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A high fidelity and user-friendly equation-oriented optimization model for carbon capture using a novel water-lean solvent

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Abstract

A novel water-lean solvent technology, developed by Research Triangle Institute (RTI) International and being commercialized by SLB, achieved low energy demand which is represented by its low specific reboiler duty (SRD) values at carbon capture rates beyond 90%. This technology demonstrated a SRD of 2.55 GJ/t-CO_2 at 95% capture, using one intercooler for absorber and five degrees Centigrade (5^0C) temperature approach in the lean/rich solvent cross exchanger at the Technology Centre Mongstad (TCM) pilot plant (two hundred tonnes per day of carbon capture capacity). Prospective adopters of this technology requested different target capture rates for the FEED (Front End Engineering and Design) studies based on their location and their company's emission reduction targets. These requests demanded an optimization model that minimizes energy demand for a target carbon capture rate. Also, the model needs to determine optimal operating parameters for carbon capture process based on frequently fluctuating flue gas conditions and flowrate, to be used for real time optimization and advanced process control applications. RTI and SLB previously developed an Aspen Plus process simulation model, which matches the TCM plant data. However, that model was prohibitively slow to be used as a tool for real time optimization and advanced process control applications.

The model slowness is because of the default "Sequential Modular (SM) strategy" adopted by Aspen Plus in the presence of recycle streams and tight heat integration commonly found in solvent-based carbon capture processes. The equation-oriented (EO) modeling strategy is more suitable for optimizing these processes. However, the adoption of the EO strategy might have been hindered by the following reasons:

(1) **Feature availability:** Aspen Plus EO mode does not have all the features available in SM mode. E.g., Balance blocks (commonly used in legacy carbon capture models) are not supported. Also, specifications are not always consistent between SM and EO modes.
(2) **User-friendliness**: Aspen Plus EO feature forms are not user-friendly, such as forms for identification of the correct EO variables and solving the recycle loops.
(3) **Troubleshooting:** Troubleshooting model convergence problems is complex as one cannot associate the source of the error to a particular block, unlike in SM mode.
(4) **Initial Values:** EO model needs good initial values.

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This paper discusses the methodology used to build this optimization model, addressing the above issues.

Keywords: Equation-oriented; Carbon Capture optimization model; Water-lean solvent; Optimization model

Nomenclature

ENRTL	electrolyte non-random two liquid
EO	Equation-oriented
FEED	Front-end engineering design
L/G	ratio of mass flowrates of lean solvent to flue gas in the absorber
RK	Redlich-Kwong
SM	Sequential Modular
SRD	specific reboiler duty
TCM	Technology Centre, Mongstad
VLE	Vapor-Liquid Equilibrium
WLS	water-lean solvent

1. Introduction

Post-combustion emissions account for over 75% of total industrial emissions, with the largest contributions from the power generation, cement, iron & steel, and petrochemical sectors. The high levelized cost of current commercial technologies for post-combustion capture poses a significant challenge to the economic feasibility of decarbonizing these industries, highlighting the need for more cost-effective solutions.

Advanced water-lean solvents (WLS) for post-combustion CO_2 capture offer several advantages over the aqueous amine solvents. WLS have lower parasitic energy penalty, lower corrosion, lower temperature and high-pressure CO_2 regeneration leading to lower cost of CO_2 capture [1, 2]. RTI International, with funding from the US Department of Energy, has been developing its water-lean solvent technology, that has shown specific reboiler duty (SRD) of 2.3 GJ/t-CO_2 at the 60-kWe/ 1 tonne/day CO_2 capture capacity pilot testing unit (Tiller Plant, SINTEF, Norway) and 2.6 GJ/t-CO_2 at the engineering scale testing system (12 Mwe/200 tonne/day CO_2 capture capacity) at the Technology Centre Mongstad (TCM) in Norway [3-5]. Prospective adopters of this technology requested different target capture rates for the FEED (Front End Engineering and Design) studies based on their location and their company's emission reduction targets. These requests demanded an optimization model that minimizes energy demand for a target carbon capture rate. Also, the model needs to determine optimal operating parameters for carbon capture process based on the prospects' frequently fluctuating flue gas conditions and flowrates, for the model to be used for real time optimization and advanced process control applications. RTI and SLB previously developed an Aspen Plus process simulation model, which matches the TCM plant data [6]. However, that model was inherently slow to be used as a tool for real time optimization or advanced process control.

The model slowness is the result of the default "Sequential Modular (SM) strategy" adopted by Aspen Plus in the presence of recycle streams and tight heat integration commonly found in solvent-based carbon capture processes. In the sequential modular strategy, each unit operation is solved independently and in sequence, therefore additional iterations are required for loops with recycle streams. On the other hand, the equation-oriented (EO) modeling strategy is a modelling approach where all the unit operation models are solved simultaneously [7]. By nature, EO modelling is more suitable for optimizing these processes in a timely manner. However, the adoption of the EO strategy might have been hindered by the following reasons:

(1) **Feature availability:** Aspen Plus EO mode does not have all the features available in SM mode. E.g.,

Balance blocks (commonly used in legacy carbon capture models) are not supported [8]. Also, specifications are not always consistent between SM and EO modes.

(2) **User-friendliness**: Aspen Plus EO feature forms are not user-friendly, such as forms for identification of the correct EO variables and solving the recycle loops.

(3) **Troubleshooting:** Troubleshooting model convergence problems is complex as one cannot associate the source of the error to a particular block, unlike in SM mode [7].

(4) **Initial Values:** EO model needs good initial values.

In this work, a general strategy will be proposed to address the aforementioned issues, illustrated by an implementation of EO model in a post combustion carbon capture application. The objectives of the work will be described in the second section. In section three, the details of the proposed methodology will be discussed, followed by the results and discussions, conclusions.

2. Objective

Objective of the work is to build an optimization model that minimizes the energy demand to determine the optimal operating conditions (reboiler temperature and solvent circulation flowrate) while meeting the capture rate target. The model is required to use rigorous electrolyte property methods and rate-based modeling framework for absorber. The model needs to have a user-friendly interface and converge quickly for different feed flue gas conditions, compositions, and flowrates, while meeting the capture rate target and other constraints

3. Methodology

Figure 1 is a screenshot of the Aspen Plus flowsheet. Flowsheet scope is from flue gas entering the Direct Contact Cooling section to CO_2 product at the desorber outlet.

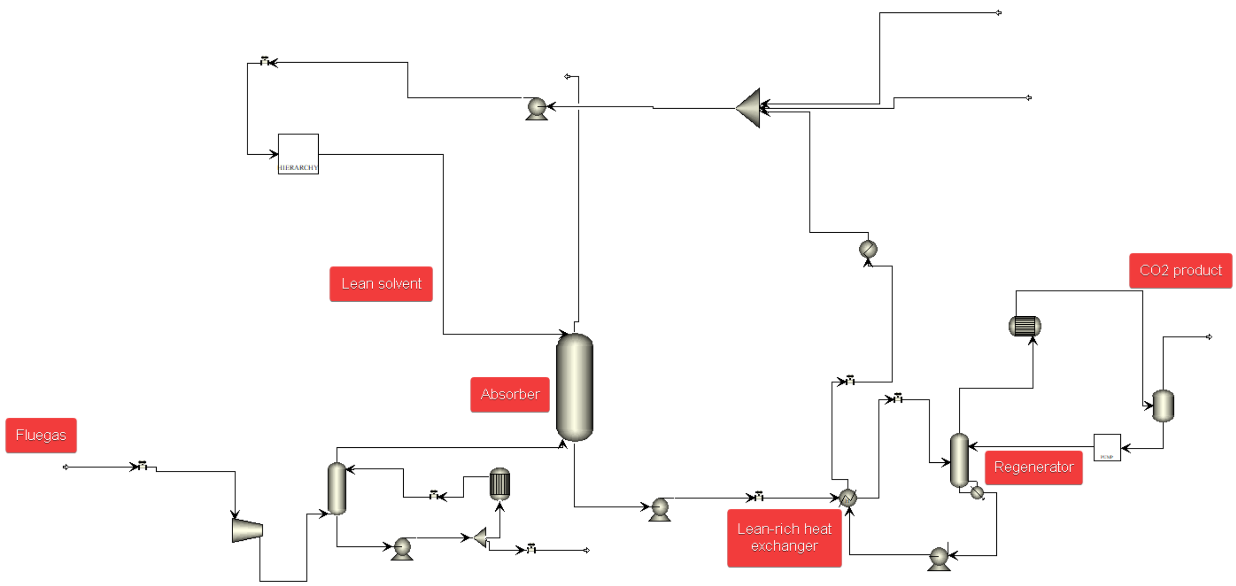

Figure 1: Aspen Plus flowsheet

The ENRTL-RK, a rigorous unsymmetric electrolyte property method with the Redlich-Kwong equation of state for vapor phase properties, is used in the EO model [8]. Rate-based modeling strategy with kinetics is adopted for absorber.

EO model needs a starting point SM flowsheet for initialization. When we selected capture rate as input in SM initialization model, a design spec on capture rate while varying solvent circulation flowrate was difficult to converge. So, we selected solvent circulation rate and lean loading/reboiler temperature inputs and capture rate as output in the SM model. In the EO model, we setup a spec group to make capture rate variable as constant and solvent circulation rate variable as calculated and did not face any convergence issues.

Initially, we considered total energy demand to be objective function for the EO optimization model. Total energy demand for carbon capture process comprises of thermal energy and electrical energy. Reboiler duty contributes to thermal energy demand. Blower duty, pumps' power requirements contribute to electrical energy demand. Thermal energy demand (reboiler duty) was found to be significantly higher than electrical energy demand from the model results. Therefore, we chose specific reboiler duty (SRD) as the objective function to be minimized to simplify the optimization problem.

Objective Function: Minimize SRD

Varied variables: L/G (ratio of mass flowrates of lean solvent to flue gas in the absorber), CO_2 loading

Constraints:

- Capture percent needs to meet the specified target
- Reboiler temperature should not exceed the specified limit

We addressed the issues, mentioned in the background section, by

(1) **Feature availability:** Using alternate but accurate specifications. E.g., (1) Balance blocks are replaced by the default EO variable specs to calculate makeup flows. (2) L/G is setup as a global parameter in the SM mode. Global parameters acquire "calculated" specification in the EO mode, even if they are inputs. So, L/G is setup as a local parameter to overcome this issue

(2) **User-friendliness**: Creating a user-friendly interface using "Custom Table" and "Layout" features [9].

- Key Model Inputs: Capture rate target, Flue gas flowrate, temperature, pressure, and composition, Lean Rich Heat exchanger approach temperature
- Key Model Outputs: SRD, Reboiler temperature, and Solvent circulation flowrate

Figure 2 shows the user-interface. Inputs are clearly indicated by their font (bold and blue). Results are displayed in black color font.

KPI

Name	Units	Value
Carbon Capture Rate Target (percentage)	UNITLESS	95
LRHX approach T	C	5
Flue Gas flowrate	KG/HR	603299
Flue Gas Water molefraction	FRACTION	0.13
Flue Gas O2 molefraction	FRACTION	0.09
Flue Gas CO2 molefraction	FRACTION	0.2
Flue Gas N2 molefraction	FRACTION	
optimized SRD		
Reboiler T	C	
Lean Loading	*	
LBYG (optimized)	UNITLESS	

Figure 2: User-Interface

(3) **Troubleshooting:** Testing if model converges over a wide range of inputs and documenting the troubleshooting steps. EO mode sensitivity feature only shows derivatives, unlike SM mode sensitivity analysis. Therefore, Aspen Simulation Workbook EXCEL add-in scenario analysis table feature was used to vary the model inputs over a wide range and test convergence [9].

(4) **Initial Values:** Setting up SM simulation model such that it always converges fast to provide initial values. Spec to honor the target capture rate is not activated in the simulation model, thus aiding in convergence. SM simulation model is tested over a wide range of inputs to ensure convergence.

4. Results and Discussion

For flue gas with 12 percent CO_2, target carbon capture rate is varied in the model between 90 and 95 percent to observe the effect on L/G and SRD. SRD remained almost the same with capture rate change for this solvent. Required L/G increased with capture rate. Figure 2 illustrates the trends with normalized variable values.

Normalized variable value is the ratio of current variable value and variable value at 90 percent capture rate in Figures 3 and 4.

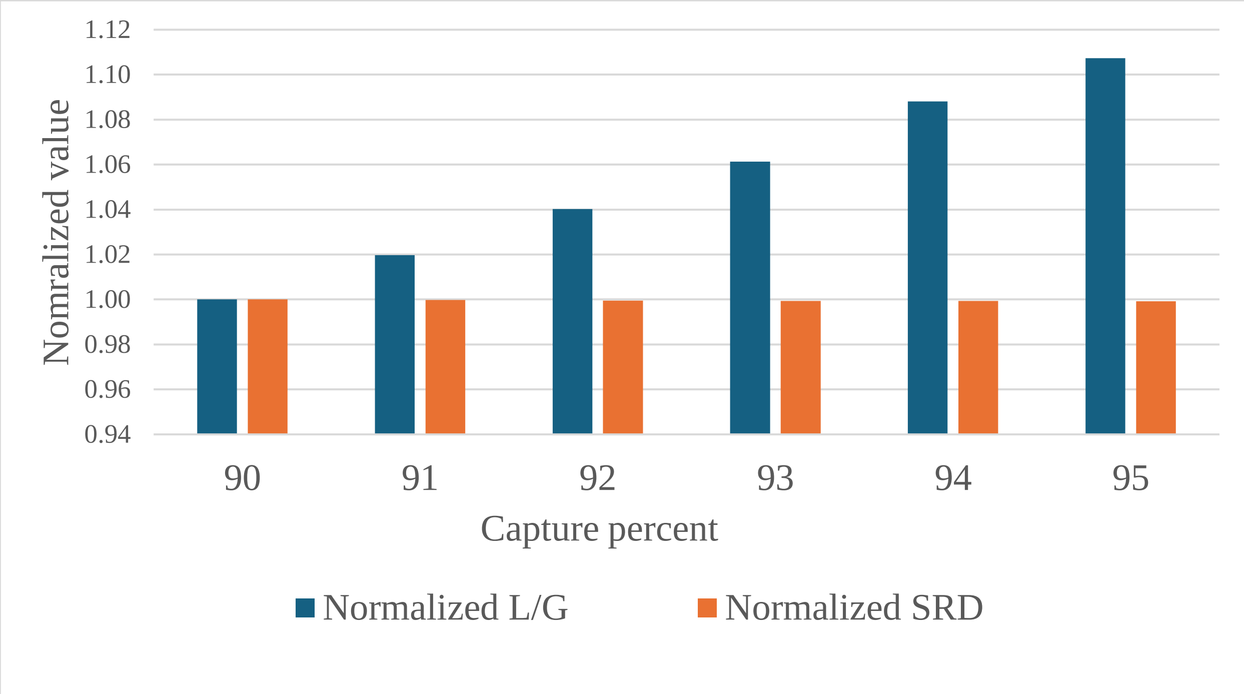

Figure 3: SRD and L/G vs capture rate

Since required L/G increases with capture rate, power requirement for pumps increase. So, we investigated effect of capture rate on electricity demand and specific electrical duty (electrical duty/tonne CO_2), plotted in Figure 3.

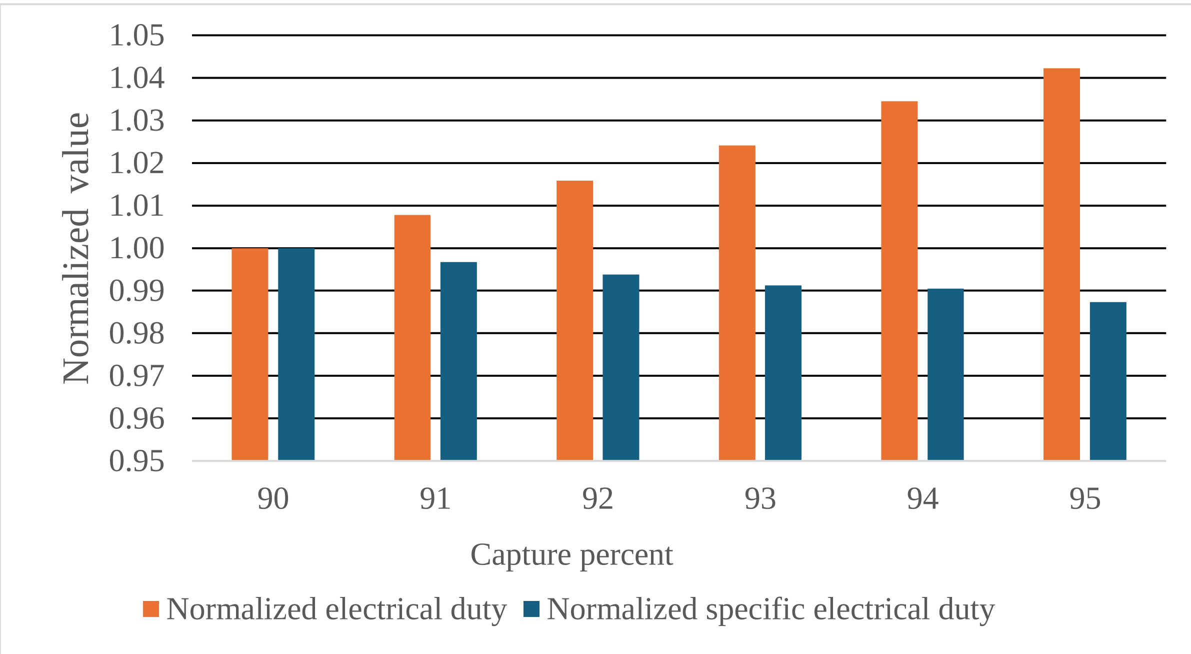

Figure 4: Electrical duty and specific electrical duty vs capture rate

Figure 4 illustrates that total electricity demand increases with capture rate. However, specific electrical duty (electricity demand/tonne CO_2) decreases slightly with capture rate increase.

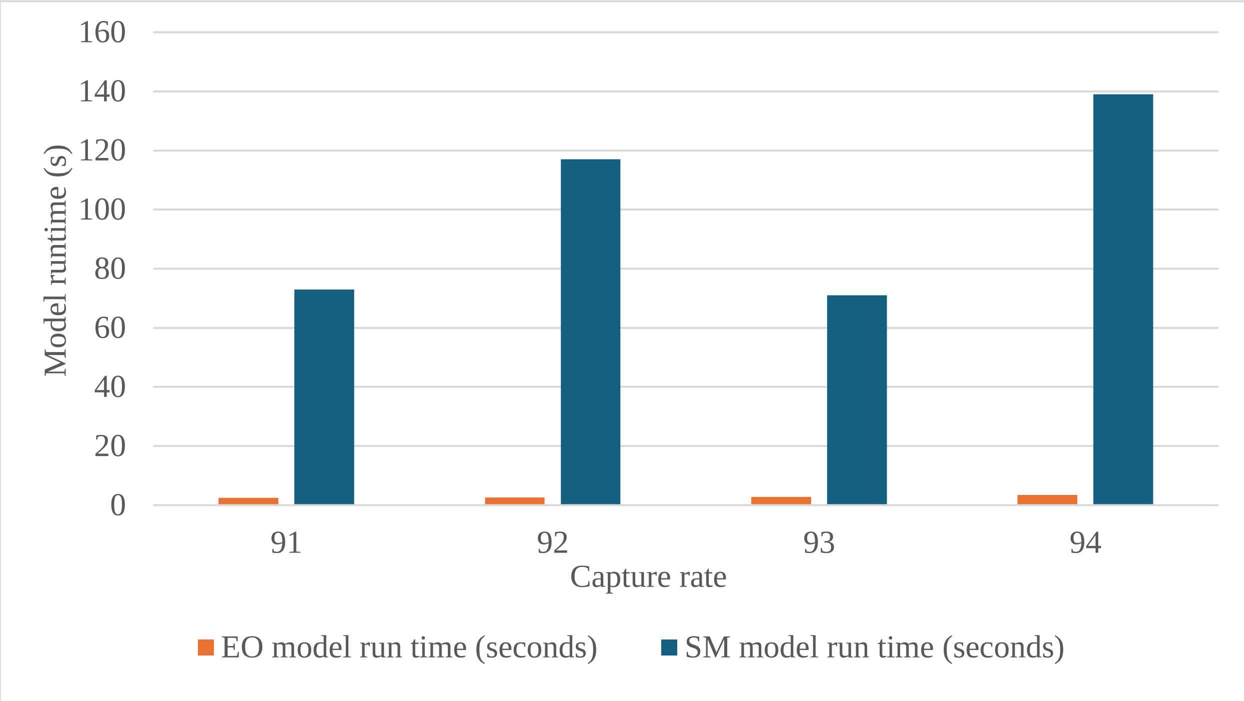

Figure 5: Model runtimes – EO vs SM modes

With respect to model performance, Figure 5 compares the SM and EO model runtimes at different capture rates. EO model runtime is consistently lower than SM model. We performed the model runs using Aspen Plus V12.1 on a PC with 12th Gen Intel® Core™ i7-12800H 2.40 GHz processor and 32 GB RAM.

5. Conclusions

In this work, we developed an equation-oriented model for a novel water-lean solvent-based post combustion carbon capture process. We used rigorous ENRTL-RK property method and rate-based modeling strategy for absorber in the model. We developed a user-friendly interface to enable model adoption. Model objective was to minimize SRD while varying L/G and lean loading/reboiler temperature to achieve the desired carbon capture rate. SRD remained almost the same with change in target capture rate. Specific electrical duty slightly decreased with increase in target capture rate. In terms of performance, EO model was observed to be consistently faster when compared to the SM model.

References

1. Heldebrant, D.J., et al., *Water-Lean Solvents for Post-Combustion CO_2 Capture: Fundamentals, Uncertainties, Opportunities, and Outlook.* Chemical Reviews, 2017. **117**(14): p. 9594-9624.
2. Wanderley, R.R., D.D.D. Pinto, and H.K. Knuutila, *From hybrid solvents to water-lean solvents – A critical and historical review.* Separation and Purification Technology, 2021. **260**: p. 118193.
3. Gupta, V., et al., *Engineering-scale testing of non-aqueous solvent for CO_2 capture at Technology Centre Mongstad*, in *IEAGHG 7th Post Combustion Capture Conference*. 2023: Pittsburgh, USA.

4. Mejdell, T., et al., *Pilot plant testing using a Non-Aqueous Solvent (NAS)* in *PCCC-5*. 2019: Kyoto, Japan.
5. Zhou, S.J., et al., *Pilot Testing of a Non-Aqueous Solvent (NAS) CO_2 Capture Process*, in *14th International Conference on Greenhouse Gas Control Technologies, GHGT-14*. 2018: Melbourne, Australia.
6. Gupta, V., et al., *Development of a Rate-Based ENRTL-RK Process Model for a Water-Lean Solvent (December 15, 2024), in 17th International Conference on Greenhouse Gas Control Technologies, GHGT-17. 2017: Calgary, Canada*. Available at SSRN: https://ssrn.com/abstract=5056807 or http://dx.doi.org/10.2139/ssrn.5056807
7. Lee A., et al., *Model Diagnostics for Equation-Oriented Models: Roadblocks and the Path Forward.(2024). LAPSE:2024*.1632
8. Chen, C.C. and L.B. Evans, *A local composition model for the excess Gibbs energy of aqueous electrolyte systems.* AIChE Journal, 1986. **32**(3): p. 444-454. AIChE Journal, 1986. 32(3): p. 444-454
9. Aspen Technology, Inc. (2021). *Aspen Plus: User Guide*. *program documentation*, Bedford, MA