ION Validation of Transformational CO_2 Capture Solvent Technology with Revolutionary Stability "Project Apollo"

Final Scientific/Technical Report

Reporting Period Start Date: June 2019

Reporting Period End Date: May 2023

Prepared by: ION Clean Energy, Inc.
(formally ION Engineering, LLC)

3052 Sterling Circle

Boulder, CO, USA 80301

Date Issued: August 2023

Acknowledgement:

This material is based upon work supported by the Department of Energy National Energy Technology Laboratory under cooperative award number DE-FE0031727

Disclaimer:

Executive Summary

This final report presents all the work and tests performed during ION Engineering's carbon dioxide (CO_2) capture pilot test campaign at the 0.6 MWe scale in the Pilot Solvent Test Unit (PSTU) at the National Carbon Capture Center (NCCC): "Validation of Transformational CO_2 Capture Solvent Technology with Revolutionary Stability," referred to as the "Apollo" Project (DE-FE-0031727). The Department of Energy's National Energy and Technology Laboratory (DOE/NETL) awarded ION Engineering (rebranded to ION Clean Energy, Inc., during the project herein) a single budget period (BP) of $3 million with $750,000 of in-kind contribution from all project members to further develop ION's "ICE-31" carbon capture solvent.

ION Clean Energy, Inc (ION) plans to decarbonize the electrical grid and carbon intensive industries by deploying solvent-based CO_2 capture. The Apollo project herein further developed ION's third-generation solvent technology, called ICE-31. The experimental program began in June 2019 and concluded in October 2021. The first major tasks consisted of collecting lab-scale empirical data to demonstrate its unique physical and chemical properties (namely, low energy requirements and exceptional solvent stability) and then creating a new proprietary module in ProTreat®, an acid-gas simulation software from Optimized Gas Treating (OGT). ION used the new module in ProTreat® to develop the test plan. Part of the test plan development task involved attentive work with Southern Company Services (SCS) staff to modify the existing PSTU and to validate modeling efforts that enhanced specific performance indicators of solvent-based carbon capture research. Of primary note, these modifications included a cold-rich bypass (CRB) to the regenerator and an additional bed of structured packing installed within the absorption tower. ION commenced its campaign with parametric testing to determine Key Performance Indicators (KPIs). Then, ION performed an extended, steady-state run to observe solvent performance and degradation rates using natural gas-fired flue gas. The test campaign finished with coal-fired flue gas to determine solvent performance KPIs. ION compiled the results from the test campaign and contracted Sargent & Lundy (S&L) to develop a Techno-Economic Assessment (TEA) to compare ION's technology with the Case B12B Rev 4. The study shows over 17% reduction in cost of CO_2 capture while simultaneously capturing 6.7% more CO_2.

ION began testing their ICE-31 solvent at the PSTU in March 2021, after a one year delay due to COVID-19. ION continued testing through the beginning of October 2021, resulting in 4,000 operational hours where ION captured over 750 tonnes of CO_2 from natural gas combined-cycle (NGCC) type flue gas (4.4% CO_2), real gas-fired boiler-gas (7.8% CO_2), and real coal-fired flue gas (13% CO_2). Using a simple stripper configuration at the PSTU, ION demonstrated 95% CO_2 capture on the three flue gases setting respective baselines. With NGCC flue gas, ION increased to 98% capture and observed an increase in the Specific Reboiler Duty (SRD) by 2-3%. Using the PSTU heat-integrated advanced flash stripper (AFS) configuration, ION demonstrated a minimum SRD of 2.6 GJ/tCO_2 at 91% CO_2 capture for NGCC flue gas with a slight increase to 2.7

GJ/tCO_2 at 97% capture. With the AFS configuration testing coal-fired flue gas, ION achieved an SRD of 2.5 GJ/tCO_2 at 91% CO_2 capture.

ION modeled the PSTU simple stripper results in OGT's ProTreat® process simulator utilizing default parameters for all heat and mass-transfer equipment. The model predicted SRDs with an average error of 0.4% ± 1.7%, lending confidence to ION's ability to scale to a commercial facility with minimal process risk. ProTreat® modeling indicated that when utilizing ION's advanced process design with ICE-31, typical U.S. facilities could expect SRDs of 2.6 GJ/tCO_2 for NGCC and 2.4 GJ/tCO_2 for coal-fired flue gas at 95% CO_2 capture. ION also demonstrated that up to 99% CO_2 capture on NGCC flue gas has a minimal impact on both equipment and operating costs.

ION conducted a comprehensive and successful program with its project partners. With ICE-31, ION confirmed its understanding of process design improvements and operational knowledge with a strong analytical backbone to successfully operate carbon capture facilities. ION demonstrated successful operation at lower L/G circulation rates, lower regeneration energies, and with improved solvent stability, thereby requiring lower make-up rates for a more viable and economically incentivizing carbon capture system at a larger scale and with multiple gas compositions.

After more than 1,200 hours of parametric testing, ION executed a long-term test on NGCC gas at 95% CO_2 capture for 1,500 hours. PSTU operation was stable and reliable with over 99% uptime and no solvent reclamation or addition. The overall mass balance for original solvent components was 100 ± 2% for the entire long-term test. Heat stable salts, mainly originating from flue gas SO_x and NO_x, increased at about 5 ppmw/day. Extractive sampling after the water wash for NH_3 was below 1 ppm and the solvent was below the limit of detection of 0.04 ppm.

The performance and stability of ICE-31 were measured and monitored by ION's Multi-component Liquid Analyzer (MLA). The MLA tracks real-time solvent component and CO_2 concentrations during process operation. The MLA can also track degradation product build up as the solvent matures. The data trends of the MLA, as verified by multiple labs and instruments during the campaign, were consistent with expectations during transitions between test cases and process disturbances.

The process performance results confirm and expand ION's expectation that ICE-31 is an exceptional solvent for flue gases with high oxidative potential, such as those at NGCC facilities. ION will continue to advance the commercial readiness of ICE-31 at the new 10 tonnes CO_2-per-day pilot facility (Enterprise) being constructed at Calpine's Los Medanos Energy Center in Pittsburg, California, and at Technology Center Mongstad's 12 MW large scale pilot in Norway. The Enterprise facility is specifically designed to optimize capture at an operating NGCC power plant and will begin operations in the third quarter of 2023.

Table of Contents

Table of Figures

Introduction

Carbon Capture Utilization and Storage (CCUS) technologies continue to be of great interest to point-source emitters as mechanisms to reduce their carbon footprint. Post-combustion CO_2 capture (PCC) is an affordable decarbonization technology today compared to other carbon removal technologies such as direct air capture. However, the effective and widespread use of CCUS today is limited almost exclusively because of economic considerations. There has been increased interest in the United States over the past few years with the announcement of tax credits for CCUS deployment which help to offset costs, but a key focus of technology developers is to reduce capital costs (CAPEX) and operating costs (OPEX) to create a successful business case to support deployment on a large-scale, commercial level.

ION Clean Energy, Inc. (ION) is developing and deploying solvent-based CO_2 capture technologies with aims of capturing 1 billion tonnes of CO_2 by 2050 to decarbonize the electrical grid and carbon-intensive industries. As part of its continuous development of solvent-based capture systems, ION completed a six-month testing campaign with its third-generation solvent technology, ICE-31, at the National Carbon Capture Center (NCCC) (Figure 1) as part of U.S. Department of Energy project DE-FE0031727 "Validation of Transformational CO_2 Capture Solvent Technology with Revolutionary Stability." The objective for the project was to scale up ICE-31 from the bench scale to the pilot scale in an industrially relevant environment.

This report covers the results and conclusions of ION's test campaign at the NCCC's Pilot Solvent Test Unit (PSTU) using ICE-31. ION is the first technology developer to test at the PSTU using the test facility's newly configured natural gas-fired boiler as part of its "Apollo" project. The test results from this test program demonstrate a reduction in both capital and operating expenses to support large-scale carbon capture deployment within the next decade.

Figure 1: NCCC's PSTU (center and right) and the new gas-fired boiler (left); photo courtesy of NCCC

Project Organization and Structure

ION was the prime contractor for this project and managed the project as shown in the organizational Figure 2 below. The project consisted of a single budget period with project award starting in June 2019 and finishing in May 2022. The period accounts for COVID-related and reporting adjustments to the timeline via two No-Cost Extensions (NCE) and Project Modifications to the Statement of Project Objectives (SOPO).

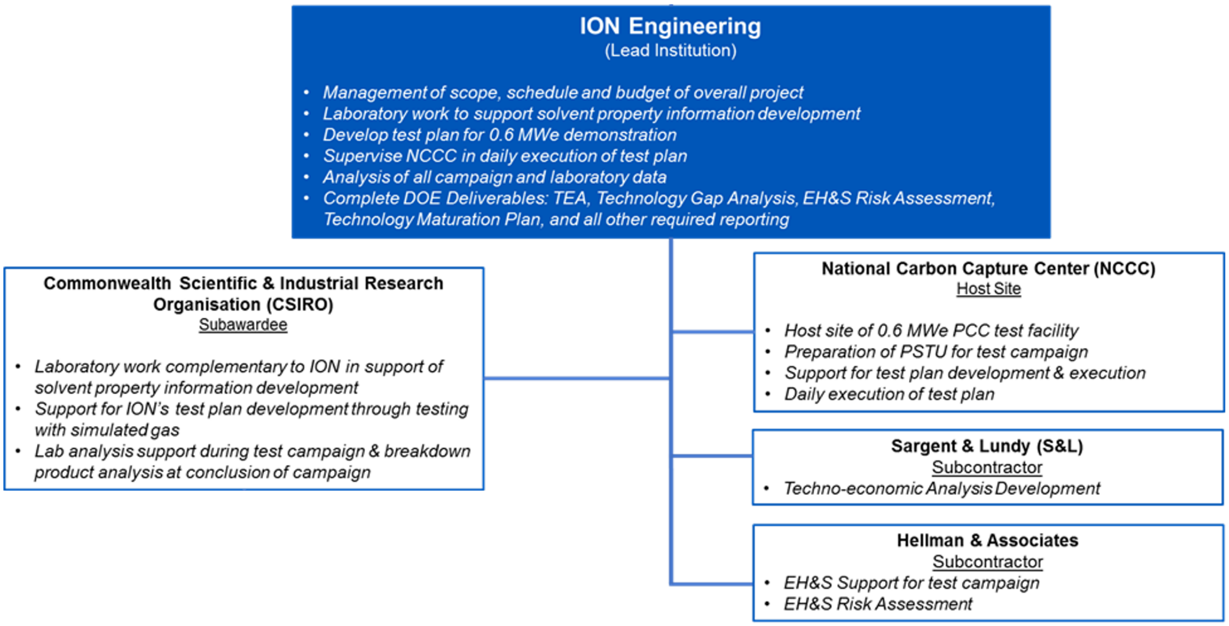

Figure 2: Overview of Integrated Project Team & Roles

ION collaborated and managed work with CSIRO to collect empirical physical properties of the ICE-31 solvent. OGT custom built a new module within OGT's software modeler, ProTreat®, to predict solvent behavior at pilot-scale operations. ION was the principal model and test plan creator before testing ICE-31 with real flue gas at the PSTU at NCCC. ION and NCCC staff closely worked together to carry out the test plan to collect meaningful data. ION contracted and utilized the expertise of S&L and Hellman & Associates to develop additional reports for large-scale design and economic development. Lastly, ION and DOE managers regularly communicated project progress and results.

Project Summary

Statement of Project Objectives

The overall objective of this project was to conduct a comprehensive bench-scale test campaign utilizing U.S. coal and natural gas fired flue gas to further understand the key performance indicators of the novel ION Capture Solvent "ICE-31" technology. The output from the test campaign, supporting laboratory work, and process modeling facilitated continued up-scaling of the technology.

Scope of Work

ION initially performed laboratory scale work to fill critical knowledge gaps of physical-chemical properties of ICE-31. This work supported the creation of the ICE-31 process module in ProTreat®. Additional lab-scale testing was performed on a 0.01 MWe test rig with simulated flue gas to provide data for early validation of the process model and support the test plan development for the bench-scale field testing. Preparations for field-testing began with test plan development and any required modifications to the NCCC's PSTU to prepare for the test campaign. Analysis of test data and reporting immediately followed the test campaign.

Project Tasks and Accomplishments

Task 1.0 – Project Management

This task included all work elements required to maintain and revise the Project Management Plan, and to manage and report on activities in accordance with the plan. It also included the necessary activities to ensure coordination and planning of the project with DOE/NETL and other project participants. These included, but were not limited to, the submission and approval of required NEPA documentation, preparation, submission, and approval of documentation in support of the Go/No-Go Decision Point.

Task 2.0 – Laboratory Scale Evaluations

Previous work has resulted in significant preliminary data on ICE-31. ION filled in critical knowledge gaps for safe and efficient plant operation as well as providing data for the development of a new module in OGT's ProTreat®.

Subtask 2.1: Lab-work for ICE-31 Properties – Using existing capabilities at the Recipient's team labs, the team filled in gaps in physical-chemical property information such as viscosity, density, kinetics, pH, vapor-liquid equilibrium, heat of reaction, material compatibility, corrosion, chemical, and thermal stability. This data supported Subtask 2.2.

Subtask 2.2: Develop ICE-31 Process Model – A new module in ProTreat® was developed for process modeling to support the techno-economic analysis (TEA) and development of a comprehensive test plan for efficient field-testing.

Subtask 2.3: Thermal and Oxidative Stability Study – Thermal and oxidative degradation studies was through a collaborative effort of the team. In the Solvent Degradation Rig (SDR), the solvent was exposed to various simulated flue gas compositions while held at typical operating temperatures. The information obtained from these studies led to a better understanding of the breakdown reaction pathways to optimize operating conditions in the field-testing campaign. Breakdown components of the ICE-31 system were identified and quantified as possible.

Subtask 2.4: PDF Operation – A 0.01 MWe test rig that utilized simulated flue gas was employed for preliminary performance evaluation of ICE-31. The data collected during this period fed forward into the test plan development for the 0.6 MWe operation with real flue gas at the NCCC PSTU and was used as preliminary data for the process model validation.

Task 3.0 – Host Site Preparation and Test Plan Development

This Recipient addressed the activities that are necessary to prepare for the field-testing.

Subtask 3.1: Develop Campaign Test Plan – A detailed test plan was developed, where the activities were defined into work packages that would address campaign objectives and provide high-quality data, resulting in essential values for the Key Performance Indicators (KPIs). KPIs of interest for this campaign included CO_2 capture efficiency, energy consumption (heating and cooling), solvent make-up rate, working capacity, column temperature profiles, emission profiles and efficacy of reclaimer. As part of the test plan, a detailed sampling plan was developed.

Subtask 3.2: Campaign related Environment, Health & Safety (EH&S) – The focus of this task was to evaluate and assemble all necessary information to determine the potential environmental, safety & health of the project and test campaign. The activity entailed assessing laboratories and the field-testing site at NCCC.

Subtask 3.3: Host Site Preparation – This subtask covered host site preparation including procurement of the solvent; identification and installation of any modifications required for the ICE-31 campaign; review and updates to any operating procedures to ensure safe operation; pilot plant recommissioning; set up of remote monitoring/ communication with the Recipient; and preparations for advanced emission related measurements.

Task 4.0 – Field Testing at 0.6 MWe PCC Plant

The Recipient conducted an extensive test campaign of ICE-31 at NCCC’s PSTU on real flue gas. The test campaign executed the detailed test plan, including emission measurements and progressive solvent evaluation to support KPIs.

Subtask 4.1: 0.6 MWe PCC Operation Phase I – This subtask covered the parametric and steady state operations of the 0.6 MWe NCCC PSTU. This operation was in accordance with the approved test plan, developed in Subtask 3.1, including the detailed sampling plan.

Subtask 4.2: Analysis and Phase I data evaluation – As per the sampling plan, developed in Subtask 3.1, samples subtask dealt with analyzing, identifying, and if possible, quantifying breakdown products and relating them to plant operation. Data of Phase I was preliminarily analyzed to determine KPI values, trends, and conclusions in preparation of Phase II (Subtask 4.3).

Go/No-Go Decision Point

In accordance with the “Go/No-Go Decision” term in this Cooperative Agreement, DOE funding was not authorized beyond Subtask 4.2 without the written approval of the Contracting Officer. DOE’s decision whether to authorize funding beyond Subtask 4.2 was specifically based on satisfactory achievement of the following success criteria:

Go/No-Go Decision Success Criteria:

- PSTU water balance within 10% of set-point targets for at least 6 hours
- Solvent make-up rate during steady-state operation below MEA baseline (< 1.5 kg/tCO_2)
- New ProTreat model converges on PSTU

ION successfully demonstrated completion of the above-mentioned tasks and, therefore, received written confirmation from the Contracting Officer to continue past this gate and continue the project with Subtask 4.3 and beyond.

Subtask 4.3: 0.6 MWe PCC Operation Phase II – This subtask covered the upsets and dynamic operations of the 0.6 MWe NCCC PSTU. This operation was in accordance with the approved test plan, developed in Subtask 3.1, including the detailed sampling plan.

Subtask 4.4: Data Evaluation – All data from plant operations was managed and stored in one database according to the Data Management Plan. Data was analyzed extensively to determine KPI values, trends, and conclusions.

Subtask 4.5: Decommissioning – Upon completion of normal operations and solvent testing, ICE-31 was removed from the PSTU and disposed of according to the host site’s disposal requirements. Relevant modifications were disassembled as agreed with host site; for example, the removal of MLAs from the host-site. Successful storage of all relevant campaign data was assessed and confirmed.

Task 5.0 – Analytical Reporting for DOE Metrics

ION utilized the data collected during the project to analyze ICE-31 performance including completion of DOE metrics.

Subtask 5.1: Process Model Validation – This subtask included all activities necessary to validate the ProTreat® module for ICE-31 with the results from the PSTU.

Subtask 5.2: Techno-Economic Analysis (TEA) – This subtask included all activities necessary to complete a TEA, as defined in Appendix D of DE-FOA-0001792.

Subtask 5.3: State Point Data Table – This subtask included all activities necessary to complete a relevant State Point Data Table, as defined in Appendix C of DE-FOA-0001792.

Subtask 5.4: Technology Gap Analysis – This subtask included all activities necessary to complete a Technology Gap Analysis, as defined in Appendix E in Section IX of DE-FOA-0001792.

Subtask 5.5: Environmental Health and Safety Risk Assessment – This subtask included all activities to complete an EH&S Risk Assessment as defined in Appendix F of DE-FOA-0001792.

Subtask 5.6: Technology Maturation Plan – This subtask included all activities necessary to complete a Technology Maturation Plan as defined in Appendix B in Section IX of DE-FOA-0001792.

Subtask 5.7: Final Reporting – This subtask included all activities necessary for completion of reporting requirements for DOE including Deep-Dive results presentation and Final Report.

Laboratory Scale Evaluations of ICE-31

Lab-work for ICE-31 Properties

Laboratory scale work was performed to fill critical knowledge gaps of physicochemical properties of ICE-31. This work supported the creation of the ICE-31 proprietary process module in ProTreat®. These physical and chemical properties included: molecular weight, heat capacity, density, viscosity, surface tension, thermal conductivity, vapor pressure, vapor-liquid equilibria (VLE), mass transfer rates, reaction kinetics, carbamate stability constants, and infinite dilution diffusivity. The empirical data of all properties were collected at various temperatures and CO_2 loading concentrations.

Develop ICE-31 Process Model in ProTreat®

In addition to the empirical data collected for the above-mentioned physical and chemical properties, additional lab-scale testing was conducted on a 0.01 MWe (equivalent) test rig with simulated flue gas to provide data that ION used for early validation of the process model and creation of the test plan for the bench-scale field testing.

From November 2019 to November 2020, Optimized Gas Treating (OGT) built and developed a new module within the carbon capture simulation software ProTreat®. This time span included their agreement formation and execution, empirical data transfer, beta versions of the new module in the software, and final initial version before testing at NCCC. ION used beta versions of the software produced by OGT and used it to create the test plan for the PSTU campaign.

Thermal and Oxidative Stability Study in the Solvent Degradation Rig

This section summarizes the performance of the ICE-31 solvent under oxidative and thermal stability stress testing. These experiments were performed using a bench scale CO_2 absorber-desorber apparatus that helped develop the Test Plan for the latter part of the testing campaign. This absorber-desorber apparatus is a Solvent Degradation Rig (SDR). The SDR consists of small-scale packed CO_2 absorption and stripping columns connected via a cross-flow heat exchanger in a typical configuration used for CO_2 capture processes. The SDR was operated continuously for four weeks with a synthetic gas mixture of air and CO_2. Other than the addition of water for level control and periodic sampling for subsequent analysis, the solvent remained in the system untouched for the duration of the operation.

The work undertaken in the SDR consisted of two experiments conducted with ICE-31 and inlet gas CO_2 and O_2 compositions representing those of a flue-gas from combined cycle gas firing and coal firing. These compositions were:

- Inlet CO_2 4 vol%, O_2 17 vol%, N_2 balance (natural gas combined cycle type flue-gas)
- Inlet CO_2 12 vol%, O_2 6 vol%, N_2 balance (coal-type flue-gas)

Samples were collected during the experiments and analyzed for the concentration of solvent and selected degradation products. ION determined the initial solvent quantities and make-up rates for the PSTU campaign from this SDR experiment.

Test Plan Overview

ION Clean Energy tested its proprietary solvent, ICE-31, at NCCC beginning in March 2021 and extending through October 2021. Prior to testing, a detailed test plan was provided by ION with the following primary objectives for technological development:

- Verify chemical reaction kinetics of the solvent at various liquid flow rates and packing heights as a function of partial CO_2 pressure
- Investigate solvent system response to transient and ramped operation
- Validate the OGT Process Model for all heating, cooling, and electrical duties needed at large scale
- Test advanced stripper heat integration such as the cold-rich bypass or the advanced flash stripper (AFS)
- Calculate the solvent consumption rate per tonne of CO_2 captured at ideal operations with NGCC or coal flue gas
- Quantify the solvent techno-economic performance throughout testing
- Determine the effect of the water wash sections on the emissions profile
- Determine process stability in response to upstream upsets such as high contaminants, high flue gas temperature, low flue gas temperature, etc.

Methodology

Overview of PSTU Standard Operations

The Pilot Solvent Test Unit (PSTU) is a 0.6 MWe CO_2 capture pilot unit at NCCC. The primary flue gas utilized for the test campaign was provided from a natural gas packaged boiler and has a concentration of roughly 7-8% CO_2 which can then be cooled and diluted with air to NGCC flue gas CO_2 content (4.4% CO_2) prior to introduction to the PSTU absorber. Pre-treated coal-derived flue gas was also used for tests at about 12% CO_2 supplied by the host site E.C. Gaston coal-fired power station. The CO_2 absorption section contains three 6-meter beds of Sulzer Mellapak^{TM} 252Y structured packing. The lean solvent travels down the column, absorbing CO_2 while the flue gas flows up the column. Due to the exothermic nature of the CO_2 absorption, the flue gas at the top of the column is significantly warmer than the inlet flue gas. Thus, a water wash vessel cools the flue gas to within a few degrees of inlet flue gas temperatures and restores water balance via recirculating, cooled wash water. The CO_2-lean flue gas exits the PSTU through an NCCC or Gaston stack for release to atmosphere, depending on sources of flue gas used.

Exiting the bottom of the absorber, the CO_2-rich solvent gravity-flows into a buffer tank. The rich solvent is then pumped through the lean-rich cross exchanger where it exchanges heat with the lean solvent and enters the top of the regenerator. The rich solvent flows down the regenerator, releasing CO_2 and absorbing water vapor while CO_2 and water vapor from the reboiler flow up the column. The semi-lean solvent falls to the stripper sump and recirculates through a forced-convection reboiler, which utilizes steam to heat the solvent and removes CO_2 to achieve lean loading. The lean solvent is then recirculated back to the absorber through the lean-rich heat exchanger for further CO_2 capture. The CO_2 out of the top of the stripper is cooled and then released to the atmosphere via the stack (Figure 3).

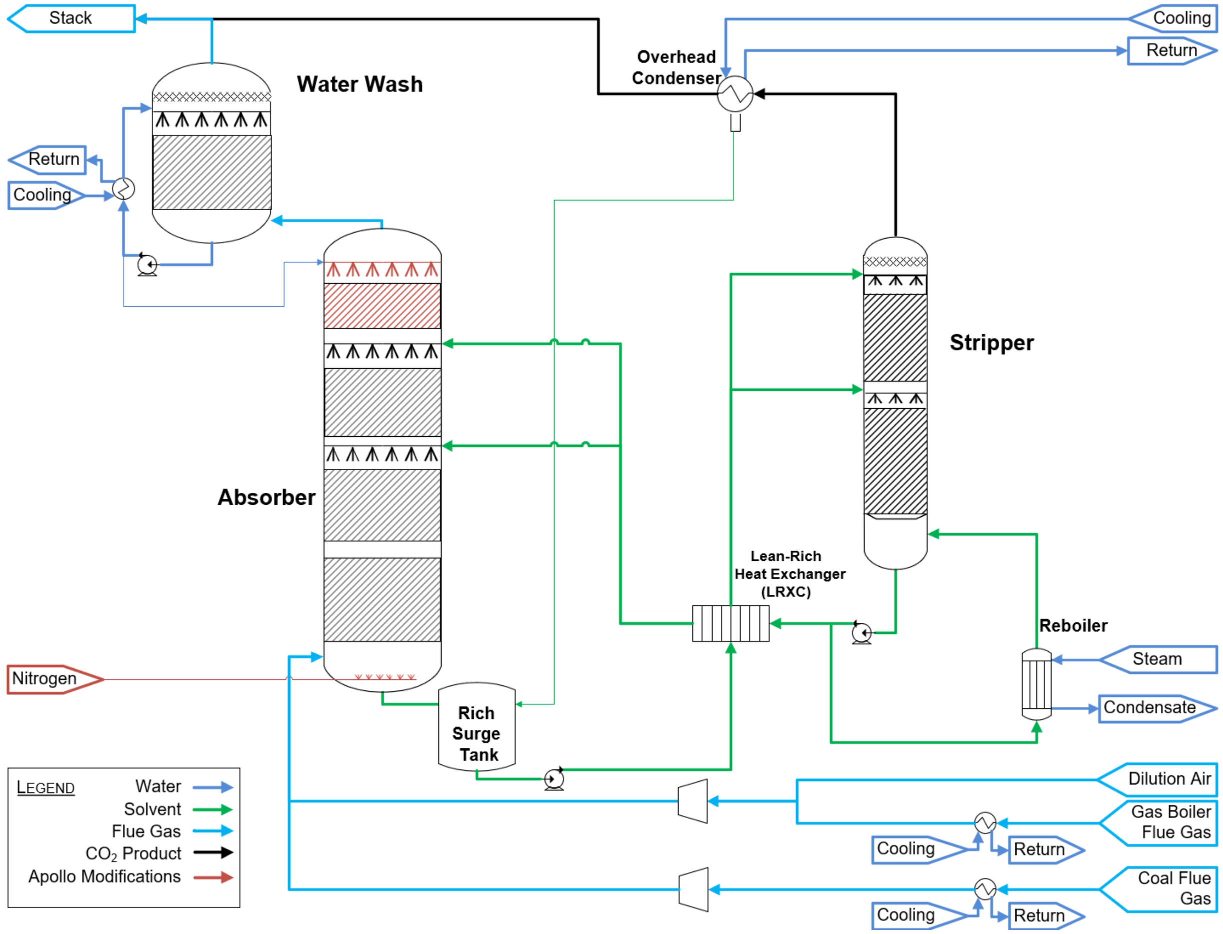

Figure 3: Process Flow Diagram for ICE-31 Operation at the PSTU

PSTU modifications for ION testing

Before testing, ION requested several modifications to the PSTU:

- Installation of a Sulzer distributor and packing system designed specifically for solvent absorption in carbon capture water washes. This fourth bed allowed for countercurrent gas-liquid mass transfer of solvent vapors into the water wash solution which significantly reduces solvent emissions.

- A bypass line feeding the regenerator from the cold-rich solvent upstream of the lean/rich heat exchanger. This cold rich bypass (CRB) was split fed to the regenerator with a portion entering above the top bed and with the main flow entering above the bottom bed.

- ION's Multi-component Liquid Analyzer (MLA) was installed on the cold lean solvent feed (immediately upstream of the absorber) to provide continuous, real-time analysis of all major solvent components including water and CO_2.

PSTU Advanced Flash Stripper Operations

In some of the work packages, ION opted to use the existing Advanced Flash Stripper (AFS) configuration which is similar to the simple regenerator but with an incorporated heat exchange system. In the AFS, the rich solvent from the buffer tank is first split, so a portion goes to a gas/liquid heat exchanger to exchange heat from the hot CO_2 out of the stripper. Similarly, after the first lean-rich heat exchanger, the other portion of warm-rich solvent bypasses the heat exchanger and enters directly in the top of the stripper. Lean solvent exchanges heat with the remaining portion of rich solvent. Finally, the hot-rich solvent passes through a once-through forced convection steam heater and then flashes into the bottom of the stripper. When operating the AFS on the PSTU, the absorber and water wash operations are identical to the simple regenerator operation.

Testing and Results Methodology

Measuring Specific Reboiler Duty (SRD)

Over the first two months of testing, ION focused on parametric testing where 70 individual test points were measured. Each data point was recorded once both the SRD and capture efficiency were constant within 1% over the course of 30 minutes. The most important output from the parametric data was the Specific Reboiler duty (SRD), defined by Equation 1.

$$SRD[=]\frac{GJ}{tonne\ CO_2} = \frac{Reboiler\ Heat\ Duty - Ambient\ Heat\ Loss}{CO_2\ Captured} \qquad \text{Eq 1}$$

The reboiler heat duty was calculated from the overall flow of steam ($\dot{m}_{steam}$) into the reboiler multiplied by the enthalpy differential between the steam conditions into the reboiler and the condensate conditions coming out (Equation 2).

$$Reboiler\ Heat\ Duty[=]\frac{GJ}{hr} = \dot{m}_{Steam}(H_{steam} - H_{condensate}) \qquad \text{Eq 2}$$

The captured CO_2 was measured on the absorber side of the process as the difference between CO_2 going in and coming out of the absorber (Equation 3).

$$CO_2\ Captured[=]\frac{tonnes}{hr} = \dot{m}_{Flue\ Gas\ in}C_{CO_2\ in} - \dot{m}_{Flue\ Gas\ Out}C_{CO_2\ out} \qquad \text{Eq 3}$$

During the campaign ION measured the heat loss for the simple stripper configuration to estimate the ambient heat losses for the PSTU. For this measurement, the simple stripper was operated at standard gas and liquid flows but at a very low steam input. Under these operating conditions, most of the heat is lost to the atmosphere and only a small portion of the reboiler heat goes towards regenerating the solvent. To isolate the effects of temperature swings throughout the day, the data was analyzed and averaged over two days. Ambient heat loss was calculated at 60 MJ/hr under heat loss conditions, which extrapolates to 80 ± 10 MJ/hr at the standard reboiler temperature. Ambient heat loss accounts for a significant amount of overall heat duty for NGCC flue gases and must be properly considered in Equation 1 above to improve the accuracy of the modeling results. During heat-loss testing, the steam rate was set at a low setpoint, and the capture efficiency was therefore lower. With a set steam rate, the capture efficiency was directly observed to fluctuate due to the ambient heat losses without any other process changes for two day/night cycles (Figure 4). Instead of attempting to account for changing ambient conditions, ION utilized an average heat loss term for all SRD calculations knowing this could add up to 1% deviation in SRD depending on the ambient losses. The same heat loss test was performed for the AFS configuration with the determined average heat loss of 70 MJ/hr.

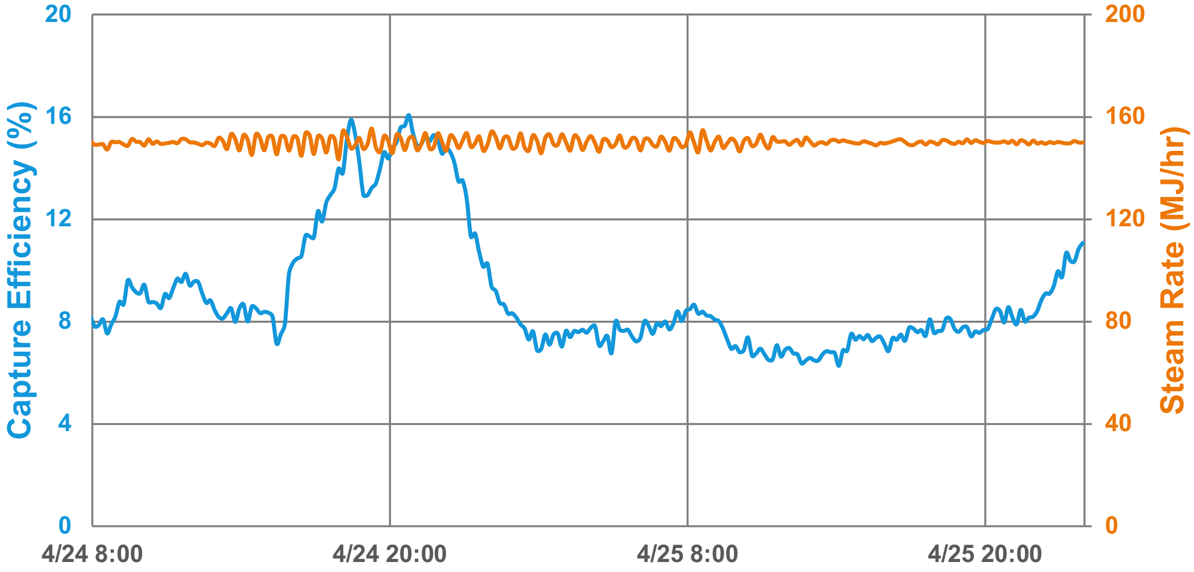

Figure 4: Capture efficiency variation during heat-loss testing due solely to ambient condition changes

Solvent Analysis

Solvent samples on both the lean and rich side were taken during each test condition throughout the parametric testing and at least three times a week during the long-term, steady-state testing. These samples were analyzed at NCCC's laboratories as well as in ION's laboratory in Boulder, CO.

The major organic components were quantified in Boulder using an Agilent 7890B gas chromatograph (GC) with a thermal conductivity detector. An Agilent capillary column was used for separation with helium as the carrier gas. A standard calibration curve was constructed using five different concentrations of known standards encompassing the full expected concentration range of components in the samples. All analyses were performed at a minimum in triplicate. Analysis of trace components and decomposition products were performed using an HP 6890 GC coupled with a 5973 mass spectrometer using electron impact ionization. The compounds were separated using a capillary column with helium as the carrier gas. For qualitative analysis, a mass range of 33 to 250 amu was scanned and for quantitative analysis the instrument was set to scan for the highest abundant fragment ion of each species using single ion monitoring. Heat-stable salts (HSS) were qualitatively and quantitatively analyzed using a Dionex ICS-5000+ ion chromatography system with a potassium hydroxide eluent generator and conductivity detector. The anions were separated using a Dionex analytical column and an AERS 500 electrolytically regenerated suppressor was used to eliminate background conductivity. A standard calibration curve was constructed using five different concentrations of known standards encompassing the full expected concentration range of anions in the samples. All analyses were performed in triplicate. The CO_2 loading of the solvent was determined using a UIC, Inc. CM-5015 coulometer in conjunction with a CM5200 acidification module. The water concentration was determined using a Mettler-Toledo V30 volumetric Karl-Fischer titrator.

Emissions Analysis

The flue gas outlet of the PSTU was equipped with a Gasmet DX4000 hot-gas FTIR. The sample was pulled through a heated line into the FTIR where the spectra was then analyzed for main solvent components as well as degradation products. Both the outlet of the lower water wash (LWW) and the upper water wash (UWW) were tested during the campaign. Table 1 provides the spectra range for the solvent-specific components analyzed along with the approximate limit of detection in the process gas. Water, CO_2, and NO were also analyzed using their standard wavenumbers. Residuals for the spectra were very low ranging from 0.001 to 0.003 for the analyzed species.

Table 1: Emissions Analysis on Outlet Flue Gas

Component	Wavenumber [cm^{-1}]	Lowest Calibration Standard [ppm]	Limit of Detection [ppm]
Solvent Component(s)	2700 – 3150	30	~ 3
NH_3	1650 – 1550	10	~ 2
CH_2O	n.d.	25	~ 3

Three extractive samples were taken during long-term testing at the UWW outlet and sent to RJ Lee Group for analysis. ICE-31 components were analyzed via OSHA PV2145 based on the actual compound; the NH_3 was quantified with OSHA ID 188 while formaldehyde was quantified following EPA TO-11A. Extractive samples for NH_3 were significantly lower than the reported FTIR results, showing that NH_3 was typically below the limit of detection throughout long-term testing.

Results and Discussion

Parametric Testing with NGCC Flue Gas

ION analyzed ICE-31 performance over a range of operating conditions with surrogate NGCC flue gas by diluting the on-site boiler flue gas with air by approximately 50%. Table 2 gives the range of conditions and baseline condition for select operating parameters.

Table 2: Operating conditions for parametric testing with NGCC flue gas

Condition	Range	Baseline
Inlet CO_2 (vol%)	4.3 – 4.5	4.4
Capture Efficiency (%)	78 – 98	95
Absorber Packing Height (m)	12 – 18	18
L/G (kg /kg)	0.7 – 1.1	0.8

Optimal L/G at 95% Capture

ION varied the L/G ratio at 95% ± 1% CO_2 capture to determine optimal performance of the solvent at the PSTU using an absorber packing height of 18 m. For each setpoint, ION modeled the steam duty needed for 95% capture prior to changing operating conditions. The steam load was then set at a determined flow rate, and the capture efficiency was allowed to reach steady state. Due to the high accuracy of the ProTreat® model, the capture efficiency was almost always within the range of the target capture rate, allowing relatively smooth and quick transitions between setpoints. The optimal lean loading is a balance between increasing carrying capacity of the solvent to limit sensible heat loss in the lean/rich cross exchanger and increasing lean loading in the stripper bottoms to better utilize stripping steam. Under these conditions, there was a wide optimal L/G range where these two effects balanced the SRD within 1% of the minimum (Figure 5). The wide range for optimal performance allows a more robust design of a large-scale facility without concern that solvent energy performance will be significantly different than the guarantees. The ProTreat® model predicted the same optimal range of performance based directly on the equipment at the PSTU.

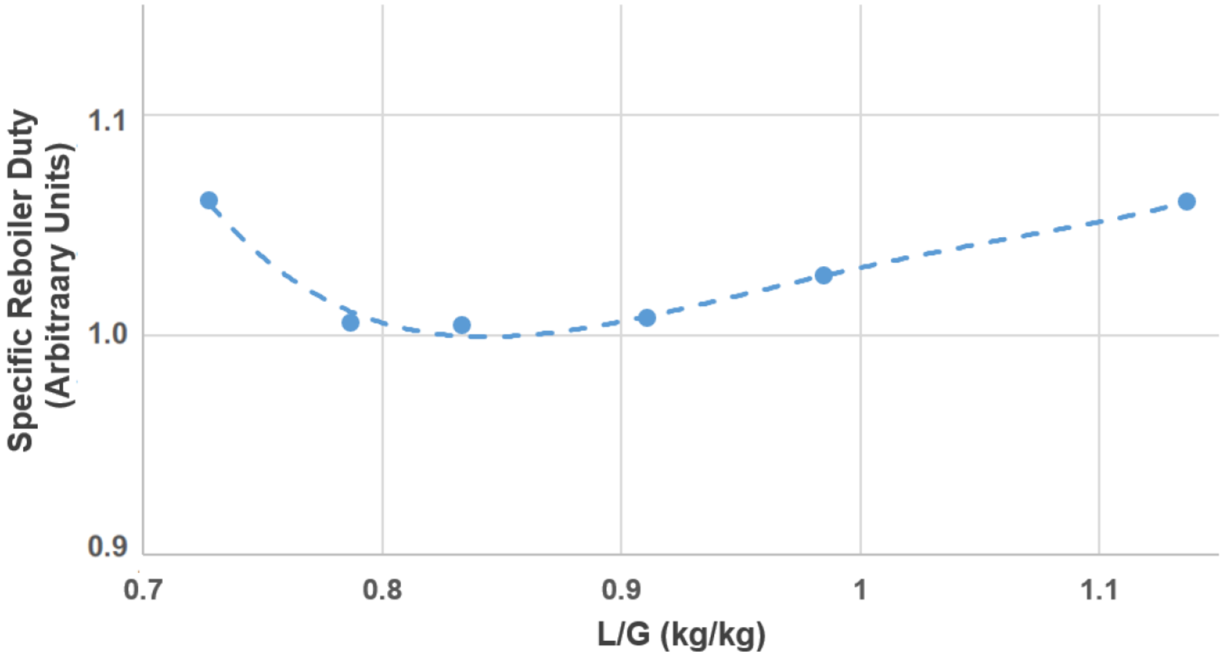

Figure 5: Optimal SRD at PSTU: 95% CO_2 capture with 4.4% inlet CO_2, 18 m of MP252.Y absorber packing

SRD versus Capture Efficiency

Another work package focused on varying the capture efficiency of the PSTU while simultaneously choosing optimal L/G ranges to determine minimum SRD performance at each capture efficiency. Both 12 m and 18 m absorber heights were tested for each capture efficiency; a 24 m absorber height was also modeled in ProTreat after parametric testing (Figure 6). With 18 m of packing, the CO_2 mass transfer into the solvent was fast enough to reach a similar rich loading across the entire capture efficiency range. The lean loading became leaner as CO_2 capture efficiency increased, but due to the high heat of absorption of the ICE-31 solvent, the stripper sump temperature increased only 5 °C going from 78 % to 98 % CO_2 capture efficiency. The overall impact of the fast kinetics and favorable thermodynamics of ION's ICE-31 solvent demonstrate that there is only a 4% SRD penalty when increasing capture from 90% to 98%, even when using a simple stripper. Further optimization with cold-rich bypass allows even leaner optimal lean loadings and a smaller penalty when increasing capture efficiency. When utilizing 12 m of packing in the absorber, the rich loading approached equilibrium for the 80% and 87% carbon capture data points. However, the solvent could not reach its optimal rich loading at higher capture efficiencies, leading to an SRD penalty of 14% when increasing capture from 87% to 95%. The large energy penalty for high capture with 12 m of packing demonstrates the importance of optimizing packing height along with capture efficiency when designing for higher capture rates. However, there is little benefit to additional absorber packing above 18 m until the facility approaches carbon-neutral capture efficiencies.

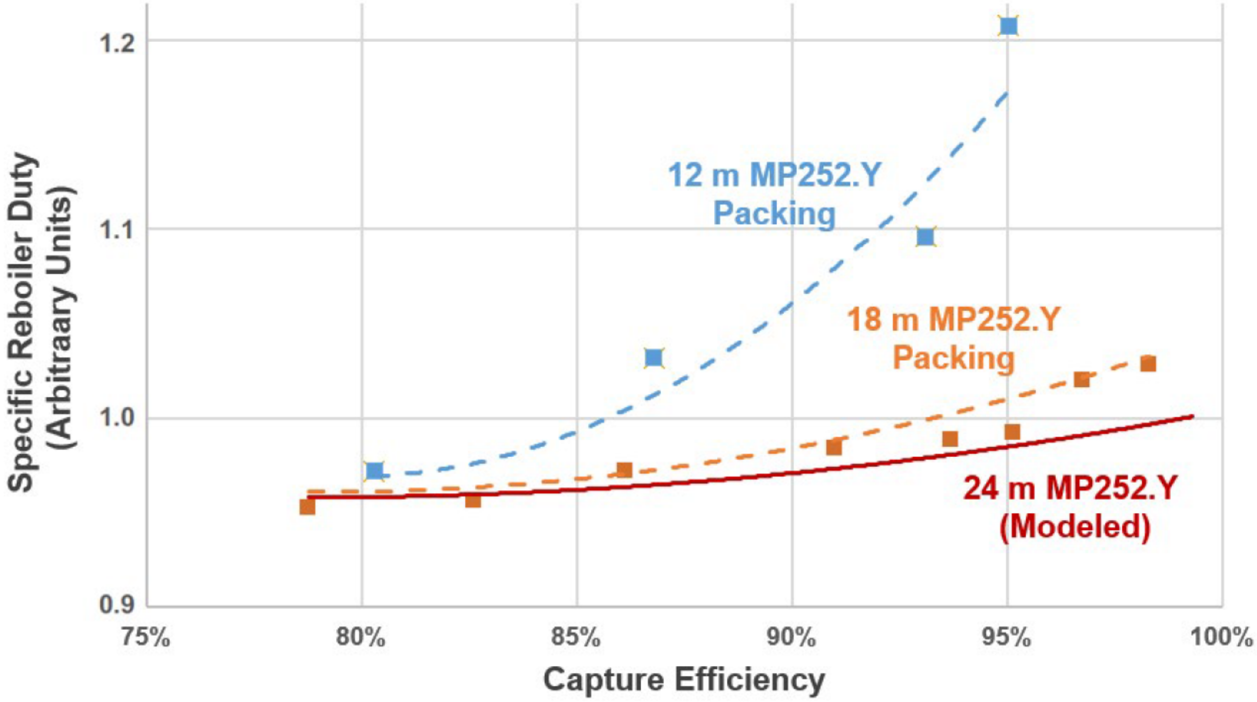

Figure 6: SRD at Optimal L/G for varying capture efficiencies with 4.4% inlet CO_2 measured at 12 m MP252.Y and 18 m MP252.Y absorber packing height and modeled at 24 m MP252.Y absorber packing height

Optimal SRD Using the Advanced Flash Stripper (AFS)

Similar to the simple stripper tests, ION ran a series of Advanced Stripper tests with varying capture efficiencies at optimal solvent flow and ratios for both the cold-rich and warm-rich bypasses. The Advanced Flash Stripper took significantly longer to stabilize than simple-stripper operation, so only one operating point was tested per day. The Advanced Flash Stripper outperformed the Simple Stripper by 12-14% across all capture efficiencies (Figure 7). The lower SRD was possible due to the lower overhead stripper temperature, which fell about 40 °C when utilizing the optimal cold-rich and warm-rich ratios. Because of the heat capacity differences between the lean and rich solvents, the bypasses shift the temperature pinch to the hot-side of the lean-rich heat exchanger but do not significantly impact the total heat exchanged. The AFS operation empirically demonstrated an SRD of 2.7 GJ/tonne CO_2 at 95% CO_2 capture from an NGCC flue gas. With optimized equipment and ION's substantially similar heat-integrated process, ICE-31 will provide an SRD of 2.6 GJ/tonne CO_2 at 95% CO_2 capture from an NGCC flue gas.

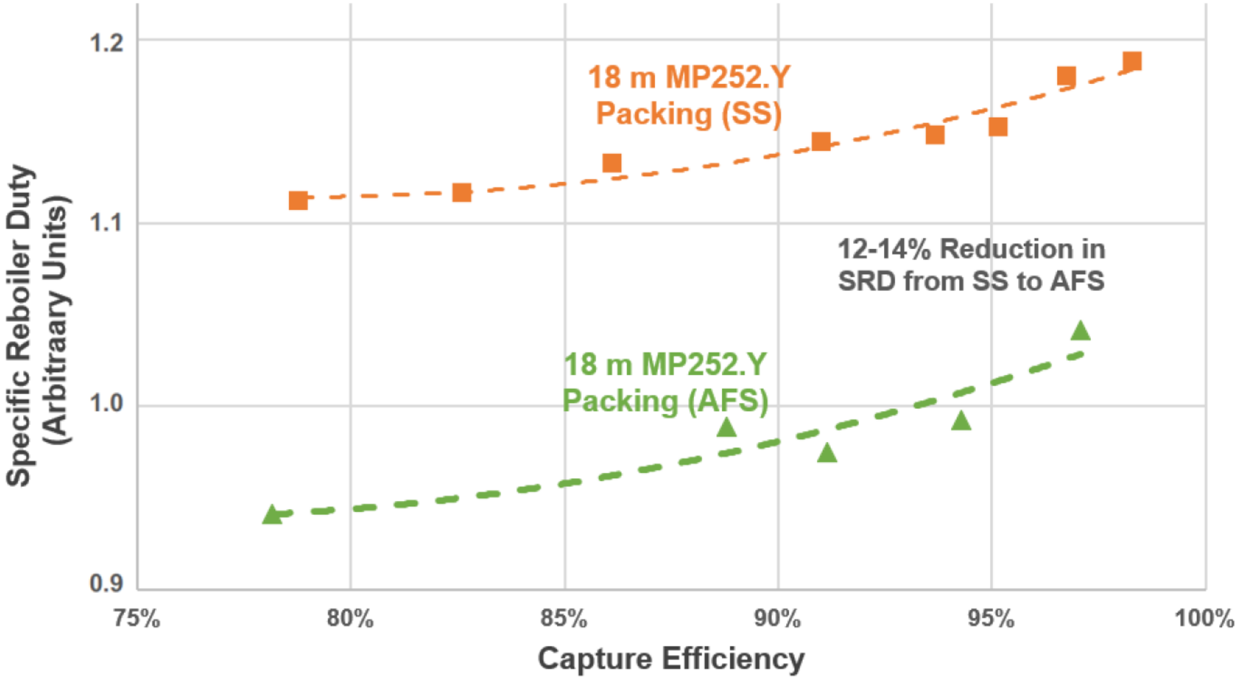

Figure 7: SRD at optimal process conditions for varying capture efficiencies utilizing both the Simple Stripper (squares) and Advanced Flash Stripper (triangles) with 4.4% inlet CO_2

Parametric Testing with Undiluted Natural Gas-Fired Boiler Flue Gas

ION analyzed ICE-31 performance over a range of operating conditions with undiluted boiler flue gas using the PSTU simple stripper to determine optimum performance both on PSTU equipment and for large-scale applications. Table 3 gives the range of conditions and baseline condition for select operating parameters.

Table 3: Operating conditions for parametric testing with undiluted boiler flue gas

Condition	Range	Baseline
Inlet CO_2 (vol%)	7.2 – 7.4	7.2
Capture Efficiency (%)	74 – 98	95
Absorber Packing Height (m of MP252Y)	12 – 18	18
L/G (kg /kg)	1.3 – 1.8	1.5

Optimal L/G at 95% Capture

Similar to the NGCC flue gas, ION varied the L/G ratio at 95% ± 1% CO_2 capture to determine optimal performance with boiler flue gas using the simple stripper and an absorber packing height of 18 m. Under these conditions, there was a wide optimal L/G range of 1.5 ± 0.1 kg/kg where the SRD was within 1% of the minimum (Figure 8). Two points at 1.4 and 1.5 kg/kg showed significant error compared to the trend, possibly due to changes in inlet flue gas temperatures, which were not controlled during this testing.

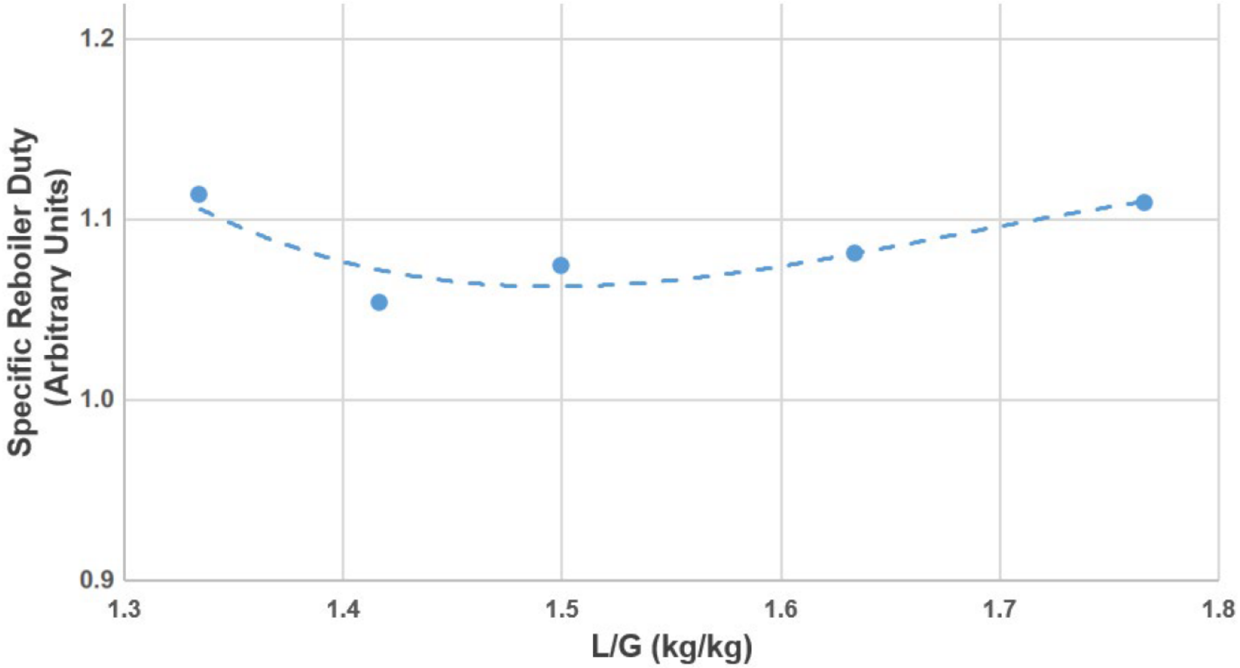

Figure 8: Optimal SRD at PSTU: 95% CO_2 capture with 7.2% inlet CO_2, 18 m of MP252.Y absorber packing

SRD Increase with Capture Efficiency

ION also varied the capture efficiency for the undiluted boiler flue gas while simultaneously choosing optimal L/G ranges for minimum SRDs. Both 12 m and 18 m absorber heights were tested for each capture efficiency (Figure 9). The overall impact of the fast kinetics and favorable thermodynamics demonstrate that there is only a 6% energy penalty in SRD when increasing capture from 90% to 98%, even when using a simple stripper. When utilizing 12 m of packing in the absorber, the rich loading approached equilibrium for the 73% and 86% capture data points. However, the solvent could not reach its optimal rich loading at higher capture efficiencies, leading to an SRD penalty of 11% when increasing capture from 86% to 93%.

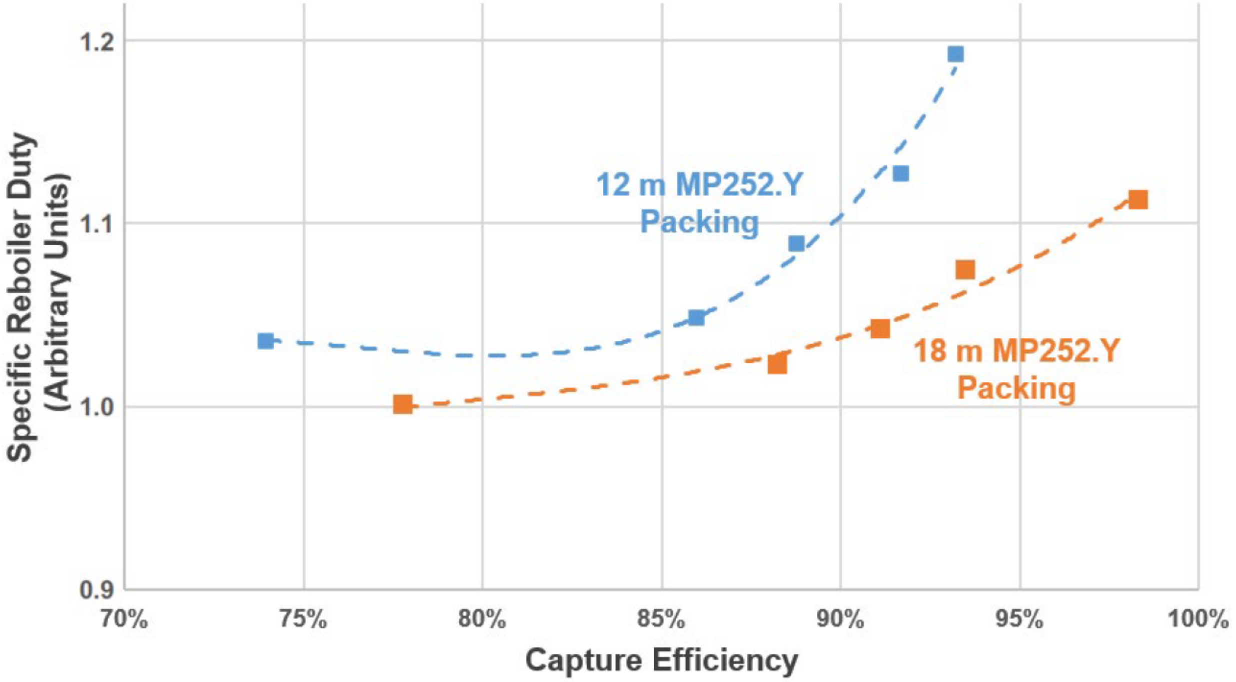

Figure 9: SRD at optimal L/G for varying capture efficiencies with 7.2% inlet CO2 measured at 12 m MP252.Y and 18 m MP252.Y absorber packing height

Parametric Testing with Coal Flue Gas

ION analyzed ICE-31 performance over a range of operating conditions with coal flue gas from Plant E.C. Gaston using the PSTU simple stripper. Table 4 gives the range of conditions and baseline condition for select operating parameters.

Table 4: Operating conditions for parametric testing with undiluted boiler flue gas

Condition	Range	Baseline
Inlet CO_2 (vol%)	10.2 – 11.7	11
Capture Efficiency (%)	94 – 96	95
Absorber Packing Height (m of MP252Y)	18	18

Optimal L/G at 95% Capture

ION again varied the L/G ratio at 95% ± 1% CO_2 capture to determine optimal performance with coal flue gas using the simple stripper and an absorber packing height of 18 m. Under these conditions, the optimal L/G was 1.9 kg/kg at an SRD of 2.9 GJ/tCO_2 (Figure 10). The coal flue gas had the lowest SRD of all flue gases due to its high CO_2 partial pressure at the absorber bottom. However, there was not a significant decrease in SRD over the NGCC and boiler flue gas cases because the solvent achieves a high rich loading with all three flue gas types.

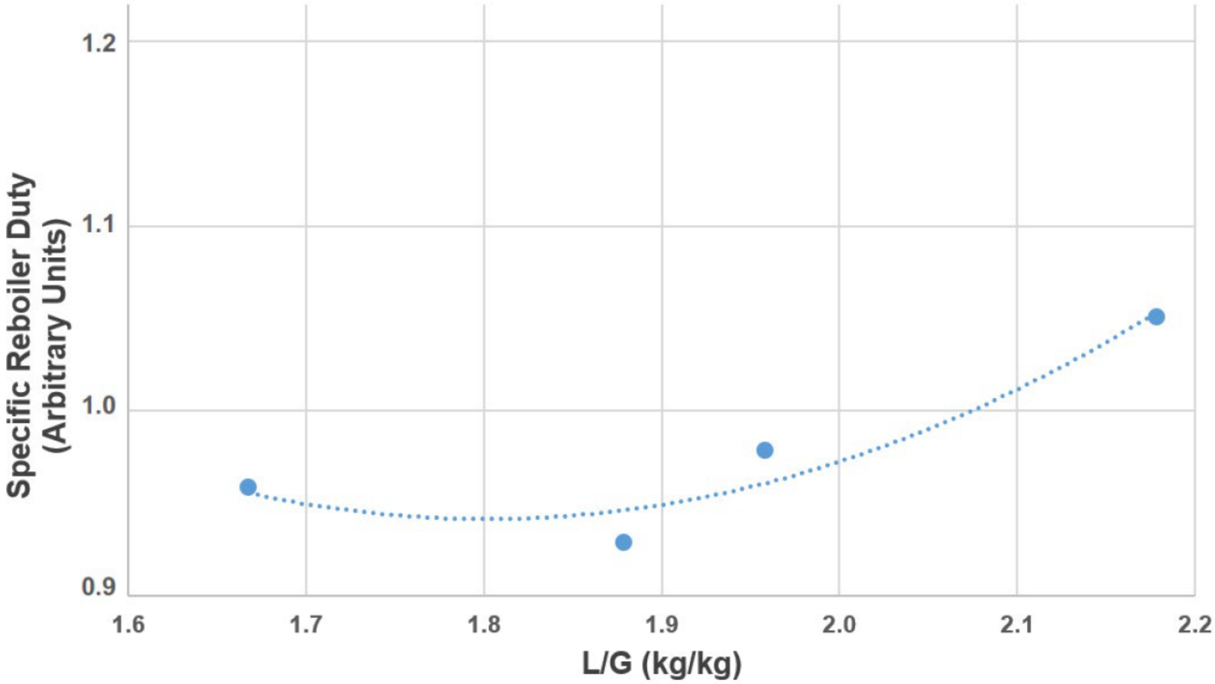

Figure 10: Optimal SRD at PSTU: 95% CO_2 capture with 11% inlet CO_2, 18 m of MP252.Y absorber packing

ProTreat® Model Validation

A two-part approach was taken for determining optimum performance of the ICE-31 solvent for the techno-economic analysis. First, the results for the simple stripper cases were thermodynamically and kinetically validated in OGT's ProTreat® process modeling tool. These validated results were then used to build a process model with stripper heat integration for the large-scale systems needed in the techno-economic evaluation of a full-scale carbon capture plant on a supercritical, coal-fired facility. Second, the benefits of heat integration were empirically tested on both coal and natural gas using the AFS equipment at the PSTU. These empirically show the 12-14% reduction in SRD compared to the simple stripper operation that the ProTreat® model predicts.

ProTreat® was validated against the simple stripper data using a process model that matches the PSTU mass and heat transfer equipment (Figure 11). Packing heights and packing types used the default values built into the ProTreat® model, which have been validated directly with Sulzer's test facilities. The lean-rich heat exchanger (LRXC) is significantly over-sized for the lower solvent flows needed for the high-capacity ICE-31. Thus, the pressure drop across the LRXC was less than 1 psi and flow was laminar. Instead of attempting to model the heat transfer coefficient so far from the LRXC design point, the shortcut heat transfer method was used with the measured temperature approach on the cold side as an input. The overall model was iteratively solved for reboiler heat duty necessary to achieve the experimental CO_2 capture as determined by the flue gas outlet mole fraction. For simple stripper and lower water wash operation, streams 202 and 304 were modeled at 1% of streams 209 and 303 respectively. Table 5 gives the other main inputs and outputs from the ProTreat® validation models. All parametric test conditions reported above were validated and reported in the ProTreat® process models.

Table 5: Select inputs and outputs for ProTreat® process model validation

Stream #	Input	Output
101 (Dilution Air In)	Flow, Pressure, Temperature, Composition	
100 (Flue Gas In)	Flow, Pressure, Temperature, Composition	
301 (Absorber Rich Outlet)	Flow	Temperature, CO_2 Loading
205 (Water Wash Recirculation)	Flow	
208 (Water Wash Recirculation)	Temperature	
104 (CO_2 Out)	CO_2 Mole Fraction	Solvent Mole Fraction, Temperature
501 (Stripper CO_2 Outlet)	Pressure	Temperature, Water Content
Absorber		Max Temperature
Stripper		Specific Reboiler Duty (SRD)
403 (Stripper Lean Outlet)		Temperature, CO_2 Loading

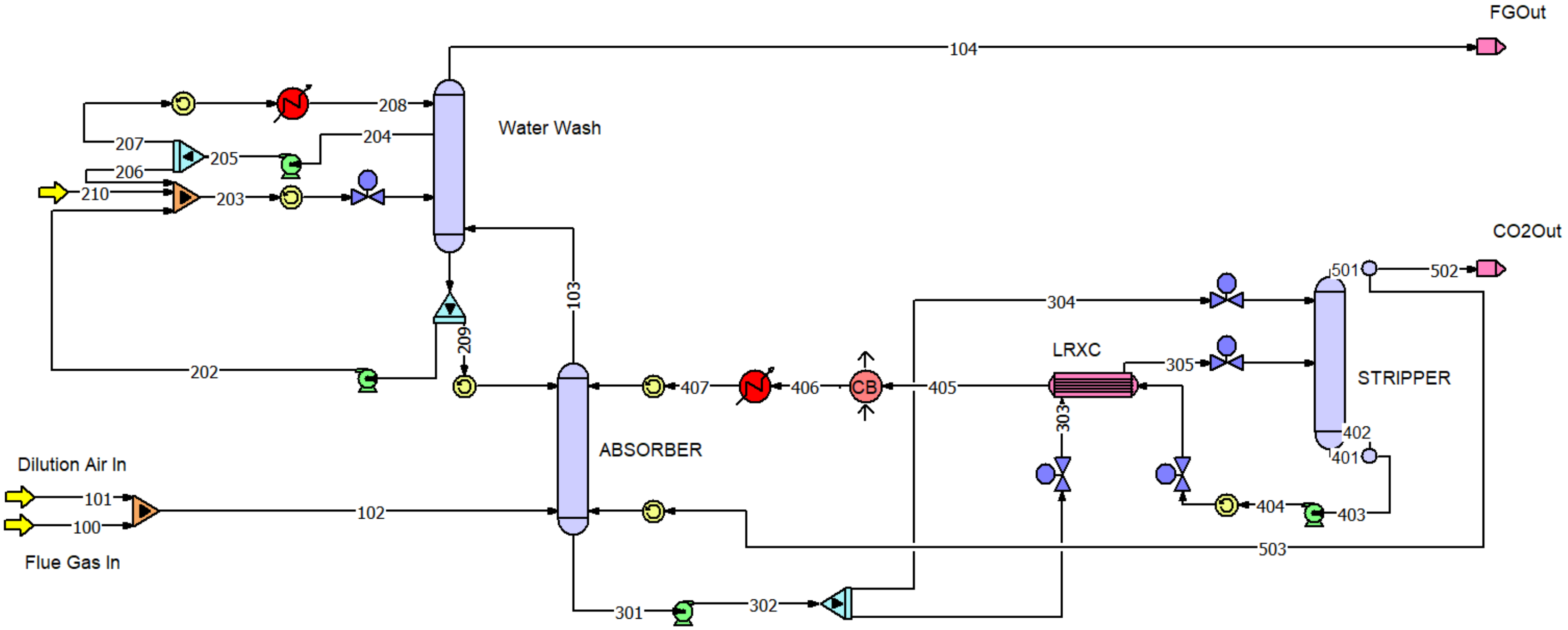

Figure 11: ProTreat® process model for simple stripper validation

Process Model Fit for SRD

ProTreat® models closely validated the NCCC results for SRD over the wide range of flue gas, capture efficiency, and flow rate parametric test conditions. The average error for SRD was only 0.4% with a standard deviation of 1.7% (Figure 12). The very close fit proves the robust nature of the thermodynamic and kinetic framework with the ICE-31 module inside OGT's ProTreat® software. This imparts strong confidence in ION's ability to model energy performance for large-scale systems and minimizes the risk in utility costs associated with those projects. The maximum error was 3% and was associated with the two outliers at high SRD's. These two points were run at the highest capture efficiency with only two absorber beds and consequently had significantly lower rich loading than the other points. These points are far away from standard operating conditions for ICE-31 and can be avoided in large-scale applications by optimizing absorber height along with capture efficiency.

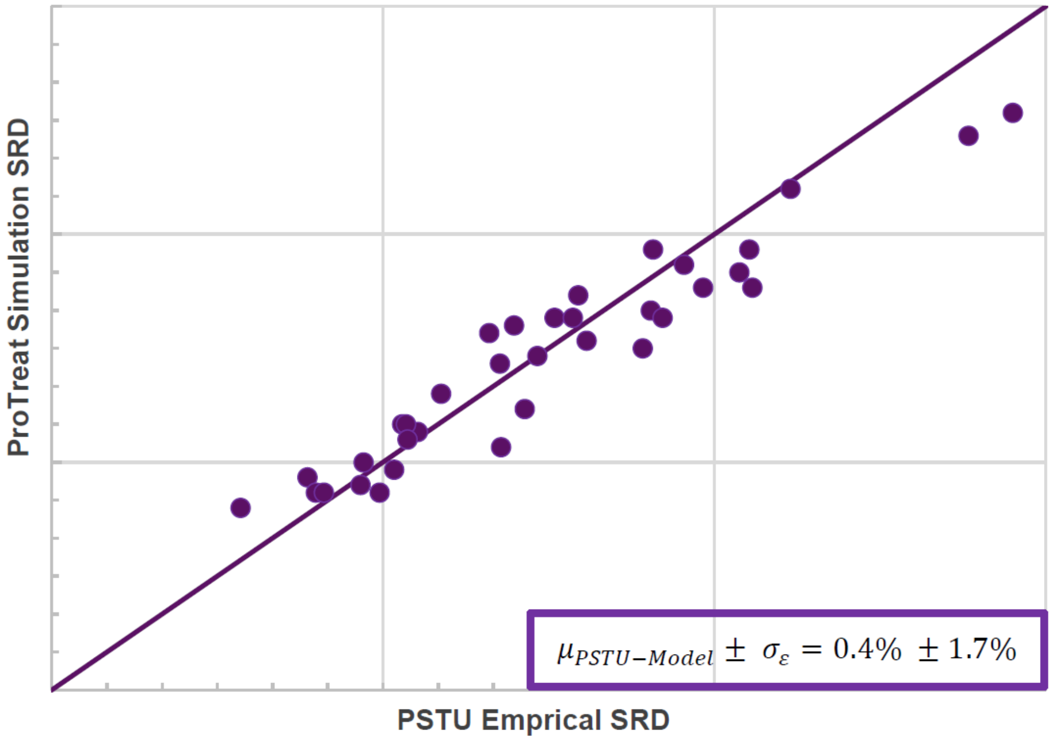

Figure 12: ProTreat® process model validation versus empirical results for SRD

ProTreat® Process Model Fit for Other Key Performance Indicators

Results from the process model were also used to validate the cooling and pumping loads for a large-scale facility. To determine this, model temperatures and solvent CO_2 capacity at key process points were compared to empirical results. ProTreat® was able to simulate process conditions at all points in the process model with extremely good fit. In all cases, the PSTU empirical results are not statistically different than the ProTreat® simulated results (Figure 13)

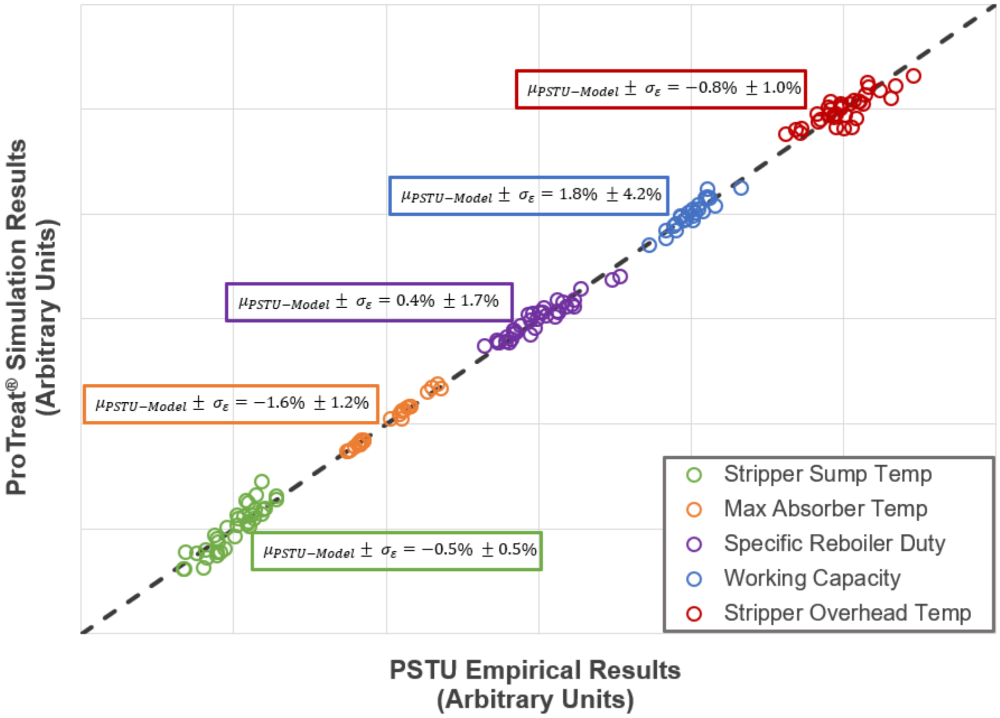

Figure 13: ProTreat® process model validation for other empirical results

Long-Term Steady State Testing

A critical test during the campaign was long term steady-state testing to determine the overall stability of the ICE-31 solvent. For this test, ION maintained optimal plant performance with NGCC flue gas for 1,500 hours. The conditions for the long-term operation are shown below (Table 6).

Table 6: Operating conditions for long-term steady state

Condition	Value
Inlet CO_2 (vol%)	4.4
Capture Efficiency (%)	95
Absorber Packing Height (m of MP252Y)	18
L/G (kg /kg)	0.8 – 0.9

PSTU on time during the long-term operation was very high with only minor operational upsets. With almost a constant steam input, ION was able to maintain 100% of expected CO_2 capture output throughout the test. Minor shutdowns due to boiler performance were made up by operating at slightly higher than 95% average capture efficiency (Figure 14 & Figure 15).

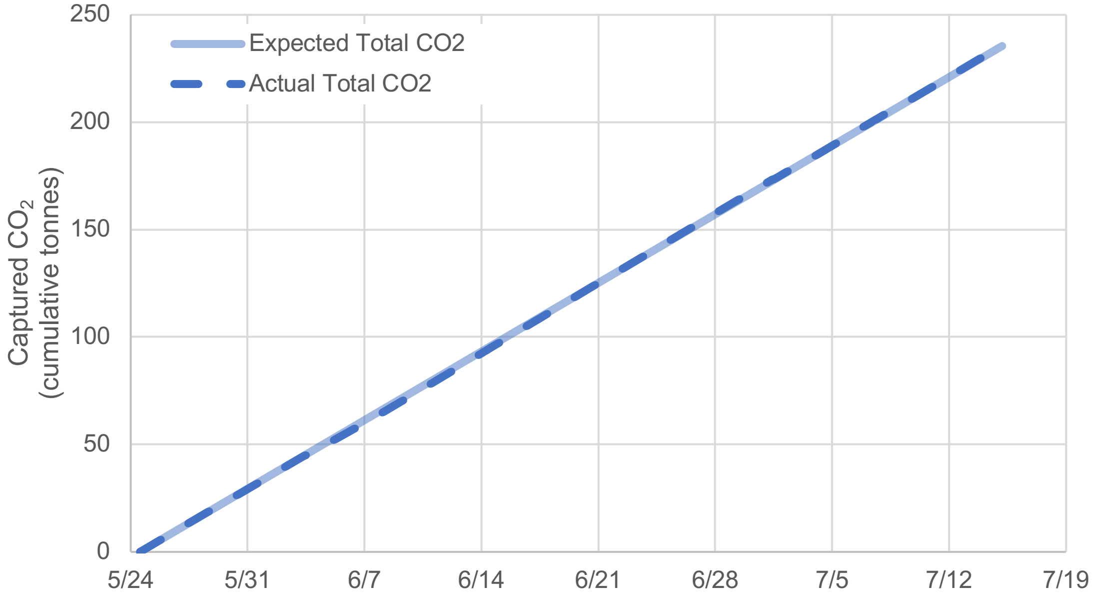

Figure 14: Total CO_2 captured during long-term steady-state operation

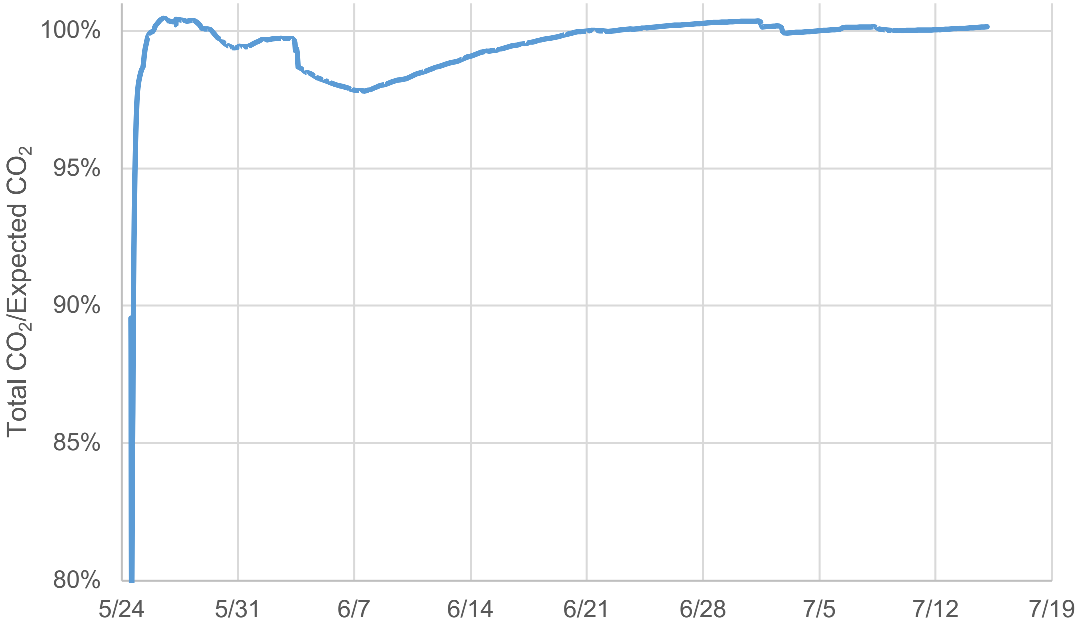

Figure 15: Comparison of Total Captured CO_2 over Expected Captured CO_2

Capture Efficiency and SRD

Since the steam rate was almost entirely constant throughout the long-term test campaign, the overall SRD at the expected capture efficiency was close to constant, only increasing 3% over the 1,500 hours of operations (Figure 16). The capture efficiency was also maintained with only minor drops. Each drop was attributed to a change in the steam flowmeter calibration that tended to drift significantly during testing. After re-calibrating the steam flowmeter, capture efficiency always returned to its previous point (Figure 17).

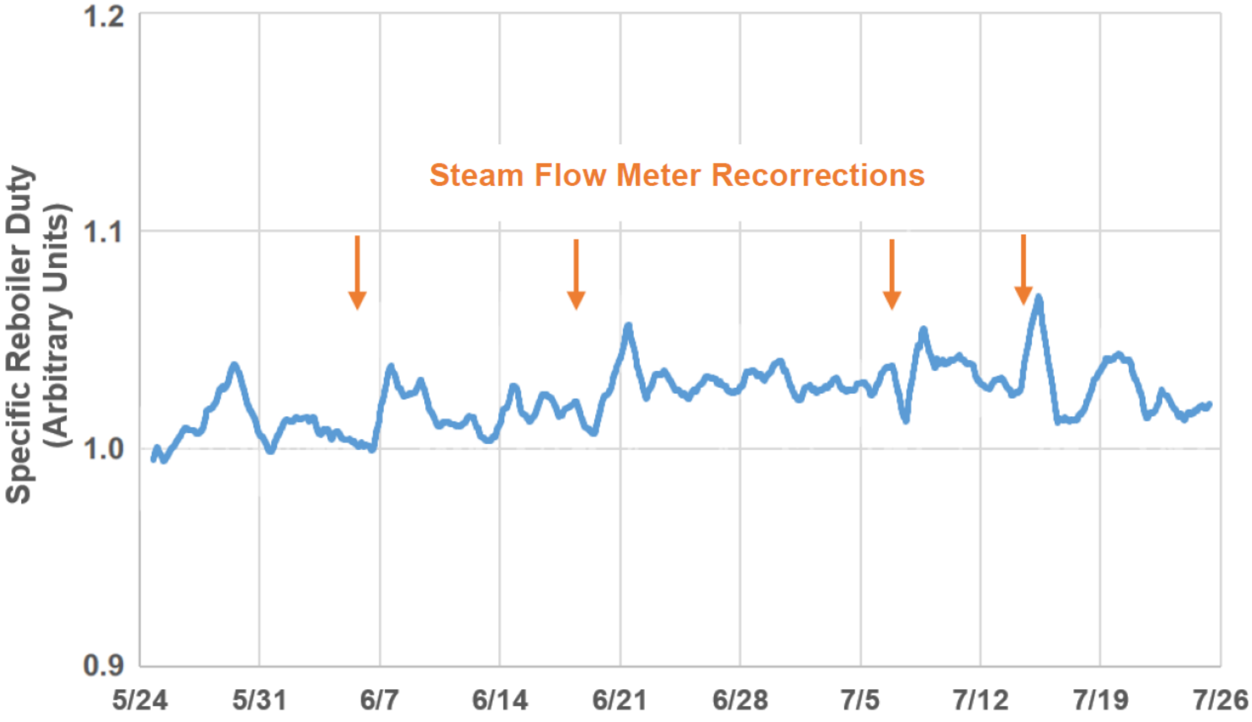

Figure 16: SRD during long-term operations; spikes in SRD correspond to suspected steam flowmeter corrections

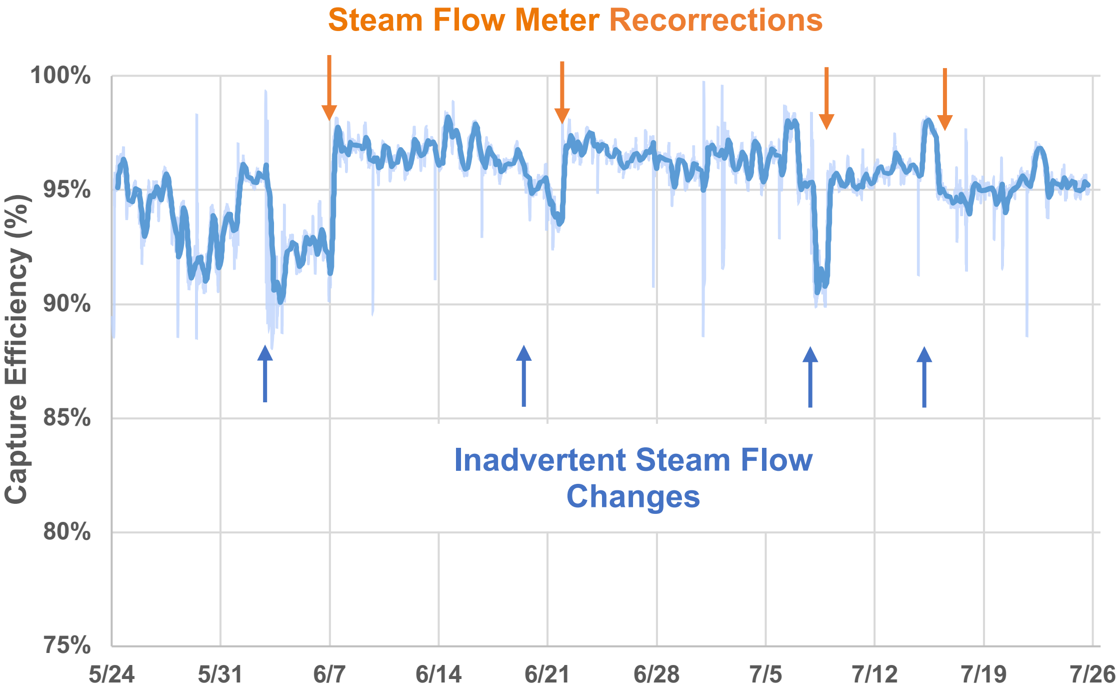

Figure 17: Capture efficiency for long-term operation (6-hr average)

Long-Term Emissions for Ammonia

The PSTU emissions were continuously monitored out of the water wash via a GASMET FTIR. Ammonia (NH_3) was the only emitted species detected by the FTIR with the overall spectra showing extremely low residuals. The FTIR typically reported NH_3 at 3-4 ppm outlet with a few days reporting as high as 7 ppm. The extractive sampling result showed NH_3 at 0.76 ppm when the FTIR reported 3.5 ppm, suggesting that the FTIR can only qualitatively determine NH_3 at the low ppm levels.

Long-Term Emissions for Solvent Components

Solvent components were also analyzed through both the FTIR and the extractive sampling. Components were below the quantitation limit of the FTIR throughout long-term testing and below the 40 ppb quantitation limit from RJ Lee. Since ION could not analyze the flue gas outlet from the UWW, the focus shifted to LWW outlet. Once again, solvent components were at the FTIR detection limit after the lower water wash. To determine the impact of the LWW, ION stopped wash water flow to the LWW for approximately an hour and then restarted flow. The FTIR showed a lag of approximately 40 minutes while the LWW packing saturated with solvent vapors. Solvent concentration in the flue gas then increased to 430 ppm before the LWW wash water flow was re-activated. Immediately, the wash water absorbed solvent emissions until they were once again below quantification (Figure 18). The LWW absorbed over 99% solvent vapors during the test, demonstrating the low volatility of the ION solvent when utilizing the dual-stage water wash.

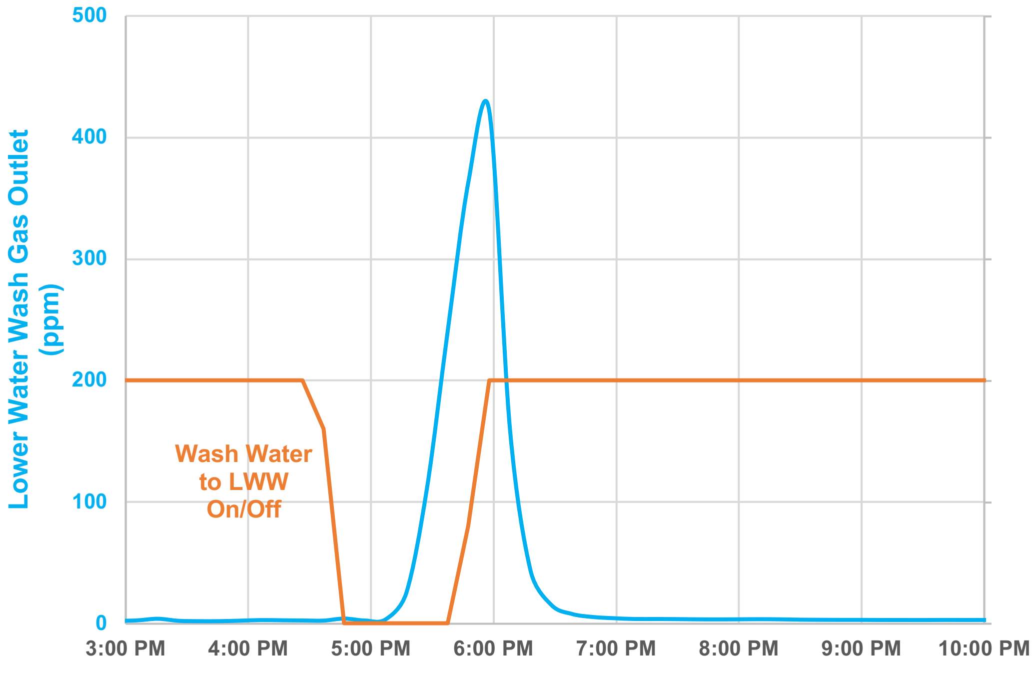

Figure 18: Solvent emissions response to LWW operation

Furthermore, the UWW circulating wash water was analyzed for solvent components to understand the amount of carryover from the LWW. During parametric operation, the wash water flow to the LWW turned off 1-5 times a day for up to half an hour at a time to maintain water balance. However, during long-term operations, the operators had a much better understanding of the wash water rate and were able to maintain continuous wash water flow for almost the entire 1,500-hour month test. When the LWW was in continuous operation, solvent component concentration in the UWW recirculating loop dropped over 50-fold from 1600 ppm to roughly 30 ppm (Figure 19). During coal testing and AFS parametric testing, the operators were able to maintain continuous wash water flow and extremely low solvent concentrations in the UWW circulating loop.

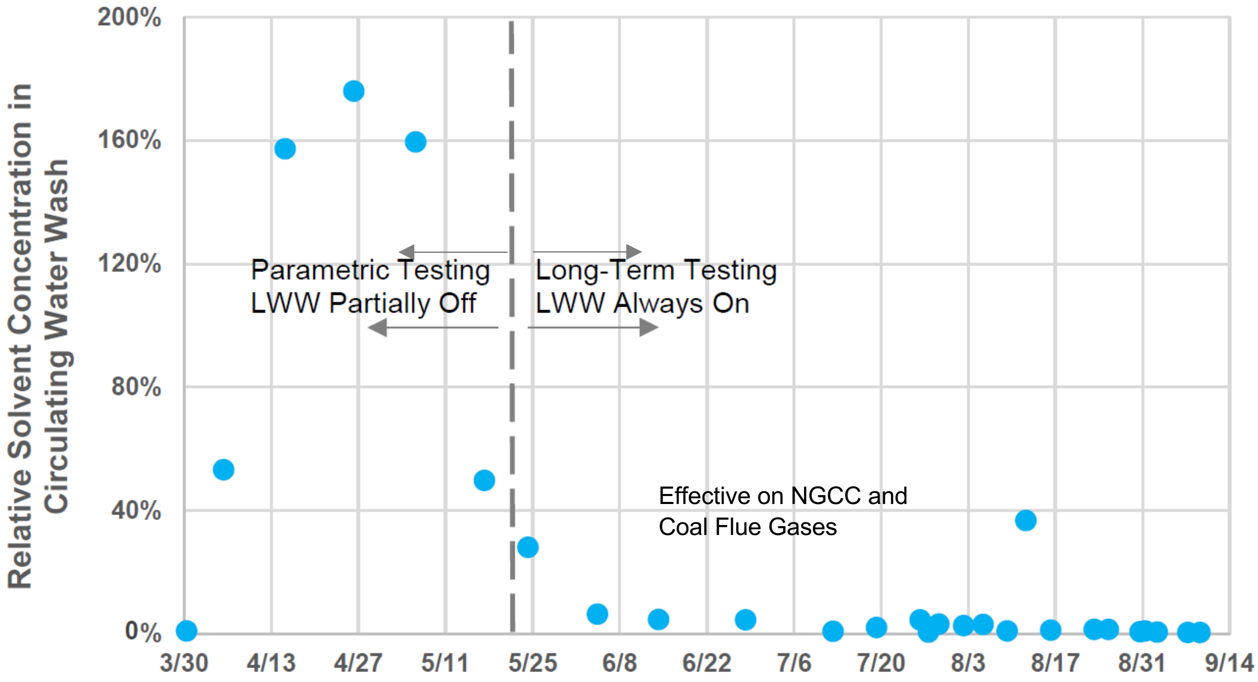

Figure 19: Solvent concentration in circulating upper wash water with different lower water wash operating conditions

Active Component Analysis

Lean samples from the long-term campaign were analyzed for all active components, CO_2, and water to determine the degradation rate of active components. Since total system inventory was constant throughout the testing, water content remained within a narrow range of 48-53% wt%. However, to account for any minor difference in water content between samples, all solvent analyses were normalized to 50 wt% water content. A linear regression was applied to the loss rate for the total active components and then normalized to the total CO_2 captured using Equation 6. Since the loss rate is calculated from changes in the total solvent inventory, it encompasses all forms of solvent losses at the facility such as oxidative degradation, thermal degradation, flue gas emissions, and solvent spills.

$$\text{Solvent } Loss[=]\frac{kg\ Active}{tonne\ CO_2} = \frac{\Delta C_{Active}}{\Delta \text{time}} * \frac{m_{Inventory}}{\dot{m}_{CO_2 captured}} = \text{slope} * \frac{4200\ kg\ Solvent}{4.5\ tonnes\ CO_2/day} \qquad \text{Eq 6}$$

The loss rate for the sum of active components was statistically insignificant with total active concentration varying randomly at 99 ± 1% of the starting composition (Figure 20). Longer-term testing is necessary to determine loss-rates for active components via the liquid-side mass balance.

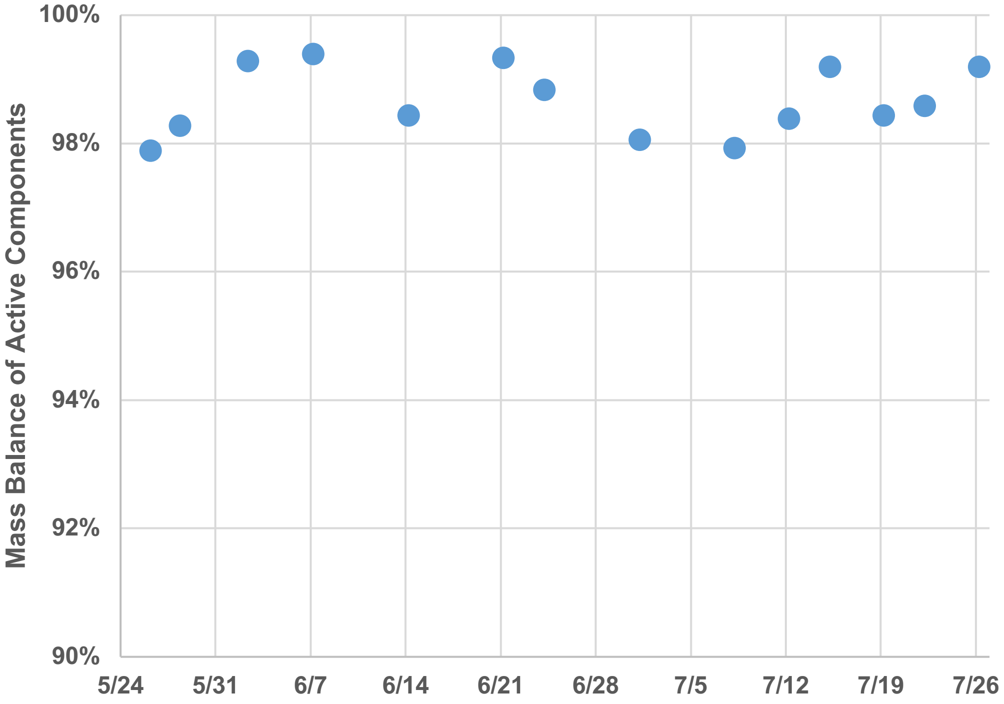

Figure 20: Total solvent component mass balance over 1,500-hour long-term campaign including active components, water, and CO_2

Heat-Stable Salt Analysis

Heat-Stable Salts (HSS) are introduced either by flue gas impurities or are the result of amine oxidation. The major HSS observed during this campaign were sulfate, Component A, nitrate, nitrite, and Component B (in order of abundance). Among them, Component A and Component B are the result of solvent degradation. Figure 21 shows the HSS content during the entire campaign; the dips in concentration on 7/28 are due to taking a significant sample after the long-term testing on natural gas-derived flue gas and replacement of that solvent with fresh solvent in preparation for testing on coal-derived flue gas.

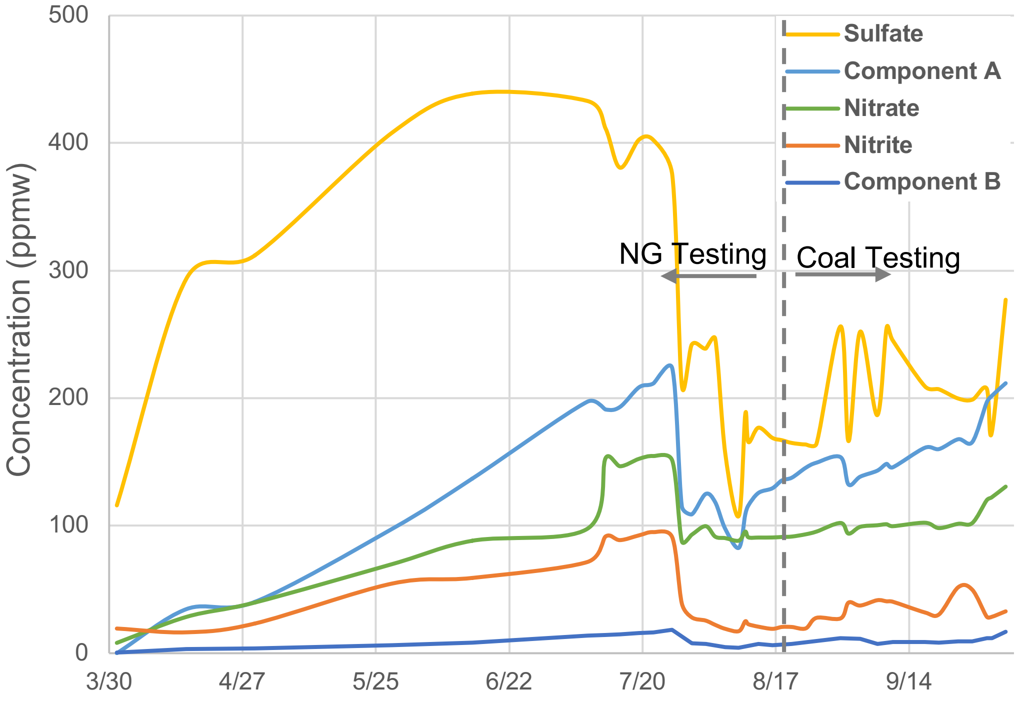

Figure 21: HSS accumulation throughout test campaign; the variation on 7/28 was due to solvent replacement upon changing from natural gas-focused to coal-focused flue gas testing

Sulfate (SO_4^{2-}) was the major HSS accumulating in the solvent. It derives from capture of SO_x (mostly SO_2) in the flue gas stream and subsequent oxidation of the intermediary sulfite (SO_3^{2-}) to sulfate. Nitrites (NO_2^-) and nitrates (NO_3^-) are the other major HSS introduced by flue gas NO_x, a mixture of gases primarily containing NO and NO_2. NO_2 is an acid gas which readily dissolves in alkaline solvents to form a mixture of nitrite and nitrate. The maximum combined nitrite/nitrate concentration was about 250 ppm at the end of the boiler gas testing (end of July) and the accumulation rate decreased thereafter.

Component A and Component B are the only HSS which were found in the solvent resulting from solvent oxidation at a maximum concentration of about 200 ppm and 20 ppm, respectively. Low heat stable salt formation demonstrates that ICE-31 does not need continuous reclaiming for flue gases with proper pretreatment.

Conclusion

ION completed a six-month testing campaign for its third-generation solvent technology, ICE-31, at the National Carbon Capture Center, confirming the remarkable performance of the solvent technology. The ICE-31 campaign at NCCC operated for over 4,000 hours including parametric and long-term steady-state testing using natural gas combined-cycle (NGCC) surrogate flue gas (4.4% CO_2), real gas-fired boiler gas (7.8% CO_2), and real coal-fired flue gas (13% CO_2).

ION demonstrated 95% CO_2 capture on all three flue gases, achieved steady-state capture efficiencies of up to 98% capture with NGCC flue gas, and reached over 99% capture during dynamic operations. Using the PSTU heat-integrated stripper (AFS) configuration, ION demonstrated a minimum SRD of 2.6 GJ/tCO_2 at 91% CO_2 capture for NGCC flue gas with a slight increase to 2.7 GJ/tCO_2 at 97% capture.

Utilizing OGT's ProTreat®, which was further validated with the empirical data from this test campaign, ION's process model predicted SRDs with an average error ± standard deviation of 0.4% ± 1.7%. The modeled performance indicates that typical U.S. facilities, where processes are optimized for capital costs due to relatively low fuel costs, ION's technology could provide SRDs of 2.6 GJ/tCO_2 for NGCC and 2.4 GJ/tCO_2 for coal-fired flue gas at 95% CO_2 capture. In high fuel cost cases, ION could further reduce SRD values.

During the long-term test on NGCC gas at 95% CO_2 capture for 1,500 hours without reclamation and without solvent make-up, the overall mass balance for original solvent components was 99 ± 1%. These results further substantiate the environmentally advantageous characteristics of the ICE-31 solvent, including extremely low solvent replacement rates in high oxygen environments. Lastly, ICE-31's stability is further demonstrated as a result of the emissions monitoring and extractive sampling – with NH_3 emissions below 1 ppm and solvent below 40 ppb, indicating very low emissions.

The process performance results confirm ION's expectations that ICE-31 is an exceptional solvent for post-combustion carbon capture in general, but more specifically is exceptionally well suited for high oxygen environments such as natural gas thermal boilers and NGCC facilities.

Appendix A: Abbreviations

AFS	Advanced Flash Stripper
CH_2O	Formaldehyde
CO_2	Carbon Dioxide
DCC	Direct Contact Cooler
FTIR	Fourier Transform Infrared spectroscopy
GC	Gas Chromatography
LRXC	Lean-Rich Heat Exchanger
HSS	Heat Stable Salts
IC	Ion Chromatography
KF	Karl Fischer water content measurement
L/G	Liquid-Gas Ratio
LLOQ	Lower Limit of Quantification
LWW	Lower Water Wash
MLA	Multi-component Liquid Analyzer
NCCC	National Carbon Capture Center
PSTU	Pilot Solvent Test Unit
SRD	Specific Reboiler Duty
TIC	Total Inorganic Carbon
UWW	Upper Water Wash
VLE	Vapor Liquid Equilibrium

Appendix B: Calculations for Capture Efficiency

CO_2 Capture Method 1:

CO_2 Capture Efficiency = $(1 - \frac{\dot{m}_{CO2,abs\,Out}}{\dot{m}_{CO2,abs\,In}}) \times 100$

<u>Tags</u> $T_{gas,\ C,\ abs\ IN}$	8610-TT-2041	$Q_{abs,IN}$	8610-FT-0150
$T_{gas,\ C,\ abs\ OUT}$	8610-TT-2035	$Q_{abs,OUT}$	8610-FT-2431A
$P_{gas,\ barg,\ abs\ IN}$	8610-PT-2040	$\%CO_{2\ IR,high,dry,abs,IN}$	8610-AI-2004A
$P_{gas,\ barg,\ abs\ OUT}$	8610-PT-2430	$\%CO_{2\ IR,high,dry,abs,OUT}$	8610-AI-2030A
$P_{ambient,\ absolute,\ mbar}$	8630-ORA-0051		

H_2O vapor pressure of both absorber in and out gas streams (P_{H2O}) are calculated from the “water97_v13.xla” Excel plugin:

P_{H2O} = pSatW($T_{gas,\ C}$+273.15)

The mole fraction of water (f_{H2O}) is taken as:

$f_{H2O} = P_{H2O}/(P_{gas,\ barg} + P_{ambient,\ absolute,\ mbar}/1000)$

The mole fraction of CO_2, corrected for water content ($f_{CO2,wet}$), is taken as:

$f_{CO2,wet} = (1-f_{H2O}) * \%CO_{2\ IR,high,dry}/100$

The CO_2 mass flow ($\dot{m}_{CO2}$) is calculated as:

$\dot{m}_{CO2,abs} = f_{CO2,wet} * Q * MW_{CO2} * P/RT$

Where Q is in Sm^3/h, T_{STD}=15°C, P_{STD}=1 bar and m_{CO2} is calculated for both inlet and outlet gas flows.

CO_2 Capture Method 2:

CO_2 Capture Efficiency = $\left(\frac{\dot{m}_{CO2,reg\ Out}}{\dot{m}_{CO2,abs\ In}}\right) \times 100$

<u>Tags</u> $T_{gas,\ C,\ abs\ IN}$	8610-TT-2041	$Q_{abs,IN}$	8610-FT-0150
$P_{gas,\ barg,\ abs\ IN}$	8610-PT-2040	$\%CO_{2\ IR,high,dry,abs,IN}$	8610-AI-2004A
$T_{gas,\ C,\ reg,\ OUT}$	8615-TT-2210	$P_{gas,\ barg,\ reg,\ OUT}$	8615-PT-2213
$P_{ambient,\ absolute,\ mbar}$	8630-ORA-0051	$\dot{m}_{reg\ Out}$	8615-FT-2215

H_2O vapor pressure of both absorber in and regenerator out gas streams (P_{H2O}) are calculated from the “water97_v13.xla” Excel plugin:

P_{H2O} = pSatW($T_{gas,\ C}$+273.15)

The mole fraction of water (f_{H2O}) is taken as:

$f_{H2O,abs} = P_{H2O}/(P_{gas,barg,abs,OUT} + P_{ambient,\ absolute,\ mbar}/1000)$

$f_{H2O,reg} = P_{H2O}/(P_{gas,barg,reg,OUT} + P_{ambient,\ absolute,\ mbar}/1000)$

The mole fraction of CO_2, corrected for water content ($f_{CO2,wet}$), is taken as:

$f_{CO2,wet,Abs\ In} = (1-f_{H2O}) * \%CO_{2\ IR\ high,dry,\ abs\ In}/100$

The CO_2 mass flow ($\dot{m}_{CO2}$) is calculated as:

$\dot{m}_{CO2,abs\ In} = f_{CO2,wet,Abs\ In} * Q * MW_{CO2} * P/RT$

Where Q is in Sm^3/h, T_{STD}=15°C, P_{STD}=1 bar and m_{CO2} is calculated for both inlet and outlet gas flows.

The mass fraction of CO_2 in the product gas (w_{CO2}) is calculated as and is needed because the CO_2 product flow is measured in mass flow (kg/hr):

$w_{CO2} = (1 - f_{H2O,reg}) * MW_{CO2} /[f_{H2O,reg} * MW_{H2O} + (1 - f_{H2O,reg}) * MW_{CO2}]$

CO_2 product mass flow ($\dot{m}_{CO2,REG}$) is calculated as:

$\dot{m}_{CO2,reg\ Out} = w_{CO2,reg\ Out} * \dot{m}_{Reg\ Out}$

CO_2 capture method 3 (inert pass-thru):

CO_2 Capture Efficiency = $\left(1 - \frac{\dot{m}_{CO2,abs\,Out}}{\dot{m}_{CO2,abs\,In}}\right) \times 100$

<u>Tags</u>

$T_{gas,\,C,\,abs\,IN}$	8610-TT-2041	$Q_{abs,IN}$	8610-FT-0150
$T_{gas,\,C,\,abs\,OUT}$	8610-TT-2035	$\%CO_{2\,IR,high,dry,abs,IN}$	8610-AI-2004A
$P_{gas,\,barg,\,abs\,IN}$	8610-PT-2040	$\%CO_{2\,IR,high,dry,abs,OUT}$	8610-AI-2030A
$P_{gas,\,barg,\,abs\,OUT}$	8610-PT-2430		
$P_{ambient,\,absolute,\,mbar}$	8630-ORA-0051		

H_2O vapor pressure of both absorber in and out gas streams (P_{H2O}) are calculated from the “water97_v13.xla” Excel plugin:

P_{H2O} = pSatW($T_{gas,\,C}$+273.15)

The mole fraction of water (f_{H2O}) is taken as:

$f_{H2O} = P_{H2O}/(P_{gas,\,barg} + P_{ambient,\,absolute,\,mbar}/1000)$

The mole fraction of CO_2, corrected for water content ($f_{CO2,wet}$), is taken as:

$f_{CO2,wet} = (1-f_{H2O}) * \%CO_{2\,IR,high,dry}/100$

The CO_2 mass flow ($\dot{m}_{CO2,\,Abs\,In}$) into the absorber is calculated as:

$\dot{m}_{CO2,abs} = f_{CO2,wet} * Q * MW_{CO2} * P/RT$

Where Q is in Sm^3/h, T_{STD}=15°C, P_{STD}=1 bar and m_{CO2} is calculated for both inlet and outlet gas flows.

To calculate the mass flow ($\dot{m}_{CO2,\,Abs\,Out}$) out of the absorber, assume inert content fraction is:

$f_{Inert} = 1 - f_{H2O} - f_{CO2,wet}$

Then the volumetric flow out of the absorber is equal to:

$Q_{\text{abs,OUT}} = Q_{\text{abs,IN}} * (T_{\text{gas, C, abs OUT}} / T_{\text{gas, C, abs IN}}) * (P_{\text{gas, barg, abs IN}} / P_{\text{gas, barg, abs OUT}}) *$

$(1 - f_{\text{H2O,Abs In}} - f_{\text{CO2,wet,abs In}}) / (1 - f_{\text{H2O,abs Out}} - f_{\text{CO2,wet,abs Out}})$

The CO_2 absorber out mass flow ($\dot{m}_{\text{CO2,abs Out}}$) is calculated as:

$\dot{m}_{\text{CO2,Abs Out}} = f_{\text{CO2,wet}} * Q_{\text{abs Out}} * MW_{\text{CO2}} * P/RT$

Where Q is in Sm^3/h, T_{STD}=15°C, P_{STD}=1 bar

Appendix C: Techno-Economic Assessment (TEA)

DE-FE0031727:

PROJECT APOLLO

Techno Economic Assessment

FOR USE, REV 3

May 30, 2023

Sargent & Lundy LLC

55 East Monroe Street • Chicago, IL 60603 USA • 312-269-2000
www.sargentlundy.com

Acknowledgement

This material is based upon work supported by the Department of Energy Funding Opportunity Announcement under cooperative award number DE-FE0031727.

Disclaimer

Executive Summary

ION Engineering L.L.C. (ION) received notification of award for a Cooperative Agreement from the U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL) under award DE-FE0031727 to evaluate the continued development of carbon capture at the engineering scale or to be applied at commercial design. Specifically, the objective of this project is to complete the initial design of a commercial-scale, post-combustion CO_2 capture system for application at an existing coal-fired generation unit. Additionally, as part of the project, ION was tasked with developing a techno-economic assessment (TEA) based on the Bituminous Baseline Study (BBS) cases developed by DOE/NETL. Sargent & Lundy LLC (S&L) was engaged by ION to prepare the TEA using performance and process design information specific to the ICE-31 solvent technology.

The purpose of the TEA is to evaluate the economic feasibility of implementing the ION carbon capture system at a greenfield power plant equipped with a supercritical coal-fired boiler. Capital costs, operating and maintenance (O&M) costs, and the cost of electricity (COE) were prepared by the Department of Energy (DOE) and National Energy Technology Laboratory (NETL) and published in the BBS in 2019. The objective of the BBS case studies is to determine the comparative costs of power facilities that generate 650 megawatts (MW) of net power. Case 12A is reflective of a supercritical coal facility without a carbon capture system; Case 12B is reflective of a supercritical coal facility utilizing carbon capture. The carbon capture system chosen for the BBS Case 12B is the Shell Cansolv system, which is considered a state-of-the-art full-scale application. The ION TEA compares the incremental increase in COE and cost of capture (in $/tonne) for the ION system with the increases estimated by the DOE between BBS Case 12A to BBS Case 12B.

This economic evaluation is conducted according to the design basis laid out in the BBS Case 12B to the best extent possible. However, several technical and operational parameters within this TEA for ION's carbon capture system as well as equipment cost basis are based on the results from ION's recently completed front-end engineering and design (FEED) study, Commercial Carbon Capture Design and Costing Phase 2 (C3DC2). As such, this TEA is based on costing and designs developed for the ICE-21 solvent, scaled for the characteristics expected for the next-generation solvent (ICE-31) based on modeling results performed by ION. The study takes into account lost generation due to CO_2 capture auxiliary power demand and heat consumption from the base plant steam cycle.

The capital costs estimate is broken into bare erected costs, total plant cost, and total overnight cost. O&M costs are broken into variable and fixed O&M. Ultimately the annualized capital costs are combined with the O&M costs to determine the lifecycle cost of the facility. The ION carbon capture TEA shows that:

- Capital expenditures are 15% lower compared to Case 12B;
- O&M expenditures are 0.4% lower compared to Case 12B;
- COE is $101.7/MWh, 3.4% lower compared to Case 12B; and
- Cost of capture is $38.3/tonne, 16.4% lower compared to Case 12B.
- 8% more carbon capture and 60% lower CO_2 emissions

Table ES-1: TEA Lifecycle Costs and Cost of Electricity Analysis

Description	**DOE/NETL BBS Case 12A**	**DOE/NETL BBS Case 12B**	**ION TEA w/ CO_2 Capture**	**ION vs. Case 12B**
Total Overnight Capital Cost	$1,678,413,000	$3,023,051,000	$2,821,020000	-6.7%
	$2,582/kW$_{net}$	$4,651/kW$_{net}$	$4,340/kW$_{net}$	
Incremental Capital Cost of CO_2 Capture	BASE	$1,344,638,000	$1,142,607,000	-15.0%
		$2,069/kW$_{net}$	$1,758kW$_{net}$	
Total Annual O&M Cost	$174,548,000	$262,533,000	$261,585,000	-0.4%
	$269/kW$_{net}$	$404/kW$_{net}$	$402/kW$_{net}$	
Incremental Annual O&M Cost of CO_2 Capture	BASE	$88,005,000	$87,037,000	-1.1%
		$135/kW$_{net}$	$134/kW$_{net}$	
Total COE without Transportation Storage & Monitoring (TS&M)	$64.4/MWh	$105.3/MWh	$101.7/MWh	-3.4%
Differential COE	BASE	$40.9/MWh	$37.3/MWh	-8.8%
Total Cost of Capture without TS&M	BASE	$45.8/tonne	$38.3/tonne	-16.4%

This work was generated with financial support from the U.S. Government through Contract/Award No. DEFE0031727, and as such the U.S. Government retains a paid-up, nonexclusive, irrevocable, world-wide license to reproduce, prepare derivative works, distribute copies to the public, and display publicly, by or on behalf of the Government, this work in whole or in part, or otherwise use the work for Federal purposes.