Thermodynamic modelling of nonaqueous carbon capture systems with the s-SAFT-γ Mie EoS

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Introduction

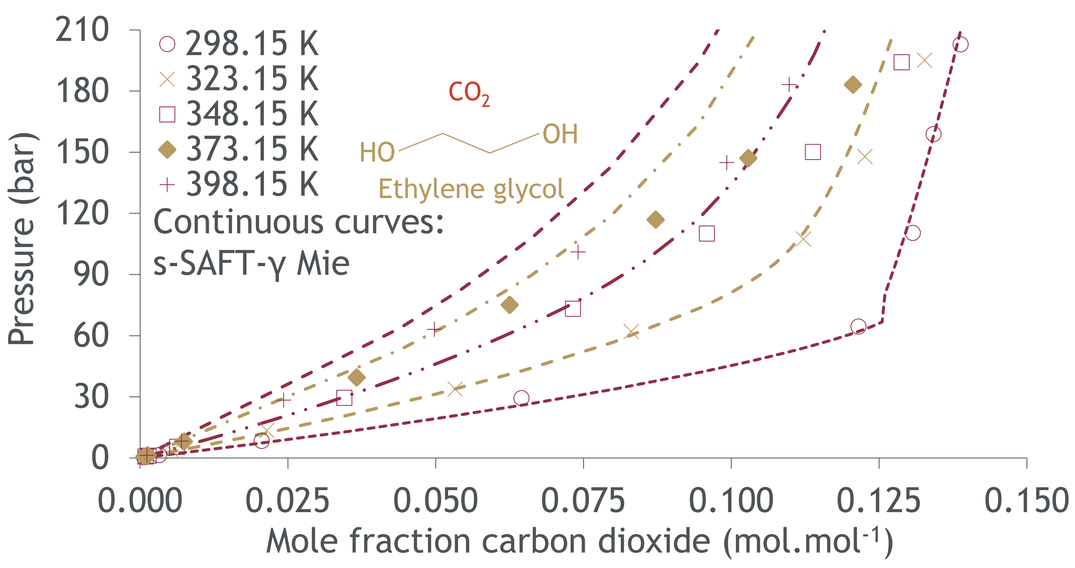
- Carbon capture by means of post-combustion chemical absorption of CO_2 with alkanolamines is a mature and promising technology for urgently-needed decarbonisation of heavy industry and fossil-fuel fired power stations
- However, high energy requirements remain a key hurdle for wide-scale adoption of the technology
- Use of nonaqueous carbon capture fluids is a promising route for reducing energy requirements of current post-combustion carbon capture processes

Motivation and aim

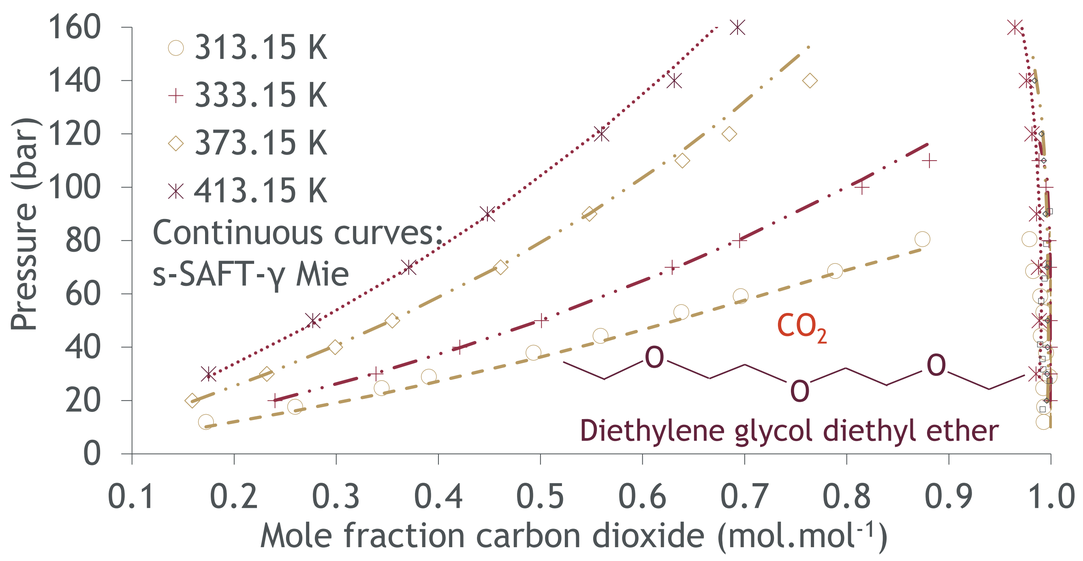
- Experimental determination of an optimal nonaqueous alkanolamine is highly impractical
- Aim: Develop a predictive thermodynamic modelling tool for use in screening nonaqueous fluids for use in alkanolamine-based carbon capture
- This entails parameterising the s-SAFT-γ Mie EoS towards describing alkanolamine/CO_2/organic systems according to a systematic and consistent approach

Results: binary systems

- Unique parameters required for the CH_2OH group in glycols, and for glycol/CO_2 systems, as shown[1]



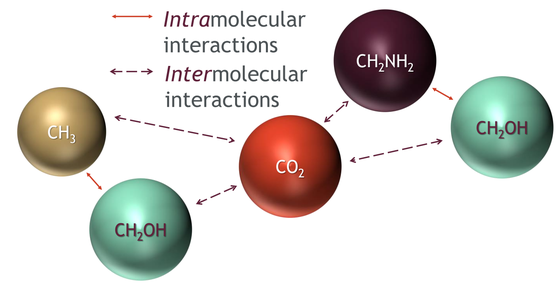
- Accurate description of highly asymmetric diethylene glycol dibutyl ether/CO_2 system, as shown[2]



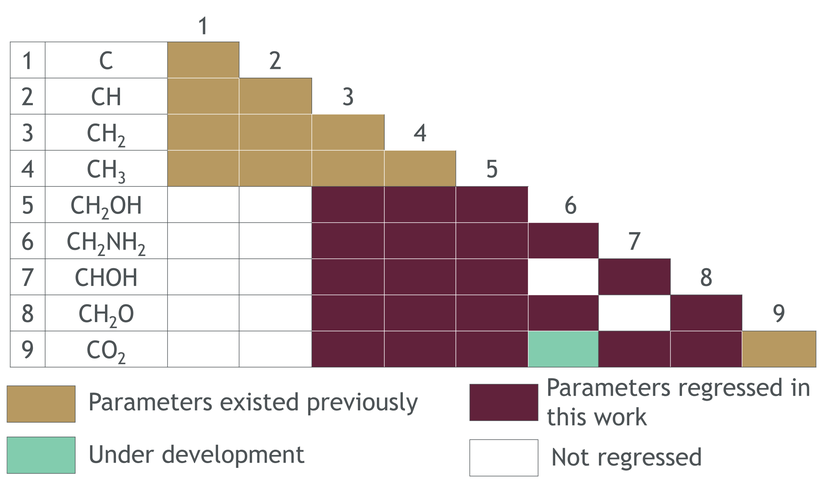
- Parameters regressed to pure and binary mixture data transferred to ternary-component systems

The s-SAFT-γ Mie equation of state

- Group-contribution approach → inherently predictive

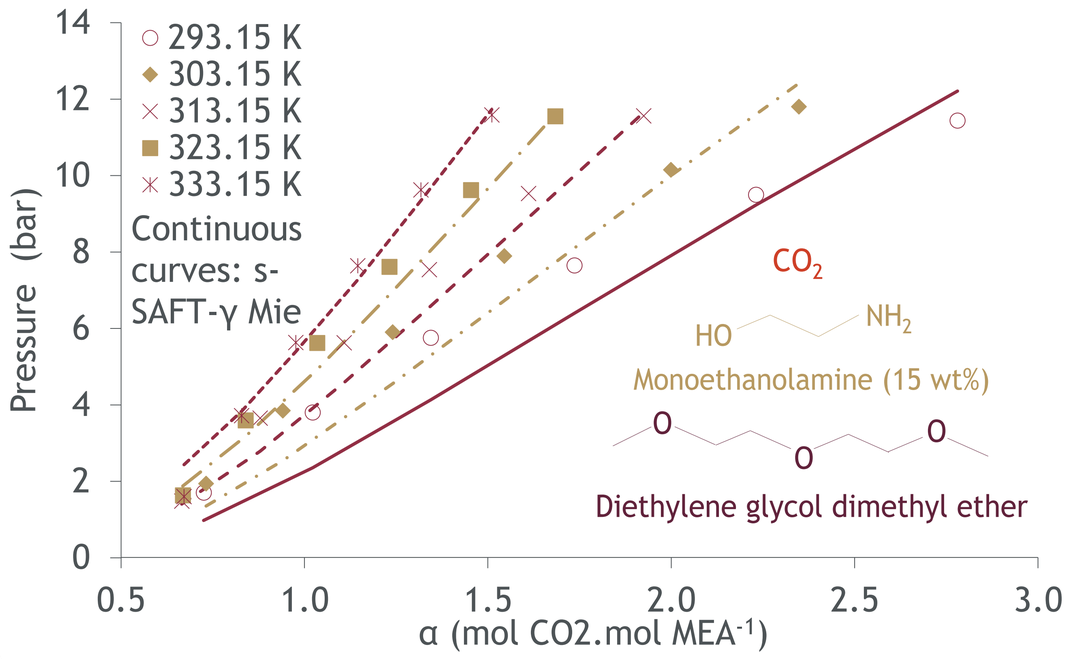


- EoS still in its infancy, as evidenced by parameter matrix shown below



Results: ternary systems

- Qualitatively accurate model description of CO_2 solubility, as shown[3]
- This is expected, given the model's predictive nature and the complexity of the ternary system



Key preliminary conclusions

- Unique parameters required for glycols
- s-SAFT-γ Mie provides robust descriptions of thermodynamic systems related to nonaqueous alkanolamine-based carbon capture → good foundation for a predictive modelling tool

References: [1] Jou *et al*. Chem. Eng. Commun. 1990;87(1):223-231. [2] Lin *et al*. Fluid Phase Equilib. 2003;209:131-145. [3] Huang *et al*. Ind. Eng. Chem. Res. 2015;54(13):3430-7.

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