

Greener Solvent Selection and Solvent Recycling for CO₂ Capture

Economically removing CO₂ from the flue gases of coal-fired power plants would alleviate concerns about their contribution to global climate change. CO₂ can be removed by several methods including absorption using solvents, adsorption onto solid sorbents, pressure or temperature swing adsorption, cryogenic distillation and membrane separation. Of these methods absorption by solvents is considered to be highly promising. Amine solvents are currently used to remove CO₂ from dilute gas streams because they have very high affinity for CO₂. Unfortunately high affinity for CO₂ makes solvent recovery for reuse very expensive [1, 2]. This project's goal is to find new solvents that balance high affinity for CO₂ with ease of solvent recovery and reuse. Because the number of candidate solvents and solvent blends is very large, a purely experimental search is impossible. In recent years, researchers have demonstrated the advantage of integrating computational solvent design with computational process synthesis to guide the experimentation needed to find new solvent absorption processes possessing good environmental and economic performance[3]. This project presents a coupled solvent selection and process synthesis approach to identify a cost-effective, environmentally friendly technology for CO₂ capture, separation and solvent recovery. Integrating solvent design and process synthesis poses the challenging problems of multiple conflicting objectives, a combinatorial explosion of alternatives, and uncertainties arising from thermodynamic model uncertainties, variations in market conditions and flue gas composition. This project will use a combinatorial chemical design algorithm to recommend new solvents and solvent blends and a new and efficient multiobjective optimization (MOP) framework under uncertainty[4], coupled with the ASPEN simulator [5], to computationally evaluate solvent candidates. Only those solvent candidates that have been computationally determined to have promising performance will be evaluated further. The goals of the proposed project are presented below.

- Using a multiple objective optimization framework and process simulation, identify the target solvent properties needed for optimal economic performance. Targets for chemical stability, health, safety and environmental properties will also be established. Identify the structural groups to be used to design new solvent molecules. Proper selection of these groups will ensure the design of stable, high performance solvents.
- Characterize and quantify uncertainties and risks in environmental and economic impacts, thermodynamic models, cost models and data. Computationally design candidate solvents and solvent blends that satisfy the performance, environmental, health and safety targets previously identified.
- Develop efficient algorithmic framework for solvent selection and solvent recycling.
- Find multiobjective solvent and process designs for CO₂ capture (Figure 3).

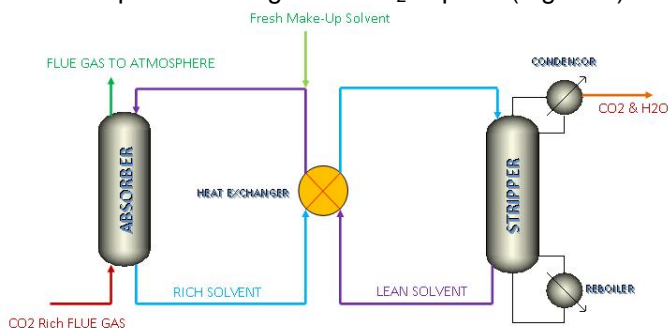


Figure 3 shows the CO₂ capture and solvent recycling absorption distillation process flowsheet. The solvent recycling consumes tremendous amount of energy and other resources like water.

Specific tasks of the REU fellows include identifying decision variables for optimization of solvent selection and solvent recycling system by carrying out simulation runs of ASPEN models and using statistical techniques, understanding the difference between rate-based models and equilibrium models, identifying optimal solvent blends, and writing report. With this project, the REU fellows will be exposed to various simulation tools, mathematical and statistical methods and algorithms, and physics based modeling. The REU students activities will be alongside graduate students who are pursuing their PhD

degrees in this area, and Post-doctoral fellows. The research contributes to the important area of carbon capture and is likely to be implemented soon in near future.

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