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Improving on the CCSI model for MEA-based CO₂ capture

Ryan Cownden, Mathieu Lucquiaud, & Jon Gibbins
University of Sheffield, UK

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Background

- Carbon Capture Simulation Initiative (U.S. DoE)
 - “gold-standard” MEA-CO₂ capture process model (2018)
 - publicly available Aspen Plus source file
 - widely used
- Underreported issues/limitations
 - interfacial area correlation – Weber dependence, Froude omitted
 - simplified chemistry
 - single packing – 250Y/252Y
 - regression based on limited dataset from lab-scale equipment

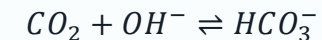
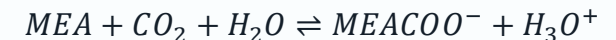
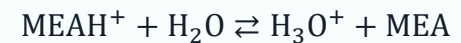
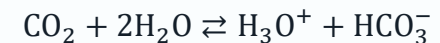
$$A_e = C_1 \left(\frac{We}{Fr} \right)^{C_2}$$

New model

- Thermodynamic/chemistry model
- Widely applicable correlations
- Validated v. large-scale pilot plants
 - 5 datasets
 - 4 facilities
 - wide range of operating conditions and scale
 - 0.1 – 78 tCO₂/d

Methodology

- Aspen Plus
 - full system model
 - rate-based absorber/regenerator
- ELECNRTL framework
 - rigorous chemistry
 - custom parameter regression v. VLE
 - 15-45%wt MEA, 40-120°C, 0.05-0.50 mol_{CO2}/mol_{MEA}
- Absorber CO₂ reaction kinetics
 - Hikita et al.
 - Pinsent et al.

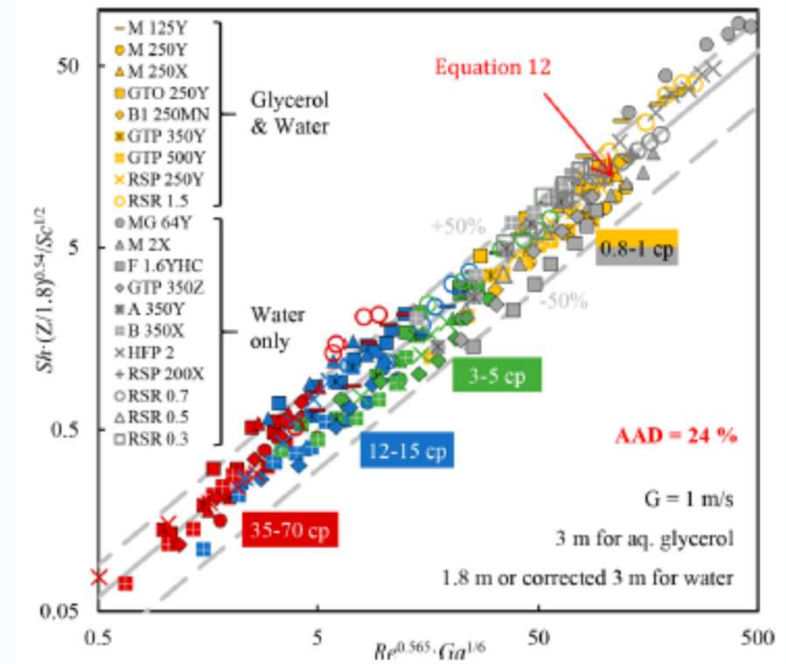


Hikita et al. (1977) – doi:10.1016/0300-9467(77)80002-6

Pinsent et al. (1956) - doi:10.1039/tf9565201512

Methodology

- Mass transfer coefficients & A_e
 - Song et al. (2018)
- Liquid holdup
 - Tsai (2010)
- Closed-loop model validation



k_L correlation v. experimental data from Song et al. (2018)

Song et al. (2018) – DOI: 10.1021/acs.iecr.7b04396
 Tsai (2010) – <http://hdl.handle.net/2152/ETD-UT-2010-05-1412>

Pilot plant data

	Stuttgart	NCCC	Haifeng	TCM
Captured CO ₂ (tCO ₂ /d)	0.11-0.16	4.9-7.8	38	49-80
Absorber liquid flux (m ³ /m ² -h)	6.1-20	9.7-35	7.0	3.9-7.8
Inlet vapour CO ₂ (%mol)	5.2-10.9	9.2-11	13	3.6-4.1
→ Rich loading (mol/mol)	0.30-0.42	0.28-0.39	0.50	0.48-0.53
CO ₂ capture rate	75-91%	93-98%	98%	86-97%
→ Absorber height (m)	4.2	6.1-12.2	15.9	24
Regenerator height (m)	2.52	12.2	8.52	9.6

Stuttgart: Notz et al. (2012) – doi:10.1016/j.ijggc.2011.11.004

NCCC: Morgan et al. (2018) – doi: 10.1021/acs.iecr.8b01472

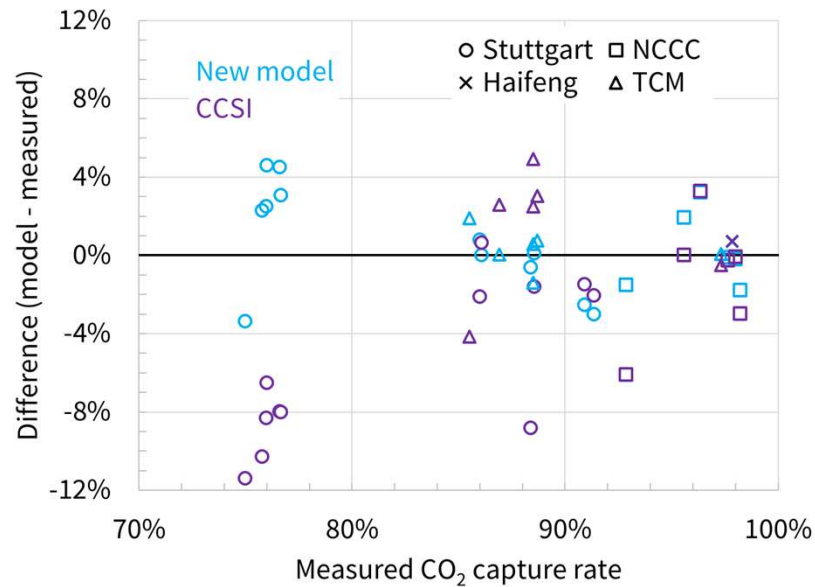
TCM: Faramarzi et al. (2017) – doi:10.1016/j.egypro.2017.03.1271

TCM: Bui et al. (2020) – doi:10.1016/j.ijggc.2019.102879

Capture rate predictions

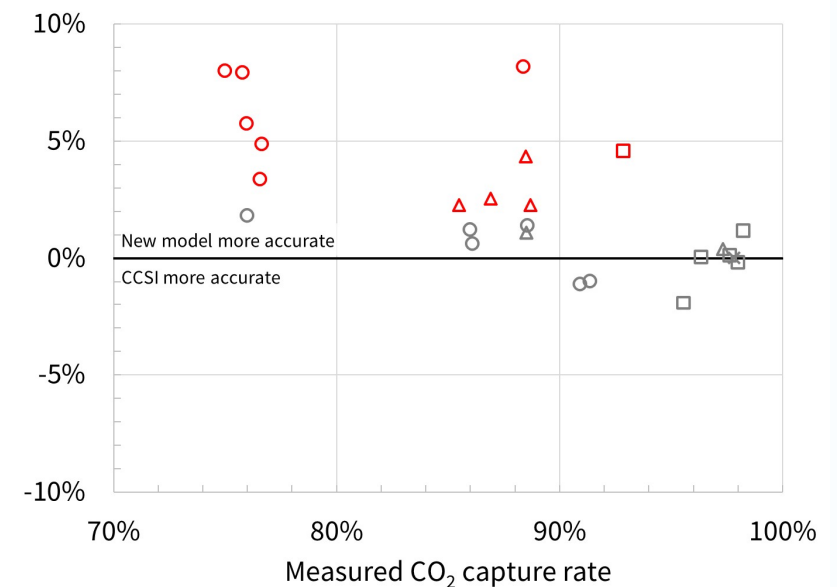
New model more accurately predicts capture rate

RMSD v. experimental data: 2.2 pp (new), 5.2 pp (CCSI)



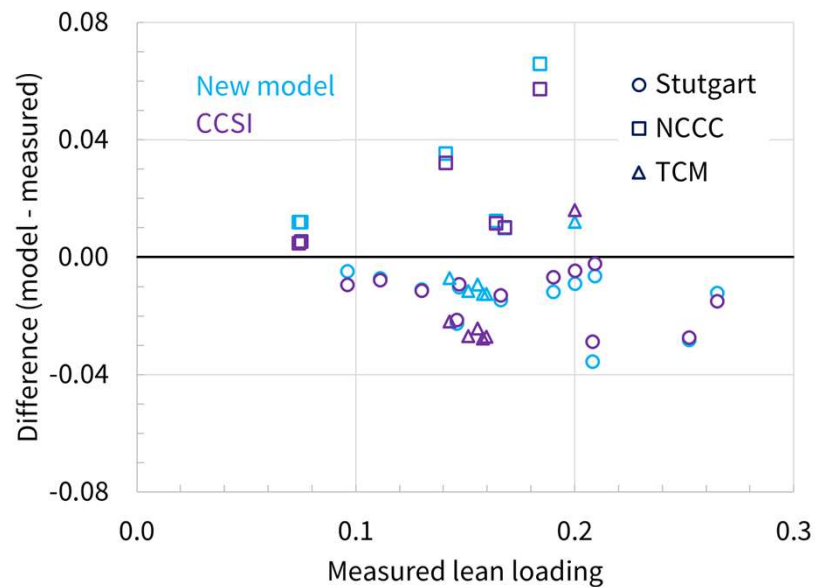
Substantial improvements for some conditions

Reduction in absolute deviation (pp) from experimental data v. CCSI

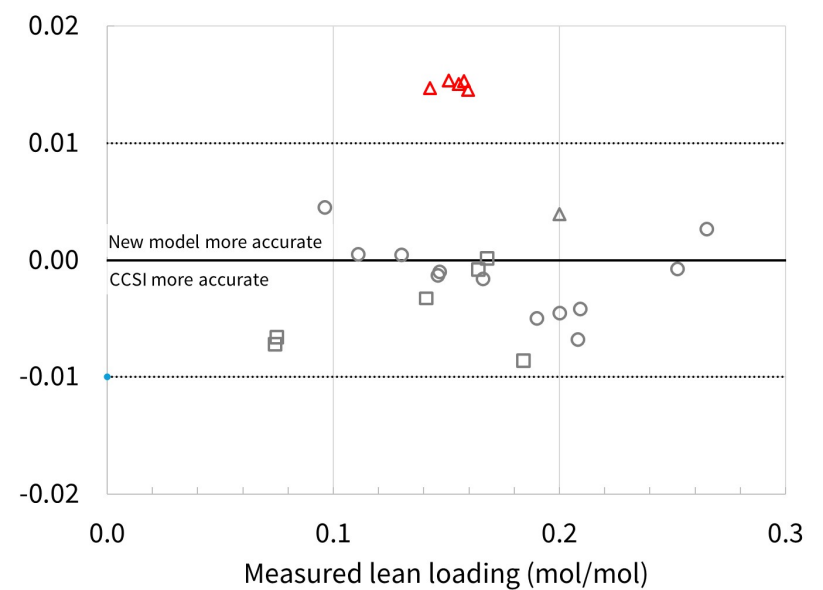


Lean loading predictions

New model & CCSI predict similar lean loadings
RMSD v. experimental data: 0.021 mol/mol (both)



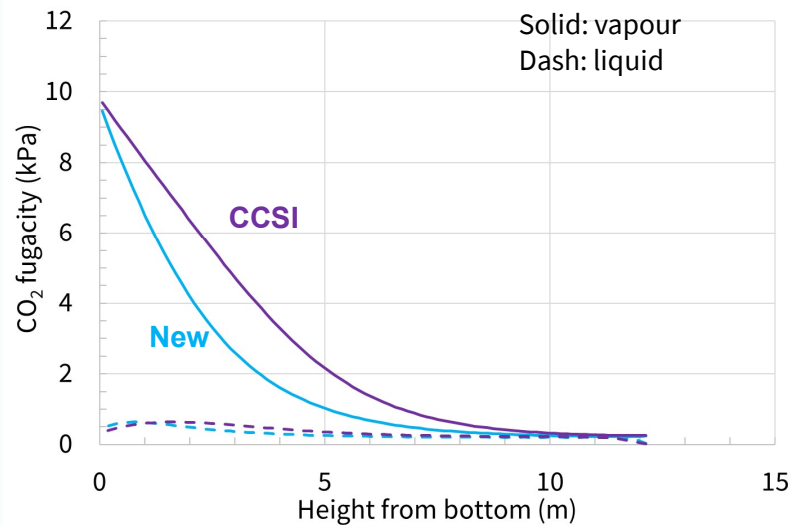
Most cases within 0.01 mol/mol, some TCM outliers
Reduction in absolute deviation (mol/mol) from experimental data v. CCSI



Column height

12m absorber – similar predicted capture rate
Loss of driving force constrains CO₂ capture

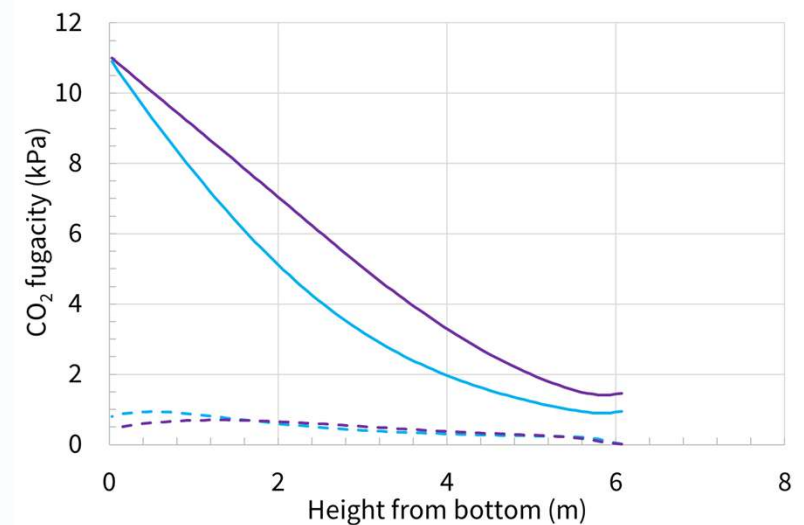
K17, 98% capture



Capture: 97.5% v 97.4%
Measured: 97.6%

6 m absorber – new model more accurate
CCSI mass transfer coefficients too low to predict CO₂ capture rate

K18, 93% capture

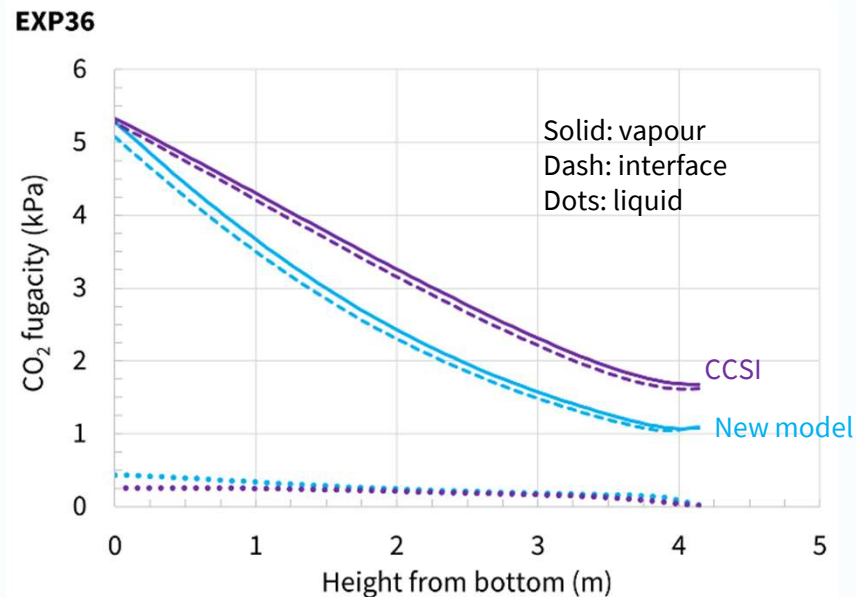


Capture: 91.4% v. 86.8%
Measured: 92.9%

- NCCC, 9/10%mol CO₂ gas inlet
- lean loading: c. 0.18 mol/mol
- same gas/liquid flow rates

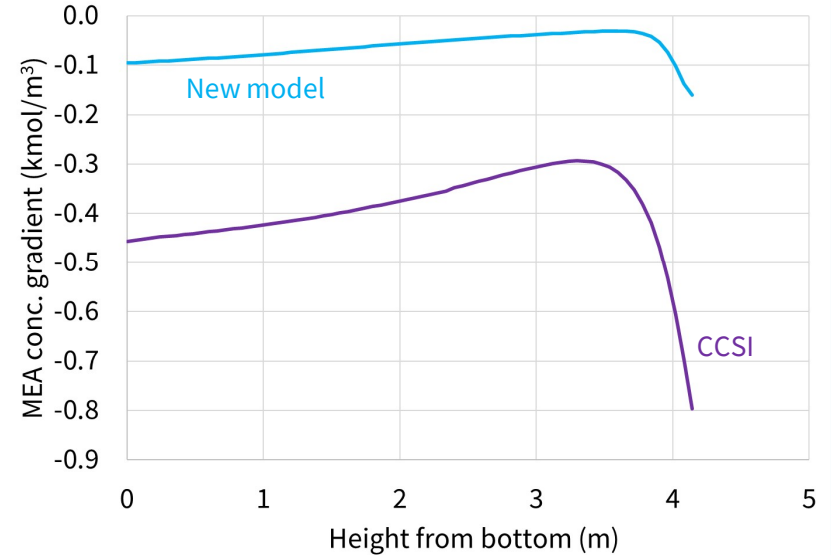
Liquid side mass transfer resistance

CCSI liquid mass transfer coefficients much lower
Leads to higher interface CO_2 fugacity, low capture rate predictions



- Stuttgart case 36: 5.3%mol CO₂ gas inlet
- lean loading: 0.224/0.225 mol/mol
- CO₂ capture rate: 79.7%/68.6% v. 76.6%

CCSI has larger liquid concentration gradients
Relative depletion of MEA at the interface

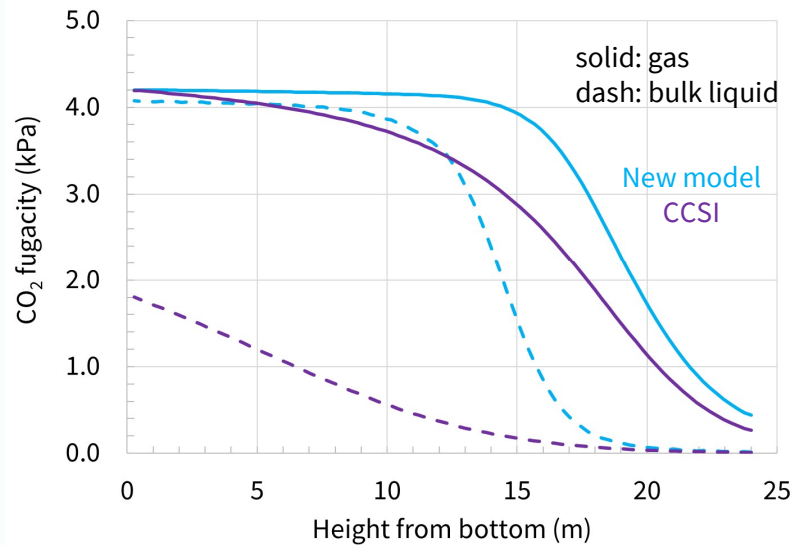


$$\Delta C = C_{\text{interface}} - C_{\text{bulk}}$$

Low temperature absorption

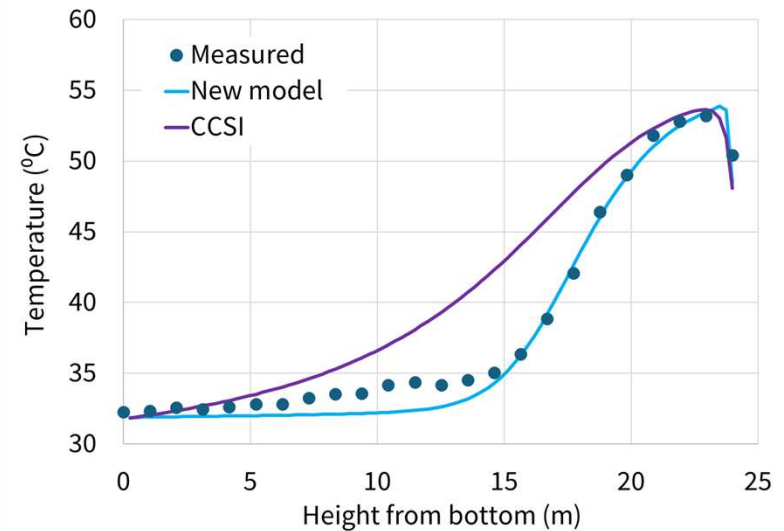
New model has slower reaction kinetics

Capture rate deviation: 0.6 pp (new model) v. 4.9 pp (CCSI)



Absorber temperature profile

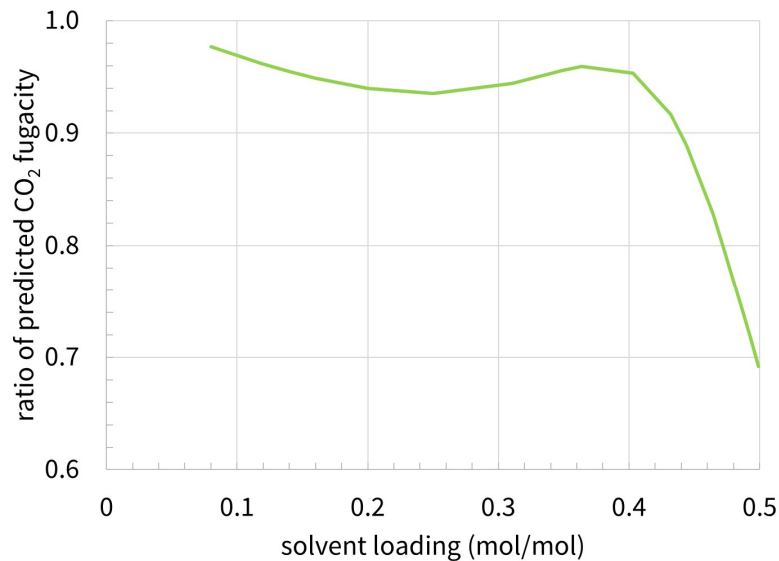
Corroborates new model reaction kinetics



- TCM (Bui et al. ICL11)
- 4.1%mol CO₂ gas inlet
- lean loading: 0.136/0.121 mol/mol
- CO₂ capture rate: 89.1%/93.4% v. 88.5%

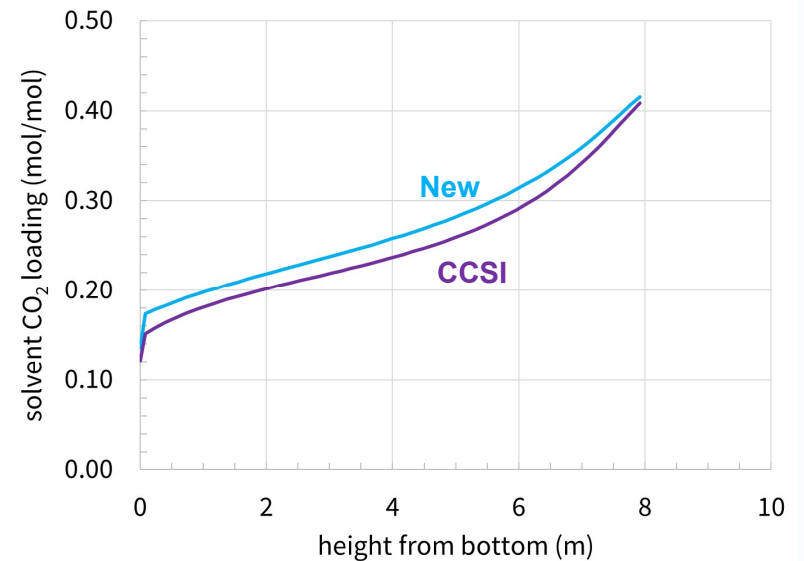
Regeneration – high rich load/temperature

New model predicts lower CO₂ fugacity @ 120°C



CO₂-MEA-water VLE
120°C, 30%wt MEA
Ratio of predicted CO₂ fugacity (new model/CCSI)

More accurate lean loading prediction
Less CO₂ flashing off at inlet, higher loading throughout



- TCM (Bui et al. ICL11)
- rich loading: 0.494/0.497 mol/mol
- lean loading: 0.136/0.121 mol/mol v. 0.143 (measured)

Concluding remarks

- New model predicts capture rate more accurately than CCSI
 - overall RMSD for CO₂ capture 2.2 pp v. 5.2 pp
- Substantial improvement for:
 - high rich solvent CO₂ loading + low gas CO₂ concentration
 - low absorber temperature
 - short columns
- Correlations more widely applicable
 - unconstrained by small sample regression
- Intend to publish model

Questions?

racownden1@sheffield.ac.uk

connect:

