Imperial College London, Department of Chemical Engineering

Advanced Process Optimisation

Project description

October 2024

Problem description

Developing suitable solvents for carbon capture is crucial for addressing the global challenge of reducing greenhouse gas emissions, particularly carbon dioxide (CO_2), from industrial processes and power generation. It is a challenge to identify such solvents due to the vast number of potential molecules. In this project, your task is to use computer-aided molecular design (CAMD) principles to suggest suitable solvents for a chemisorption-based carbon capture process. A good solvent should provide good process performance (e.g., meeting purity and throughput constraints), minimise environmental impact (e.g., solvent losses, energy use), have a positive societal impact (e.g., be safe for operators and the local population), and maximise economic performance (e.g., low capital and operating costs). It is difficult to formulate a CAMD problem that captures all these aspects, so you are asked to consider the following representative properties as a basis for your design:

(a) The relative energy difference (RED) is calculated from the solubility parameter, which is used as a measure of miscibility. Minimisation of RED of the solvent is required for higher dissolution of a particular solute (here CO_2), and should preferably be less than 1.

(b) The liquid heat capacity (C_p) plays an important role in determining the heat required to regenerate the amine-based solution during desorption. Thus, solvents with a low C_p are preferred to reduce the sensible heat requirements.

(c) The liquid density (ρ) plays an important role in determining the solvent flow rate, equipment size and pumping power requirements; a solvent with high ρ is required.

The following conditions should also be met by any solvent candidate:

(e) The solvent's normal melting temperature, T_m, should be less than the average temperature of the absorption column, T_Abs (313 K), to avoid solvent solidification.

(f) The solvent's normal boiling temperature, T_bp, should be higher than the average temperature of the desorption column, T_des (393 K), to avoid excess vaporization of the pure solvent.

Assignment

In a pair, complete the following tasks:

1. Develop a mathematical formulation for the design problem. For the objective function, you can use a weighted sum of the properties in (a)-(d), with equal weight given to each property. Please note that you may need to scale some properties for the optimisation problem formulation. Use the method of Hukkerikar et al. [1] to estimate the melting temperature, boiling temperature, density and RED. Use the method of Joback and Reid [2,3] to calculate the heat capacity. Justify your choice of building blocks (atom groups) to include in your design space.

2. Implement the mathematical formulation in GAMS and identify an optimal solvent, with a solver of your choice. Comment on the performance of the solver and reliability of the solution.

3. Using 5 different weight vectors for the objective function, generate alternative solutions to the CAMD problem and comment on their suitability.

4. Propose three additional constraints that you could use to improve the mathematical formulation to obtain more likely candidate solvents, explaining why you have chosen these constraints and specifying what equations should be added to the formulation. Do not implement them.

5. Write a report of no more than 10 pages on your findings. Use margins of 2.5 cm throughout, a line spacing of 1.2- and 11-point Arial font.

Submit your report (one report per pair) and your GAMS file on Blackboard by 4 pm on 17 December 2024. Your GAMS file should include an initial guess and local solver that ensures convergence to a solution.

Note that there are previous works using CAMD to design solvents for carbon capture [4,5] but you should come up with your own formulation and explain your choices.

Marking Scheme (out of 25)

Question	Key Criteria	Marks
1	Is the mathematical formulation correct and explained clearly?	5
2	Is the GAMS file correct? Are the results and interpretations explained clearly?	5
3	Are 5 weight vectors investigated? Does the discussion demonstrate an understanding of multi-objective optimisation? Is the discussion of the solvents identified insightful?	5
4	Are the three constraints relevant and explained clearly?	5
5	Is the standard of English in the report of high quality? Is the report well structured?	5

References

1. A. S. Hukkerikar, B. Sarup, A. Ten Kate, J. Abildskov, G. Sin, and R. Gani, "Group-contribution+ (GC+) based estimation of properties of pure components: Improved property estimation and uncertainty analysis," *Fluid Phase Equilib*, vol. 321, pp. 25–43, 2012, doi: https://doi.org/10.1016/j.fluid.2012.02.010.
2. K. G. Joback and R. C. Reid, "Estimation of pure-component properties from group-contributions," *Chem Eng Commun*, vol. 57, no. 1–6, pp. 233–243, 1987, doi: https://doi.org/10.1080/00986448708960487
3. N. V Sahinidis, M. Tawarmalani, and M. Yu, "Design of alternative refrigerants via global optimization," *AIChE Journal*, vol. 49, no. 7, pp. 1761–1775, 2003, doi: https://doi.org/10.1002/aic.690490714.
4. A. I. Papadopoulos *et al.*, "Computer-aided molecular design and selection of CO2 capture solvents based on thermodynamics, reactivity and sustainability," *Mol. Syst. Des. Eng.*, vol. 1, no. 3, pp. 313–334, 2016, doi: https://doi.org/10.1039/C6ME00049E.s
5. Y. S. Lee, E. J. Graham, A. Galindo, G. Jackson, and C. S. Adjiman, "A comparative study of multi-objective optimization methodologies for molecular and process design," *Comput Chem Eng*, vol. 136, p. 106802, 2020, doi: https://doi.org/10.1016/j.compchemeng.2020.106802.