameters influencing MW efficiency

Salt effect



Possibility to **modify MW efficiency** by salt additions

Heating mode



On-off : ±10°C

Energy/CO_2 reduction of 40% vs continuous heating

WP2: Microwave Regeneration

- ✓ MW heating rate as tool for **amine screening** (amine/solution response to MW).
- ✓ In addition to MW related properties (dielectric constants, dipoles), **heat capacity, viscosity,** amine **concentration**, **salt presence** and **heating mode** were found to influence MW heating efficiency.
- ✓ The lowest Energy/CO_2 and Energy/CO_2^2 using MW were found for the **50 wt% MEA solution** (instead of the well-known 30 wt% MEA) under various conditions.
- ✓ **MW Energy consumption** for <u>small scale setup</u> **overestimate real energy consumption** as reported in literature.

→ **Bigger quartz vial vs conventional heating**

setups in construction

More insight about:

→ MW energy consumption for bigger scales

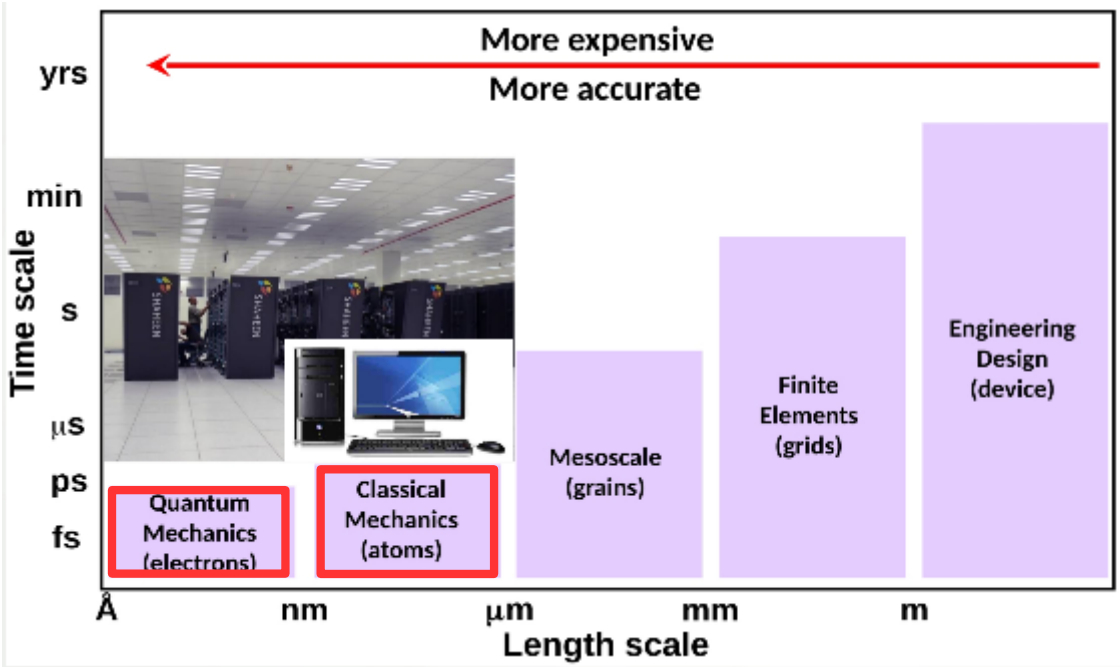
→ CO_2 regeneration fluxes (MW vs conventional)

Is MW a good alternative to conventional heating?

Is there some MW non-thermal effects?

WP3: Molecular modelling of microwave regeneration

- **Computational techniques:** different time and length scales

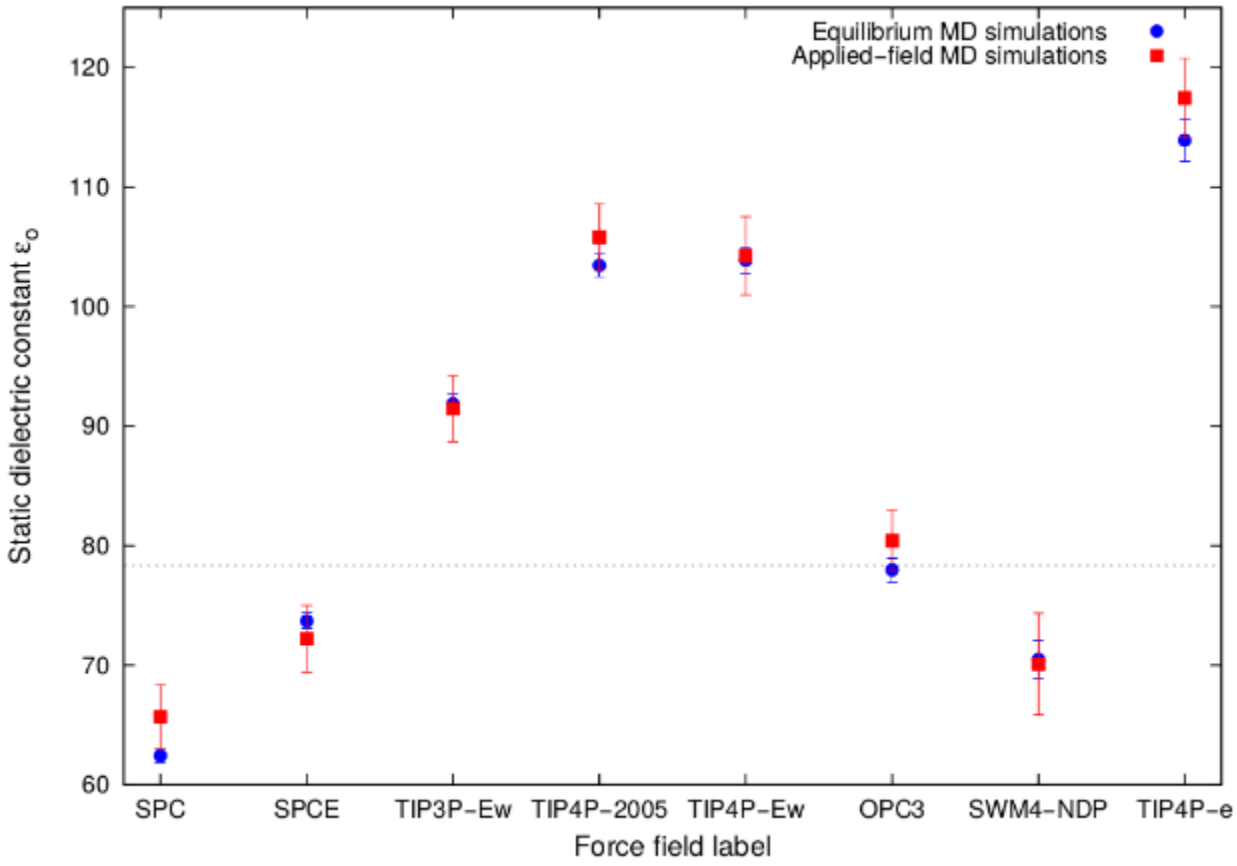


- **Classical molecular dynamics:**
  - Study dielectric response of CO_2-MEA-H_2O system to microwave
  - Prediction of static dielectric constant, frequency-dependent dielectric spectra, and heating profiles
- **Ab-initio molecular dynamics:**
  - Effect of microwave on the reactions involved in CO_2 capture

WP3: Molecular modelling of microwave regeneration

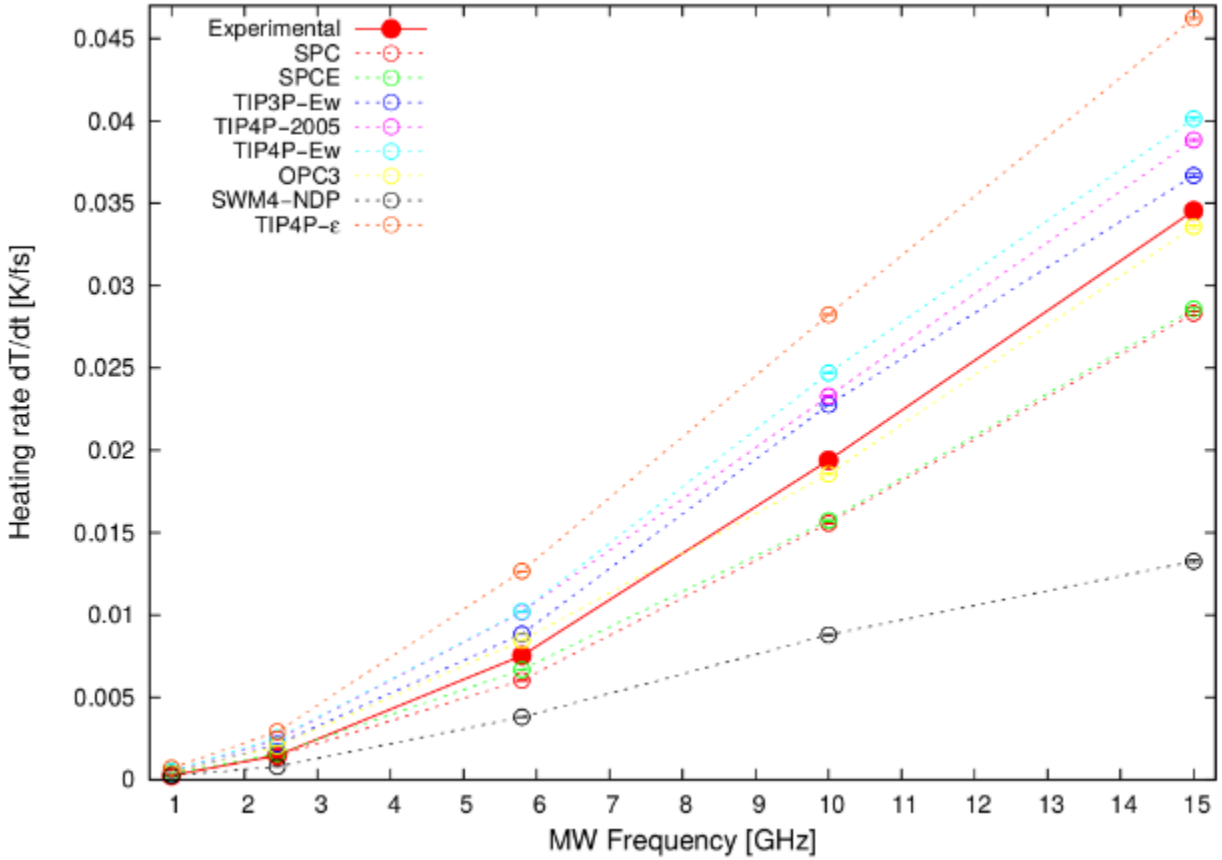
MW Heating of Water: Static Dielectric Constant

- Compare different empirical force fields
- Static dielectric constant computed using two different approaches



MW Heating of Water: Heating Rates

- Simulate heating profiles and compute heating rates at different microwave frequencies
- OPC3 is the most accurate empirical force field



MW Heating of Water: Publication

A paper on our computational methodology is currently under review

Classical molecular dynamics simulation of microwave heating of liquids: the case of water

N. D. Afify[1, a)] and M. B. Sweatman[1]
School of Engineering, The University of Edinburgh, The King's Buildings, Sanderson Building, Mayfield Road, Edinburgh EH9 3JL, United Kingdom

(Dated: 28 August 2017)

We perform a complete classical molecular dynamics study of the dielectric heating of water in the microwave region. MW frequencies ranging from 1.0 to 15.0 GHz are used together with a series of well-known empirical force fields. We show that the ability of an empirical force field to correctly predict the dielectric response of liquids to MW radiation should be evaluated on the basis of a joint comparison of the predicted and experimental static dielectric constant, frequency-dependent dielectric spectra, and heating profiles. We argue this is essential when multicomponent liquids are studied. We find the well-known SPCE and recently developed OPC3 (J. Chem. Phys.145, 074501 (2016)) empirical force fields of water are superior for reproducing dielectric properties, with the OPC3 force field particularly good for predicting heating rates at a range of MW frequencies.

Keywords: Classical molecular dynamics; Empirical force fields of water; Microwave heating of water; Dielectric spectra of water

I. INTRODUCTION

Dielectric heating of liquids using microwave (MW) radiation (0.3-300 GHz) is becoming an increasingly important research area, where many applications are emerging. One of these applications is the use of MW dielectric heating of liquids has, to our knowledge, yet to be developed. Some of us recently reported the frequency-dependent dielectric spectra of water, alcohols, glycols, and monoethanolamine using classical MD simulations[2]. In that study, several empirical force fields for each liquid were employed in an attempt to accurately predict their

Concluding Remarks for WP3

- In the CO_2 capture project we employ both classical and ab-initio molecular dynamics techniques
- The most accurate force field for each component in the CO_2-MEA-H_2O system has to be identified
- Selected force fields should reasonably predict experimental static dielectric constant, dielectric spectra, and microwave heating rates
- We have identified OPC3 as the most accurate force field available for water, a paper is currently under review
- The work on MEA is already complete but not reported here.
- None of the available MEA force fields was found accurate enough – tuning of the best force field was essential
- Ab-initio molecular dynamics calculations are underway

WP4: *Process modelling & performance assessment*

Work Delivered

- Regression of thermodynamic model (eNRTL) for concentrated MEA solution
- Comparison of mass transfer correlations through modelling and simulation
- Intercooler study (in preparation for large scale design development)

Thermodynamic modelling

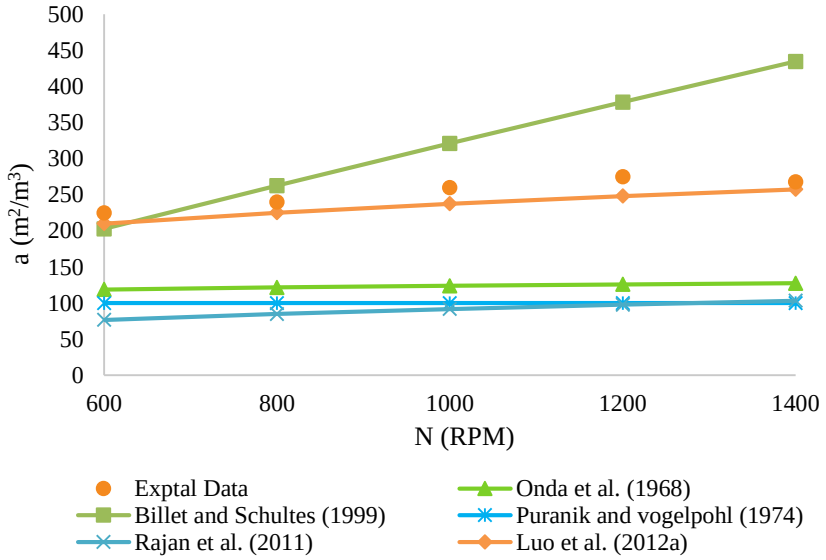
- The eNRTL model in Aspen Plus is used for thermodynamic modelling of the CO2-MEA-H2O system in the RPB
- Default binary interaction parameters of the eNRTL is unsuitable for concentrated MEA solution in RPBs
- Extensive regression conducted using data gathered from literature (Mason and dodge, 1935; Jou *et al*., 1995; Aronu *et al*., 2011)
- The predictions of the eNRTL model compared to experimental data

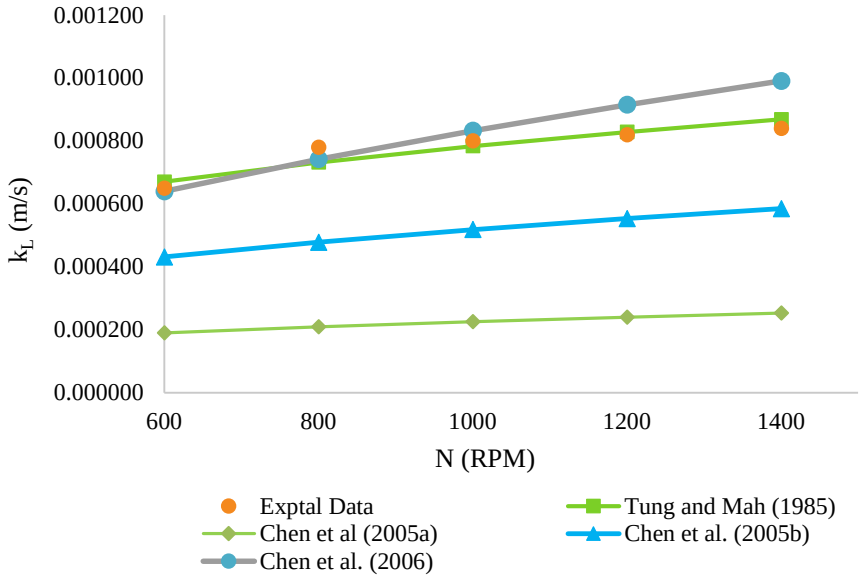
Mass transfer correlations

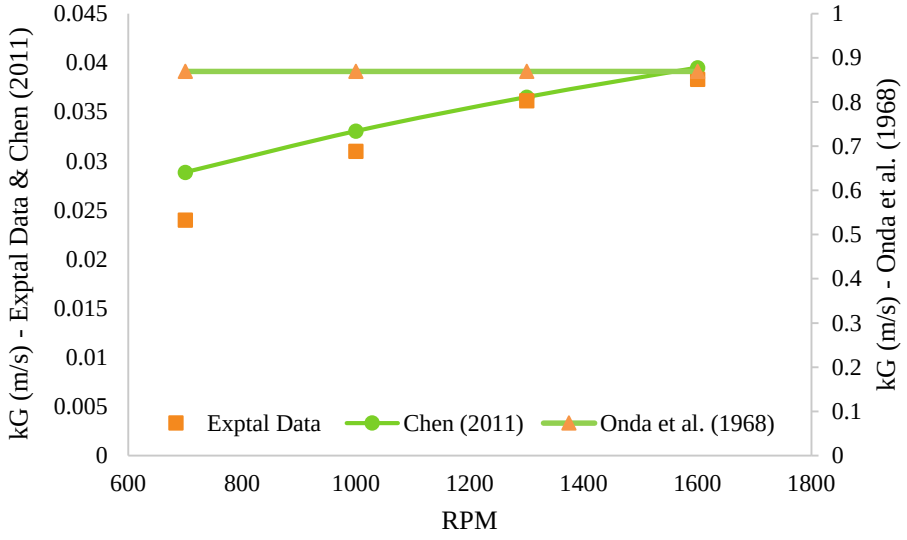
Model of RPB developed in gPROMS ModelBuilder used to test and compare mass transfer correlations:

- Effective interfacial area (including Onda et al. (1968), Billet and Schultes (1999), Puranik and Vogelpohl 91974), Rajan et al. (2011) and Luo et al. (2012))
- Liquid film mass transfer coefficients (including Onda et al. (1968), Tung and Mah 91985), Munjal et al (1989), Chen et al. (2006))
- Gas film mass transfer coefficients (including Onda et al. (1968), Chen 2011))

WP4: *Process modelling & performance assessment*







Key conclusion:

Modifying packed bed correlations such as Onda et al (1968) in RPB by replacing the "g" term (gravitational acceleration) with "$r\omega^2$" (centrifugal acceleration) do not result in good estimate of mass transfer parameters in RPBs

Thank you for your attention!