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ProTreat® simulation accurately represents experimental results for post-combustion carbon dioxide capture with novel mixed amine solvent in real process environment

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Abstract

Comparison of ProTreat® simulations to data obtained from testing ION's advanced solvent at the NCCC facility demonstrated excellent agreement between process simulations and process telemetry. ProTreat® simulations created and executed to resemble test conditions during ION's testing campaign at NCCC converged with good accuracy. The models predicted temperature profiles for absorption and stripping columns the were directly compared with real data and served to evaluate the accuracy of the simulations. Lean and rich solvent loading predictions using ProTreat® were within 6% (mass/mass) of measured results. The software-generated temperature profiles in the absorber and stripper yielded variances of less than 5 ºF (2 ºC) at any height of the packing across all periods of evaluation with real data. Comparing ProTreat® simulations with actual process data has provided confidence in using ProTreat® as a viable method for predicting ION's proprietary solvent's gas treating capabilities.

Peer-review under responsibility of the organizing committee of GHGT-13.

Keywords: ProTreat®; Advanced solvent; PCC; process model validation; CO_2 capture; Gas Processing; Power Generation

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1. Introduction

For operational expenditures during the design of a process, optimization of carbon dioxide capture technology involves maximizing the rate of carbon dioxide (CO_2) removal (absorption/desorption) capacity while simultaneously minimizing thermal and mechanical energy required to drive the process [1]. In the case of amine-based solvents, thermal energy is used to reverse the absorption of CO_2 reaction, thus regenerating the capture solvent and providing the driving force for absorption of newly arriving CO_2 in flue gas in a continuous operation [2]. For this reason, thermal energy requirements are inherently coupled to CO_2 removal capacity, resulting in a challenging and delicate optimization process which can benefit from predictive simulation tools. Rate-based process simulation tools have been shown to be highly accurate and more importantly predictive of solvent performance and have been used to facilitate engineering, design, and optimization of CO_2 removal processes and technology [3]. For a similar reason, reliable simulation tools allow developers to confidently assess economic options for plant design and specifications related to initial capital expenditures for fluctuating costs amongst different column and packing dimensions and materials of construction.

ION Engineering, LLC ("ION"), tested their leading CO_2 capture solvent at the National Carbon Capture Center ("NCCC"), located at Southern Company's Plant E.C. Gaston in Alabama, United States, in 2015. The campaign details have been reported elsewhere [4]. ION's objectives spanned an initial parametric phase followed by a steady-state period using its proprietary solvent. During both phases, individual set points implemented throughout the campaign were also mirrored as inputs into a ProTreat®-designed model of NCCC's facility for solvent-based technologies. The direct comparision of real and simulated results are presented in this paper. For reference, the testing facility provided a slipstream of post-combusted coal-fired flue gas to test CO_2 capture technologies of gas streams with CO_2 concentrations between 10 mol% and 14 mol% (dependent on plant electric loads) and is open to developers with their individual technologies [5].

ION contracted Optimized Gas Treating ("OGT") to develop a ProTreat® simulation engine specific for its proprietary amine-based solvent. ProTreat® is a true rate-based modelling engine and is built from the bottom up from first principles using fundamental chemistry, mass transfer, kinetics, and thermodynamic relations. The ProTreat® model can be used to closely estimate steady state CO_2 absorption and desorption processes, because it accurately accounts for simultaneous physical transport of CO_2 between gas and liquid phases and chemical reaction kinetics of CO_2 in the liquid phase through the specific CO_2 – amine reaction.

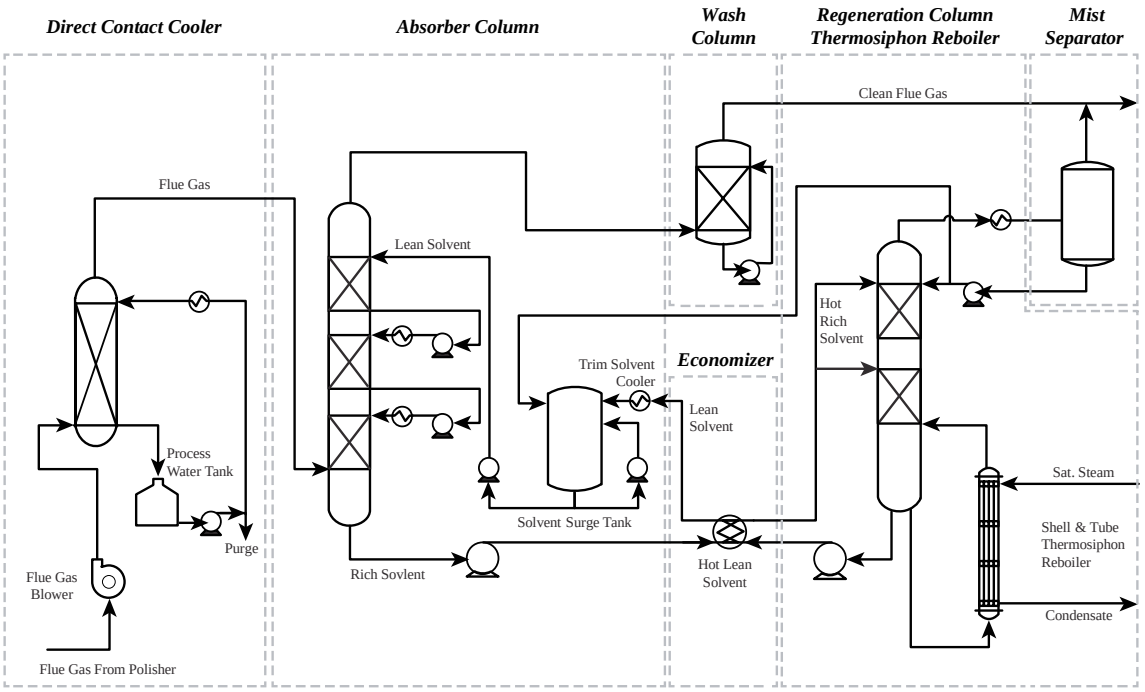


Fig. 1. General process flow diagram of the pilot solvent test unit (PSTU) at the National Carbon Capture Center (NCCC).

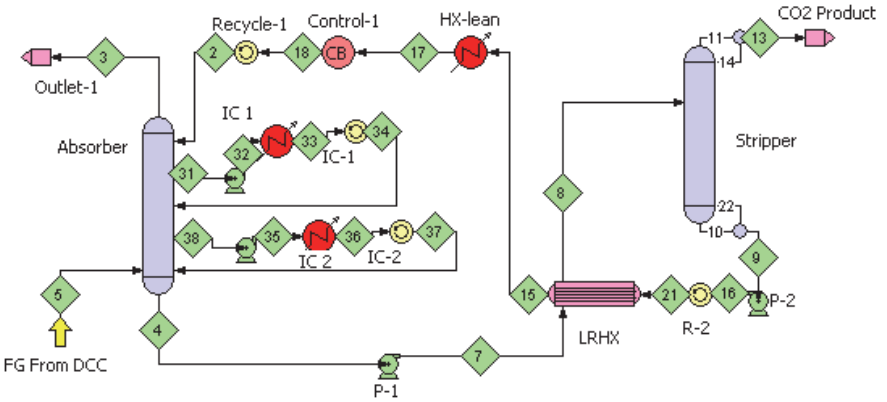
Experimental results from ION's recent test campaign at NCCC will be presented in this paper and compared to simulated results using ProTreat®. Comparison of ProTreat®-generated results to data obtained from ION's solvent at the NCCC facility will be discussed and has provided confidence in using ProTreat® as a viable method for predicting its proprietary solvent's gas treating capabilities.

A ProTreat® model of the test facility at NCCC was developed using as-built equipment including packing height and type in absorption and stripping columns, heat exchangers and key process set points (such as, intercooler temperatures and flow rates) in order to develop representative simulation cases that could be directly compared to experimental results.

2. PSTU Process Simulation

The pilot solvent testing unit (PSTU) at the NCCC facilities was designed specifically for testing amine based solvents for CO_2 removal from coal fired flue gas [5]. The general PSTU process configuration is presented (Fig. 1). The PSTU test unit (Fig. 1.) comprises of a caustic scrubber (omitted in Fig. 1. and not incorporated in the simulations discussed herein) which is the first contacting process in the PSTU test unit. Followed immediately by a blower (pictured, Fig. 1.) and direct contact cooler, absorption column, a lean-rich cross heat exchanger, an amine regenerator with a thermosiphon reboiler, and a single bed wash tower downstream of the absorber.

A ProTreat® model of the PSTU model was constructed in order to evaluate consistency of the ION-specific ProTreat® simulation tool with actual process data. The ProTreat® PSTU model (Fig. 2) was limited to CO_2 absorption and solvent regeneration operations in order to focus the evaluation on ION's specific solvent flow sheet



components. Absorption and regeneration operations were simulated in a continuous process which included the absorption column, intercoolers, lean-rich cross exchanger, lean solvent trim cooler and regeneration column with a kettle reboiler (reboiler choice is discussed Section 3.2). Column specifications used in the ProTreat simulation are presented in Table 1.

Fig. 2. ProTreat® flow sheet for PSTU at NCCC.

Table 1. PSTU Column Information

Property	Units	Absorber	Regeneration
Column diameter	mm	641	591

Packing height (total)	mm	6048	6048
Packing height (per section)	mm	2016	3024
Number of packed sections		3	2
Packing type		Mellapak 252.Y	Mellapak 252.Y
Material of construction		316 SS	316 SS

3. Experimental

Process data from four steady state test periods were used to evaluate the consistency of ProTreat® simulations specific to ION's solvent. The first two steady state test periods occurred at the beginning and end of the parametric testing period during ION testing at NCCC. The last two steady state periods of model evaluation occurred during the later portion of ION testing at NCCC. They were selected to provide two points of comparison at the beginning and at the end of the longer term steady state operation period, to potentially capture deviations occurring due to solvent aging and accumulations of heat stable salts (HSS). Simulation methodology, selection, and specification of independent process variables is discussed in this section below and is organized by major unit operation.

3.1. Absorber

Inlet flue gas conditions were specified for all time periods in the ProTreat® simulation and were based on conditions actually experienced during ION solvent testing at NCCC (Table 2). Similarly, the absorber trim cooler (Table 3), the intercoolers (Table 3) and lean solvent composition (Table 4) were also specified, with the exception of lean solvent loading which was a dependent variable given the nature of a continuous CO_2 scrubbing process. The lean solvent trim cooler was used to specify the lean solvent temperature entering the absorber, which was based on process data from NCCC testing. Absorber pressure was specified based on incoming flue gas pressure at the bottom of the first bed of packing and subsequent pressure drop was computed within the ProTreat® simulation across all beds.

Table 2. Inlet Flue Gas Conditions

Property	Units	Parametric 1, 24 hours	Parametric 2, 72 hours	Steady State 1, 72 hours	Steady State 2, 72 hours
Total flow	kg/hr	2,268	2,268	2,268	2,268
Temperature	˚C	40.3	39.2	44.2	38.3
Pressure	barg	0.09	0.09	0.09	0.09
Water	% saturated	100	100	100	100
Carbon Dioxide	% mol, dry	11.8	12.0	12.3	11.6
Nitrogen	% mol, dry	80.7	80.7	80.6	80.7
Oxygen	% mol, dry	7.5	7.3	7.1	7.7

Table 3. Absorber Process Conditions

Property	Units	Parametric 1, 24 hours	Parametric 2, 72 hours	Steady State 1, 72 hours	Steady State 2, 72 hours
Absorber pressure (bottom 1st bed)	barg	0.09	0.09	0.09	0.09
Lean solvent temperature (entering absorber)	˚C	38	44	41	42
Intercooler 1, solvent temp, exit	˚C	58	57	58	59
Intercooler 1, volumetric flow	m^3/hr	5.84	5.79	5.82	5.81

Intercooler 2, solvent temp, exit	˚C	58	57	57.6	58.9
Intercooler 2, volumetric flow	m^3/hr	5.76	5.55	5.52	5.66

Table 4. Control Block Conditions

Property	Units	Parametric 1, 24 hours	Parametric 2, 72 hours	Steady State 1, 72 hours	Steady State 2, 72 hours
Stream total flow	kg/hr	7,258	5,670	6,804	6,804
Solvent	% wt.	Specified	Specified	Specified	Specified
Water	% wt.	Remainder	Remainder	Remainder	Remainder

3.2. Regeneration Column

The physical process equipment for the regeneration column was specified in ProTreat® (Table 1). Regeneration pressure was specified at the top of the highest packed section in the ProTreat simulation and computed across all sections (Table 4). Reboiler duty was not specified, but was iterated upon to until lean solvent temperature exiting the regeneration unit was consistent with process data (Table 5). This decision was made because of PSTU reboiler configuration and regenerator internals. The PSTU reboiler was operated as a natural circulation using a thermosiphon operation, which is an appealing cost-effective option for full-scale deployment. At present, while thermosiphon reboilers can be modelled in ProTreat®, adjustments cannot be made to accurately account for increased pressure head on the solvent entering the reboiler resulting from solvent holdup in the bottom of the column. Typically in higher pressure regeneration as is typically found in pre-combustion amine treating, accurate accounting of the pressure head of the sump does not significantly impact simulation of reboiler performance. However, in post combuation CO_2 captue where overhead regeneration pressure is typically around 1.0 barg, the impact of a 2-4 m liquid head can have significant impact on evaluation of reboiler duty [6]. Secondly, when considering operational set-points for near atmospheric regeneration, solvent temperature exiting the reboiler is a more relevant variable to control to as opposed to ‘a duty’ set point which would involve computations and introduce complexity and error into the control strategy. Thus, it was of greatest interest to evaluate the accuracy of predicting lean solvent loading based on temperature.

Table 5. Reboiler Conditions

Property	Units	Parametric 1, 24 hours	Parametric 2, 72 hours	Steady State 1, 72 hours	Steady State 2, 72 hours
Regenerator overhead pressure	barg	0.62	0.71	0.70	0.70
Lean solvent temperature (exiting regenerator)	˚C	113	120	118	119

3.3. Lean Rich Cross Exchange

In ProTreat®, temperature differential across the LRXC was specified as an approach on the rich solvent stream. With lean solvent temperature entering the cross exchanger being specified (due to reboiler modelling strategy, discussed above), this methodology results in the rich solvent temp leaving the cross exchanger being specified as well. Because rich solvent temp exiting the absorber was a dependent variable, any discrepancies in the model in computing rich solvent temp exiting the absorber would then carry over and convolute the regeneration side of the process. This decision was made to isolate the two sides of the process in order to better identify where deviations are occurring so that they could be targeted and resolved in future efforts if needed.

4. Results

ProTreat® simulations converged with good accuracy producing temperature profiles for absorption and stripping columns along with other dependent process parameters that were used to evaluate the accuracy of the simulations, which was remarkable (Fig. 3).

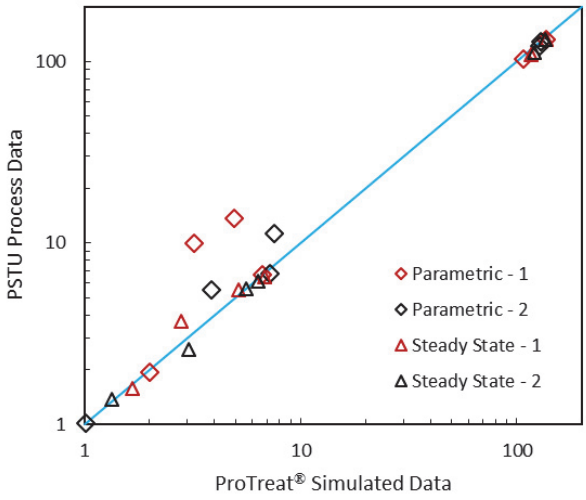


Fig. 3. Comparison of dependent process variables from PSTU testing and ProTreat® simulations.

4.1. CO_2 Mass transport

Evaluation of lean and rich solvent CO_2 loading was the first point of evaluation of the ProTreat® simulation to ensure that mass transport was accurately represented prior to entering into analysis of more complex and dependent process conditions. Lean solvent temperature was effectively specified by iterating reboiler duty in order to achieve a process set point it is not surprising that good agreement was observed for lean solvent CO_2 loading, which were within 6% of observed values. After observing good agreement with lean CO_2 loading it was easy to evaluate accuracy of absorber side CO_2 mass transfer which also excellent and within 6% of observed values in the PSTU throughout the four test conditions evaluated.

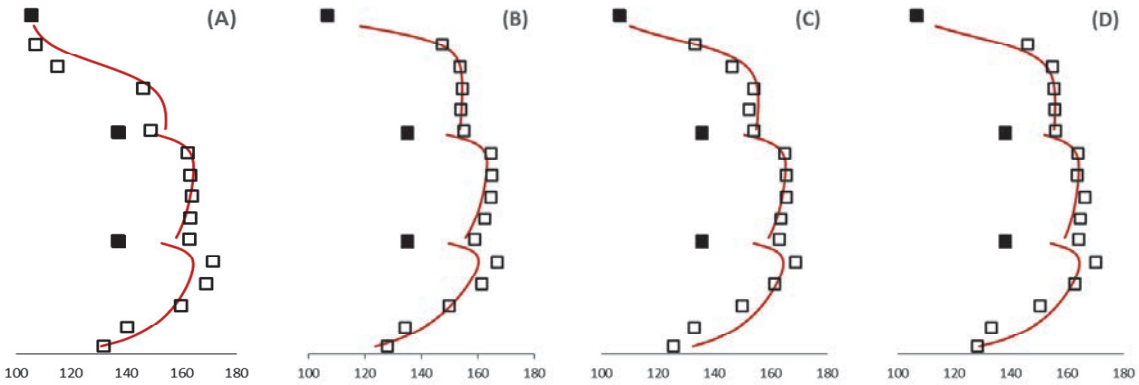


Fig. 4. Absorber temperature (ºC) profiles on abscissa. (a) Parametric Testing #1; (b) Parametric Testing #2; (c) Steady State #1; (d) Steady State #2. For all figures (a-d); Black solid squares – Specified (or controlled) liquid temperatures (from top to bottom; lean solvent entering absorber, solvent exiting top intercooler, solvent exiting bottom intercooler).

4.2. Thermal evaluations

Conformation that CO_2 mass transport was being accurately represented in the ProTreat® simulation allowed comparison of thermal data to be made easily. Temperature profiles of the absorption column are presented in Fig. 4. (above). Overall excellent agreement between process temperatures and simulations are observed.

Trends observed across all periods of evaluation:

1. Under prediction of the rate of temperature increase in the lowest bed
2. Under estimate of peak bulge temperature in the bottom absorber bed
3. Over estimate of the rate of temperature increase in the middle bed of packing

Trend 1 appears to increase in intensity (although deviations are not large in any of the four time periods) from Fig.4.a (data from 26-June, fresh solvent, shortly after start-up) to Fig.4.d (6-August, after > 1,000 hrs operation without purging solvent) which suggest that rich end viscous properties of the ION specific solvent may be changing as heat stable salts accumulate in the circulating solvent. Pattern 2 and 3 are likely related. Both suggest that some aspect of the $CO_{2(g)} – CO_{2(l)}$ – amine reaction may be underrepresented in ION specific flow sheet components.

Trend 2 alone, suggests that one of the following may be occurring;

a. more CO_2 is reacting and producing a higher peak temperature,
b. thermal capacity of the solvent may be overestimated by the simulation, or
c. heat of reaction for the CO_2 amine reaction may be underrepresented at absorption temperatures.

Consideration of Trend 2 in conjunction with trend 3, which suggests that less CO_2 is being absorbed into the ION solvent in the middle section of packing, and the knowledge that good agreement between rich and lean solvent loadings were observed strengthen the argument for (a.) which could be a result of an underrepresentation of solvent – CO_2 absorption kinetics. Furthermore, substantially greater discrepancies in rich and lean CO_2 loading would almost certainly be apparent if either (b.) and (c.) existed and were significantly influencing the simulation results.

5. Conclusions

ProTreat® process simulations performed using ION's solvent specific flow sheet components (solvent components, amines) provided highly representative simulations of the ION solvent which showed excellent agreement with process data from ION solvent testing at NCCC. Mass transport of CO_2 was accurately represented on the absorption and regeneration sides of the process. Deviations between actual and simulated absorber temperature profiles were minor, easily explained and did not significantly impact key design parameters such as lean and rich CO_2 loadings which must be simulated accurately.

ION's modelling capabilities puts itself in a prime position for scale-up and commercialization of its leading carbon capture solvent. ProTreat® is ION's preferred simulation tool for acid gas treating. In this case, its predicted results for CO_2 are backed with solid measured in-field results for both baseline MEA and its own proprietary solvent. ProTreat® is a modelling software that relies on mass transfer rates and does not introduce potential miscalculations or manipulations from user-input such as selection of property packages or adjustable parameters such as residence times, theoretical trays, and other mixing factors. ION has modelled an optimized plant created in ProTreat® with regeneration energies lower than baseline MEA and top competitors. Process modelling using ProTreat® will enable ION to assess its solvent system performance at future testing sites and design custom-built processes while providing confidence to future collaborators and investors for the common goal of reducing greenhouse gas emissions.

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Appendix A. Required Disclaimer

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