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Solvent selection and design for CO_2 capture

How we might have been missing the point

4th Post Combustion Capture Conference

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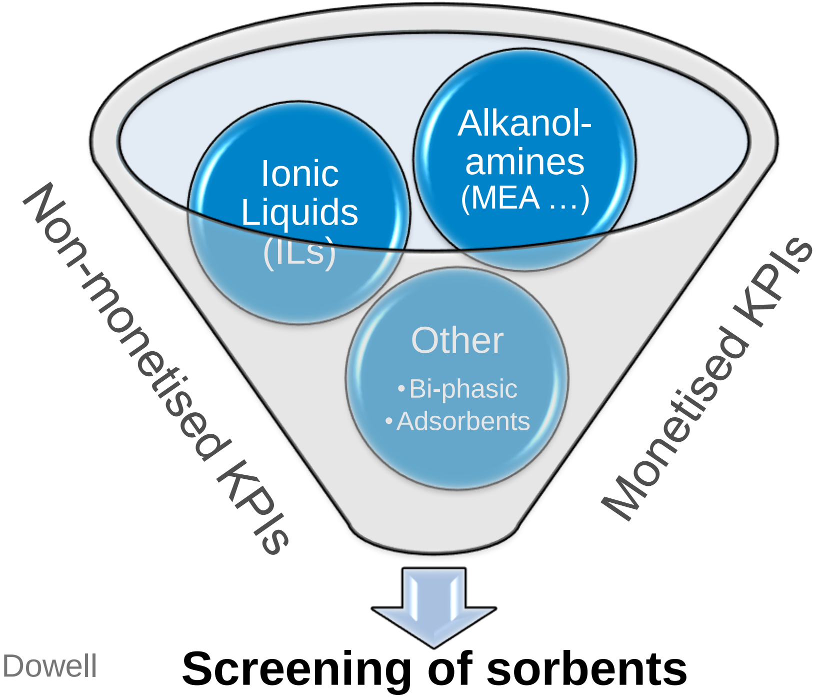
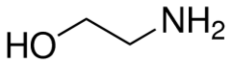


R&D scientist: "*We've developed a new solvent!*"

Properties	30wt% MEA*	New solvent
Equilibrium constant	0.015 kPa	1/3*MEA= 0.005 kPa
Viscosity	2.51mPa·s	3*MEA = 7.53mPa·s
All other properties	= new solvent	= 30wt% MEA

Is the newly developed solvent better than the standard (MEA)?

*MEA= Monoethanolamine 

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Solvent selection and design for CO_2 capture

How we might have been missing the point





Motivation: Gap between lab and field

Research Chemist

- Develops new CO_2 capture material
- Uses intuition to predict implications

Process Engineer

- Wants to reduce CO_2 footprint at best cost
- Needs to select process and solvent

Motivation: Focus on energy

Research Chemist

- Develops new CO_2 capture material
- Uses intuition to predict implications

- Thousands of new materials having been proposed
- Focused on developing solvents with either increased CO_2 capacity and/or reduced heat of regeneration
- Cost $\$/\mathrm{MWh}$ or $\$/\mathrm{ton}_{\mathrm{CO_2}}$ is composed of CAPEX* and OPEX*
- Focusing on CO_2 capacity and heat of regeneration excludes the contribution of transport and kinetic properties which determine equipment size and thus capital cost
- Reducing the energy demand ($\mathrm{GJ}/\mathrm{ton}_{\mathrm{CO_2}}$) of the capture process does not necessarily reduce the overall cost ($\$/\mathrm{ton}_{\mathrm{CO_2}}$)

→ Essential to move beyond equilibrium-based metrics of solvent performance

*CAPEX=Capital Expenditure, OPEX=Operating Expenditure

Screening model closes gap between lab and field

Research Chemist

- Develops new CO_2 capture material
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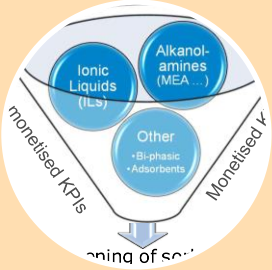


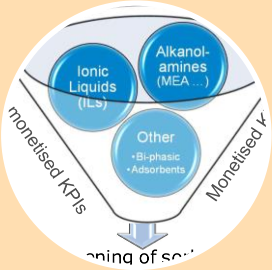
Rapid screening

- Bridges gap between lab and application
- Analyses process cost implications

Process Engineer

- Wants to reduce CO_2 footprint at best cost
- Needs to select process and solvent

Screening model closes gap between lab and field



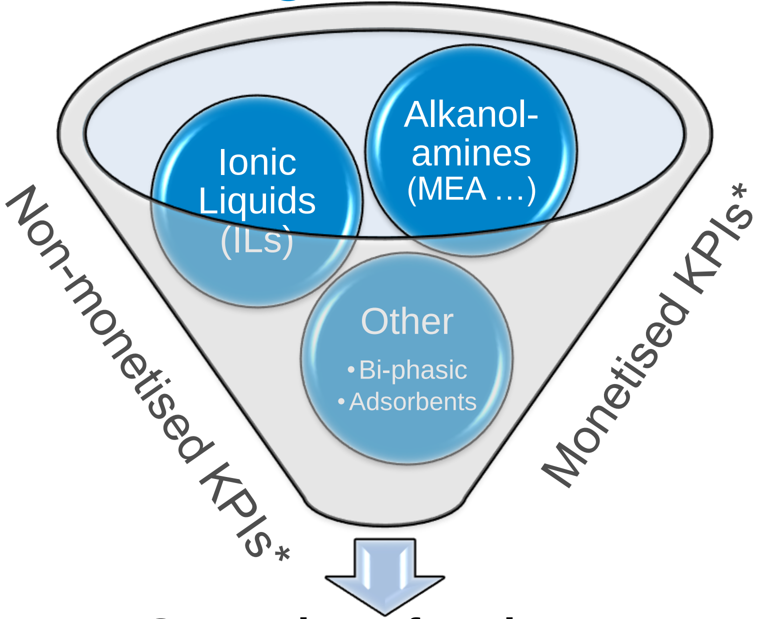
Rapid screening

- Bridges gap between lab and application
- Analyses process cost implications

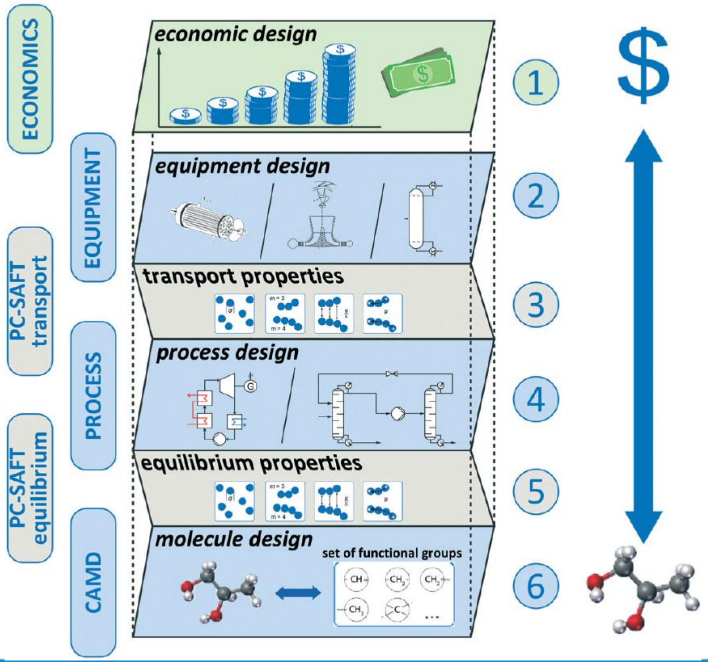
- It typically takes several decades for a technology to move "out of the lab"
- Screening approach will allow technologies to "fail quickly", thus avoiding years of costly experimentation and enables process engineers to quickly identify most promising technology
- Solvent screening uses both monetised and non-monetised performance indicators

- Challenges:
  - Identifying the minimum set of thermophysical and kinetic parameters which must be reported for evaluation
  - Dealing with uncertainty (incomplete data sets)

Screening model



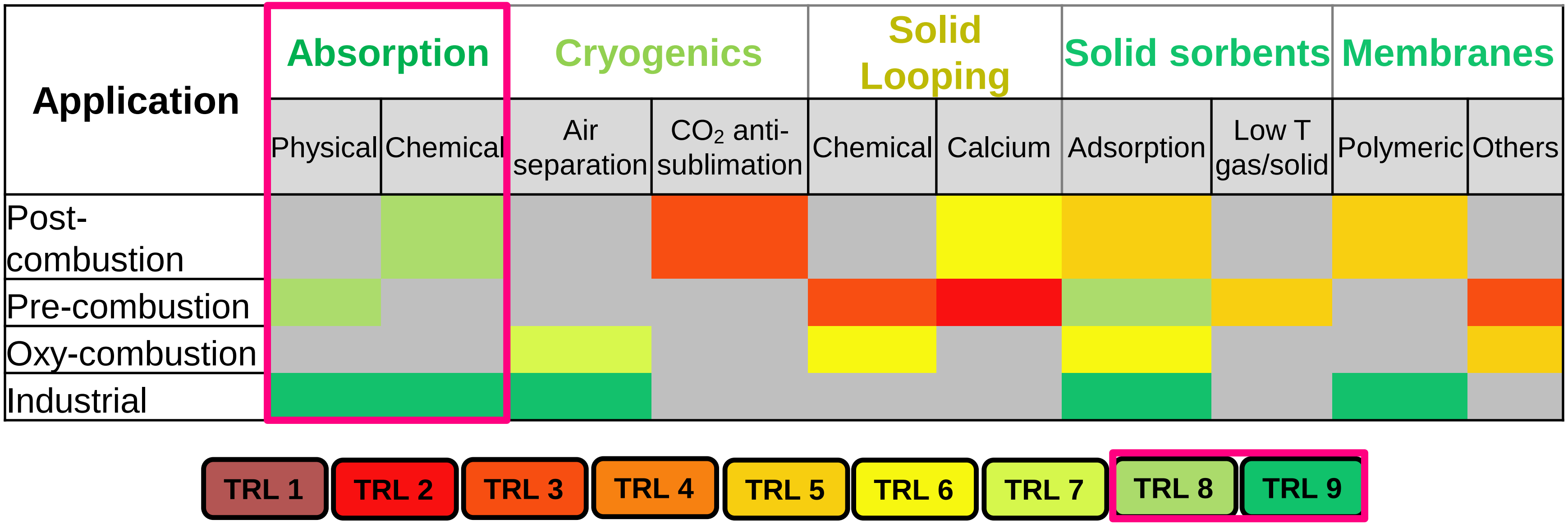
Screening of sorbents



*KPIs= Key Performance Indicators

Right figure from J. Schilling et al., *Mol. Syst. Des. Eng.*, 2017

TRL* of carbon capture technologies

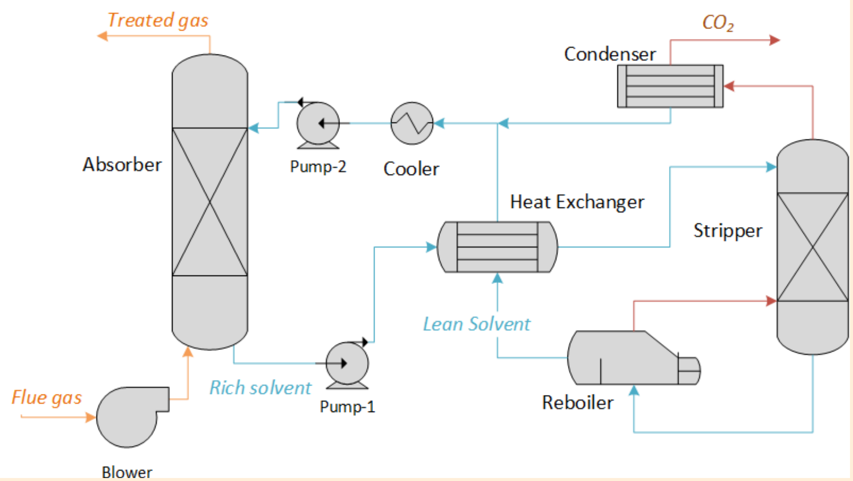


*TRL= Technology Readiness Level

Source: Abanades et al. (2015) - Emerging CO_2 capture system, Int. J. GHG Contr. 40 126-166

Approach: Rigorous process model for solvents

PFD* solvent-based CO_2 capture unit



Bespoke thermodynamic unit modelling

- Absorber
- Reboiler
- Heat exchanger
- Stripper
- Condenser
- Pumps, Blower, Mixer

Implemented in PSE's gPROMS®

*PFD = Process Flow Diagram

Interaction of model with solvent data and properties

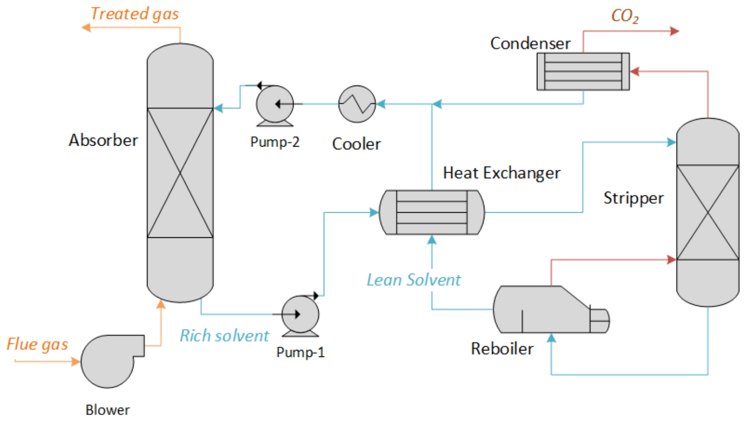
Solvent data

Minimum required properties

- Equil. CO_2
- Density
- Reaction constants
- Surface tension
- Viscosity
- Heat capacity
- Thermal conductivity

Input

Process and economics model



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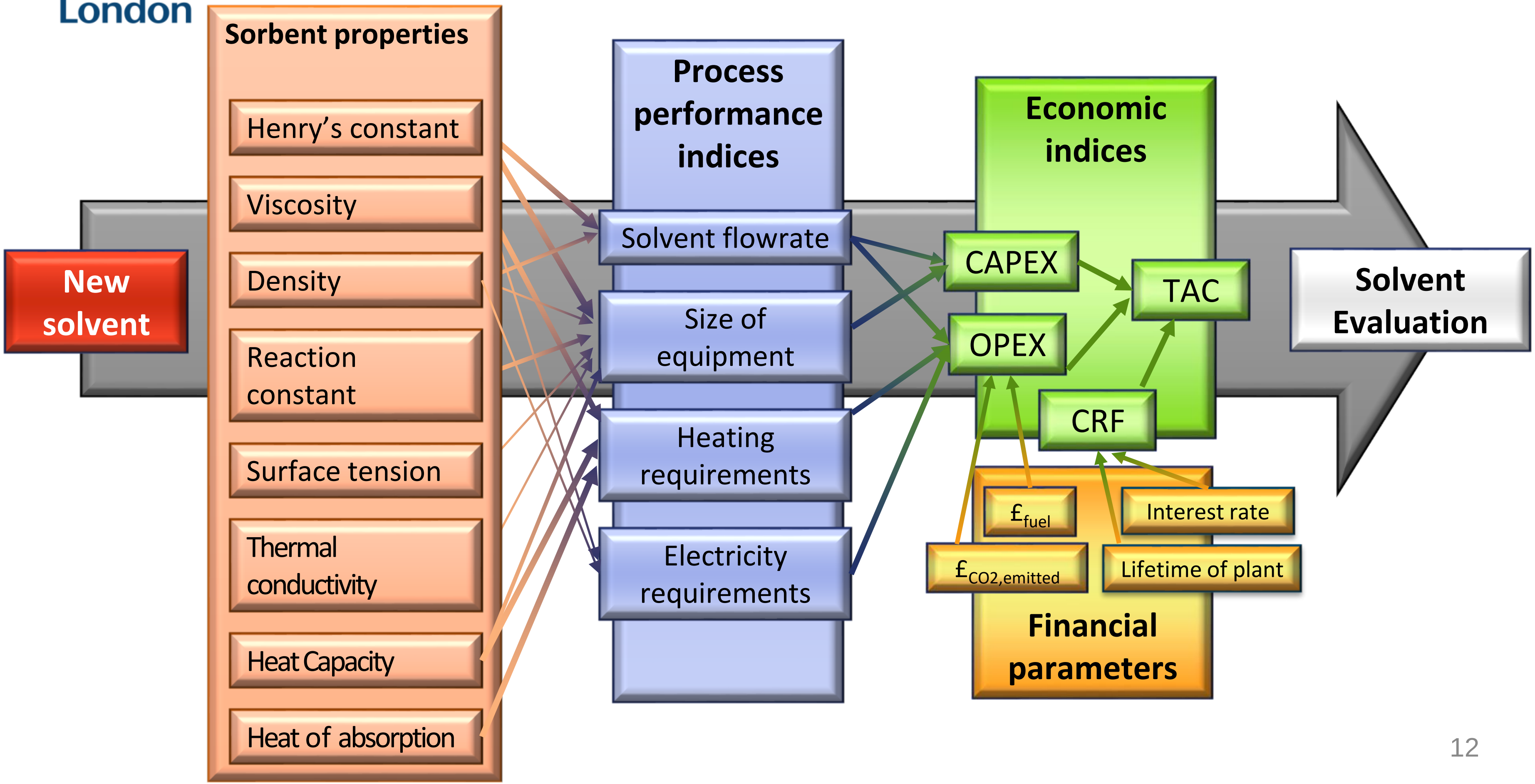


Details of thermodynamic model

$$k_L^0 \left(\frac{\rho_t^L}{\mu_L g}\right)^{1/3} = 0.0051 \frac{Re_L'^{\,2/3} (a_p d_p)^{0.4}}{Sc_L^{0.5}}$$

$$A_t = \frac{(p_t - d_0) D_s l_B}{p_t}$$

$$d_e = \frac{1.10}{d_0}\left(p_t^2 - 0.917 d_0^2\right)$$

Wilke-Chang equation: $D_{i,j}^0 = 7.4\ 10^{-8} \frac{(\phi M_i)^{1/2} T}{\eta_i V_j^{0.6}}$

Perkins and Geankoplis equation $D_i \mu^{0.8} = \sum_{j=1}^{n} x_j D_{i,j}^0 \mu^{0.8}$

laminar

$$Nu_t = 1.86 \left(Re_t\ Pr_t\right)^{\frac{1}{3}} \left(\frac{d_{in}}{L_{tube}}\right)^{\frac{1}{3}} \left(\frac{\mu}{\mu_w}\right)^{0.14}$$

turbulent

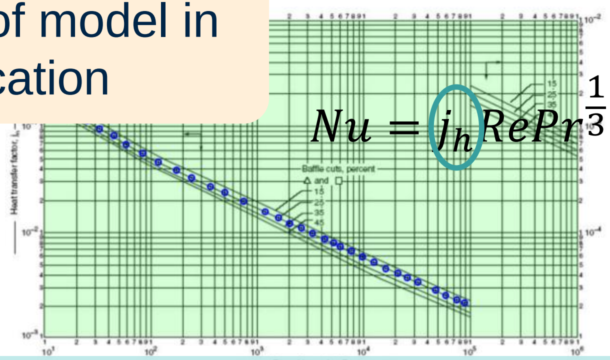
$$Nu_t = C\ Re_t^{0.8} Pr_t^{1/3} \left(\frac{\mu}{\mu_w}\right)^{0.14}$$

$$Re_t = \frac{u_t d_i \rho}{\mu}$$

$$Pr_t = \frac{Cp_t \mu}{k}$$

$$Nu_t = \frac{h_t d_i}{k}$$

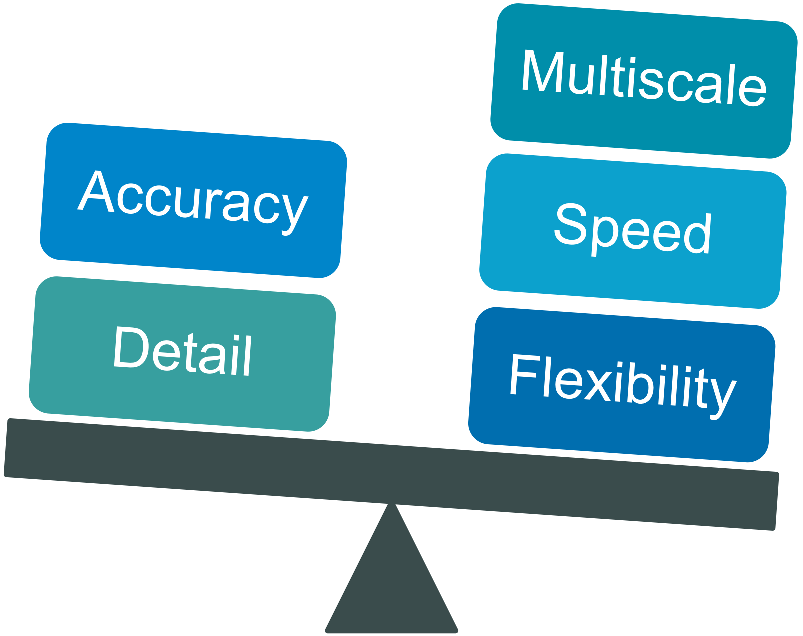
Detailed description of model in upcoming publication



$$Nu = j_h Re Pr^{\frac{1}{3}} \left(\frac{\mu}{\mu_w}\right)^{0.14}$$

$$\log_{10} j_H = -0.4714 \log_{10} Re - 0.4305$$

Trade-off: Flexibility and speed are main priorities



Economic indices

Capital Expenditure (CAPEX)

Correlations based on key characteristics of each unit.[1]

- E.g.: Heat exchangers → Area, material
- Annualised cost using the Capital Recovery Factor (CRF)

$$CRF = \frac{i(1+i)^n}{(1+i)^n - 1}$$

i = interest rate (10%)
n = years (25 years)

Operating Expenditure (OPEX)

- Energy requirements (MW) ≠ Electricity (MW) + Heat (MW)
- Short-Run Marginal Cost (SRMC) for the production of electricity and for the production of heat

$$\frac{\$^{SRMC}}{\mathrm{MWh}} = \frac{\$^{\mathrm{MWh}}_{\mathrm{fuel}}}{\eta_{\mathrm{plant}}} + \left(\frac{\$}{\mathrm{ton}_{\mathrm{CO_2}}} \cdot CI^{\mathrm{ton}_{\mathrm{CO_2}}}_{\mathrm{MWh}}\right) + \$_{\mathrm{O\&M}} + \$^{\mathrm{CO_2}}_{\mathrm{T\&S}}$$

Total Annualised Cost (TAC)

- $\mathrm{TAC} = CRF \cdot \sum_k^{\mathrm{units}} CAPEX_k + \sum_l OPEX_l$

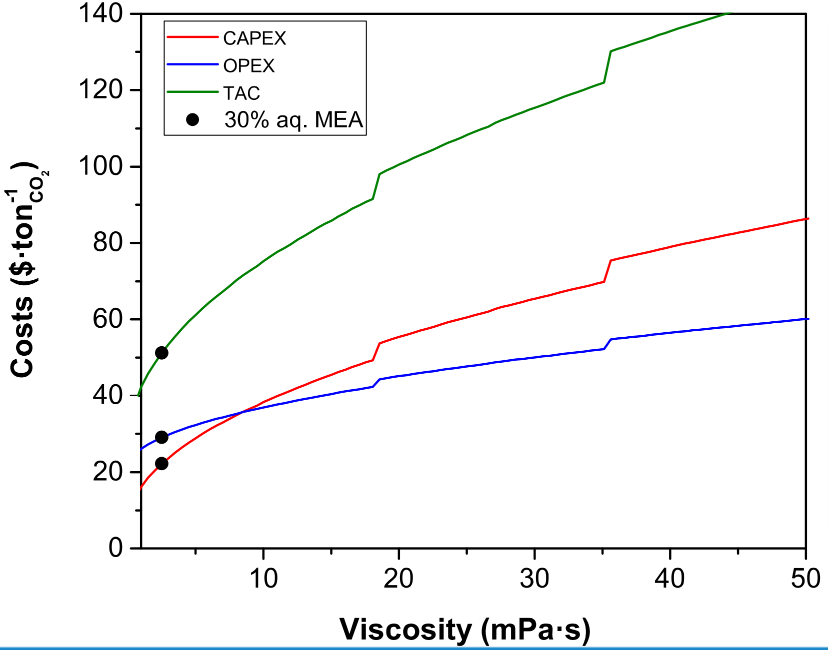
"Total cost of ownership"

J.R. Couper, W. R. Penney and J.R. Fair, Chemical process equipment revised selection and design, 2009 Gulf Professional Publishing.

Sensitivity analysis: Impact of properties on process

Key Operating Parameter (KOP)	Sensitivity study
• Flue gas: $900\frac{\mathrm{kg}}{\mathrm{s}}$, 12mol-% CO_2 725MW_g supercritical pulverized coal fired power plant • Capture rate: 90% CO_2 emitted by power plant captured • Lean loading=$0.31\frac{\mathrm{mol}_{\mathrm{CO_2}}}{\mathrm{mol}_{\mathrm{binder}}}$ • Absorber: 40°C, 1.1bar	• Single property of solvent is varied while others are fixed, *e.g.*, solvent's viscosity is increased and density, heat capacity, *etc.* stay constant • Properties depend on temperature • Fixed KOP → Effect on process performance → Effect on costs (CAPEX, OPEX, TAC)

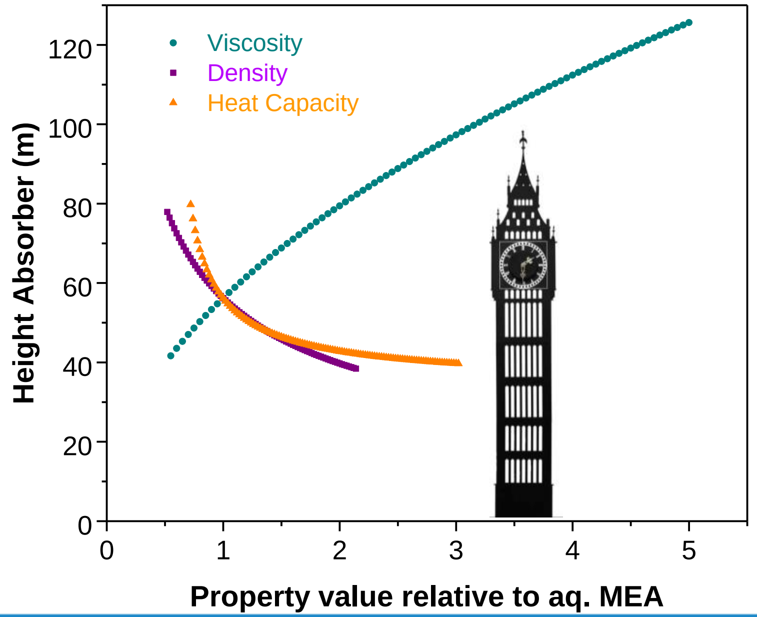
Results: Effect of changing viscosity on costs



Increasing viscosity

- hinders mass transfer of gas into liquid
  → Longer contact times required
  → Taller columns
- lowers Reynolds number
  → Reduces heat transfer in exchangers
  → Transition from turbulent to laminar flow
  → Steps in costs (lean solvent cooler and main heat exchanger)

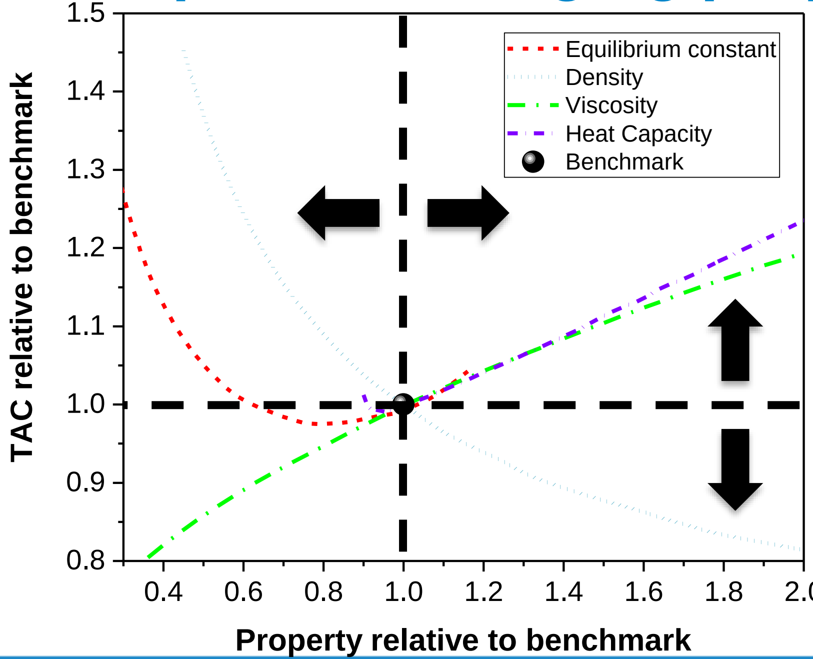
Results: Impact on height of absorber



Sensitivity study identifies limits

- If a new solvent has a high viscosity, it needs to offset the negative impact by reducing the required solvent flowrate. →trade-offs
- World's tallest distillation column ≈ 120m

Results: Relative impact of changing properties on TAC

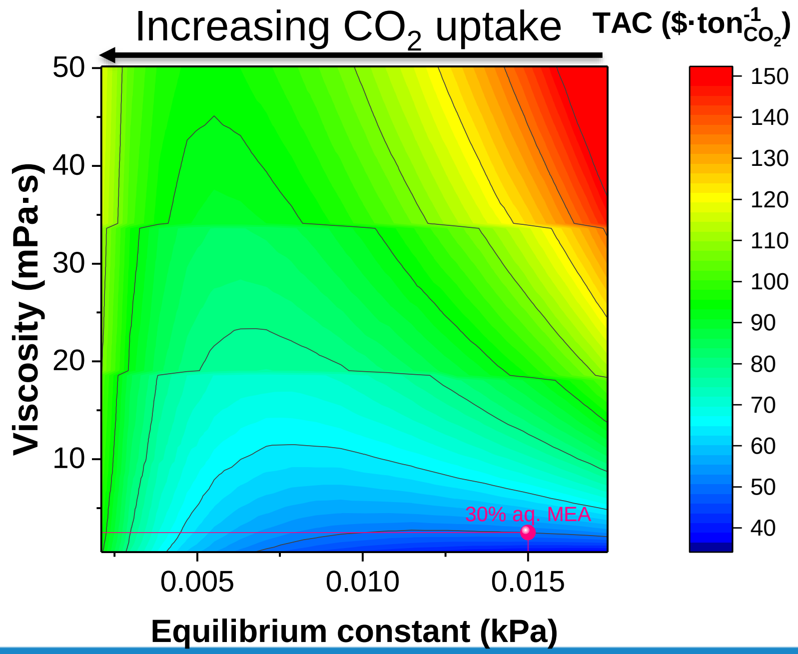


Increased capture cost

Decreased capture cost

*Benchmark= 30wt% MEA

Results: Two-dimensional impact on TAC



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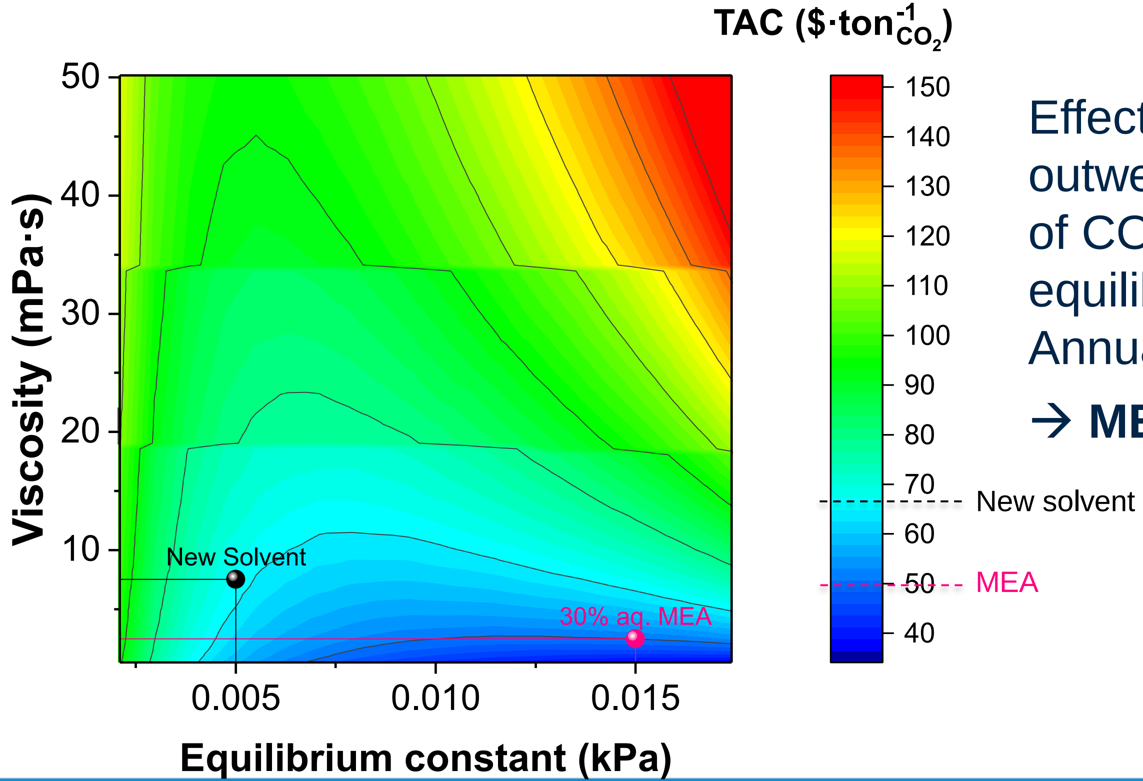
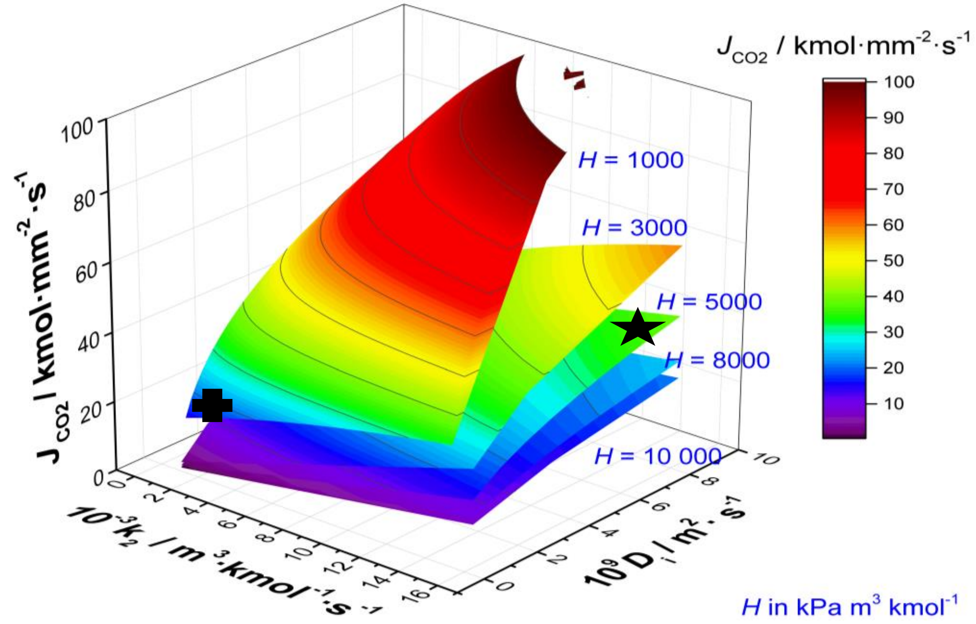


Effect of increasing viscosity outweighs beneficial increase of CO_2 uptake (decreasing equilibrium constant) on Total Annualised Costs (TAC)

→ **MEA is better solvent**

Results: Molar flux J_{CO_2} across the vapour-liquid interface



A lower soluble solvent (★) might present improved molar flux if its diffusivity is favoured over the more soluble solvent (✚).

Diffusivity (D_i) Reaction constant (k_2) Henry's constant (H)

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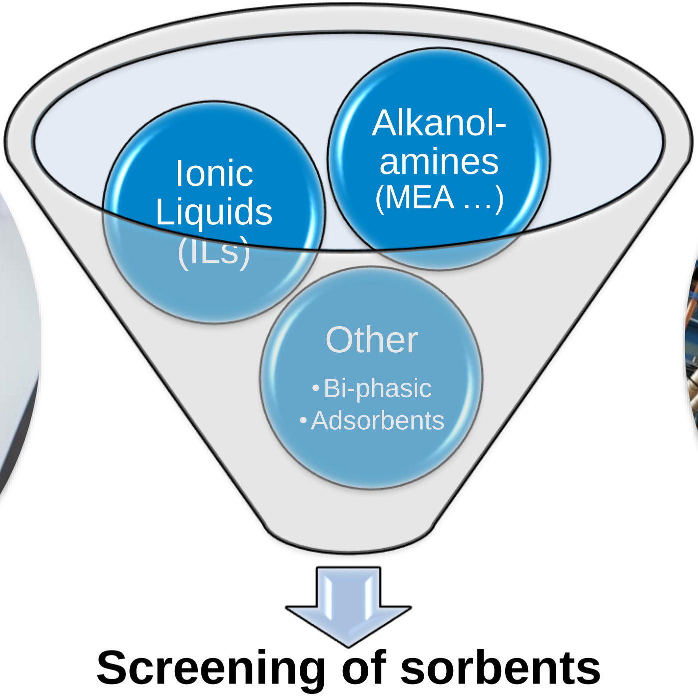
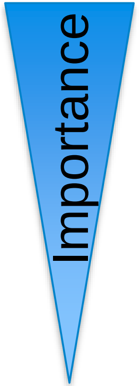
Summary



Conclusions: Holistic approach needed

- Historically focused on enhancing the CO_2 absorption and reducing the heat of reaction, neglecting the effect of the other properties on the process cost
- Properties that have a primary importance on the TAC of CO_2 capture are:



1. Viscosity
2. Equilibrium loading of CO_2
3. Reaction kinetics
4. Heat capacity
5. Heat of absorption
6. Density
7. Surface tension

*TAC=Total Annualised Cost

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