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## Disclaimer:

# Large Pilot-Scale Carbon Dioxide ($CO_2$) Capture Project Using Aminosilicone Solvent

## Final Scientific/Technical Report

Reporting Period Start Date: 10/1/2015

Reporting Period End Date: 6/30/2017

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# Executive Summary

GE Global Research has developed, over the last 8 years, a platform of cost effective $CO_2$ capture technologies based on a non-aqueous aminosilicone solvent (GAP-$1_m$). As demonstrated in previous funded DOE projects (DE-FE0007502 and DEFE0013755), the GAP-$1_m$ solvent has increased $CO_2$ working capacity, lower volatility and corrosivity than the benchmark aqueous amine technology. Performance of the GAP-$1_m$ solvent was recently demonstrated in a 0.5 $MW_e$ pilot at National Carbon Capture Center, AL with real flue gas for over 500 hours of operation using a Steam Stripper Column (SSC). The pilot-scale PSTU engineering data were used to (i) update the techno-economic analysis, and EH&S assessment, (ii) perform technology gap analysis, and (iii) conduct the solvent manufacturability and scale-up study.

(i) Techno-economic Analysis: The 0.5 $MW_e$ pilot-scale engineering data were used to update the $CO_2$ capture process models, and the techno-economic analysis was conducted for a 550 MW coal fired power plant. The 1st year $CO_2$ removal cost for the aminosilicone-based carbon-capture process was evaluated at \$46.2/tonne $CO_2$ (no solvent degradation) and at \$52.9/tonne $CO_2$ (with solvent degradation). This is a 20% reduction compared to MEA, primarily due to lower overall capital cost. Further reduction in $CO_2$ capture cost is expected by lowering the manufacturing cost of the solvent, implementing flowsheet optimization and/or implementing the next generation aminosilicone solvent with improved stability and increased $CO_2$ working capacity.

(ii) Environmental, Health, and Safety (EH&S) Assessment was updated for the GAP-$1_m$/TEG $CO_2$ capture plant with SSC. Plant-wide engineering controls were described. Five components of the solvent, CAS#2469-55-8 (GAP-0), CAS#106214-84-0 (GAP-1-4), TEG, and methanol and xylene (minor contaminants from the aminosilicone) were included in this assessment. The toxicological effects of the chemicals associated with the $CO_2$ capture system, and the solvent manufacturing process were reviewed and addressed.

(iii) GAP Analysis: Systematic analysis of the solvent loss in the GAP-$1_m$ / TEG process identified a number of areas for technology development. Solvent thermal degradation, thermal oxidation, and hydrothermal equilibration were identified as the critical technology gaps that need to be addressed in future R&D activities.

While the current GAP-$1_m$/TEG technology has many positive attributes, there are areas for improvements to enable its widespread deployment and testing in a 10 $MW_e$ pilot. Based on our process and economic models, and recent experiments performed in our laboratory, four attributes have been identified that will significantly reduce the cost of $CO_2$ capture for the aminosilicone solvents: a) increased $CO_2$ working capacity, b) improved solvent stability, c) lower solvent viscosity, and d) optimized heat of reaction. It is proposed that future R&D directions would include the design and demonstration of advanced aminosilicone solvents to meet the $CO_2$ cost target of 40 \$/t$CO_2$ at a 90% $CO_2$ capture efficiency with 95% $CO_2$ purity.

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# 1 Project Objectives

The primary objective of this cooperative agreement between GE Global Research, and the Department of Energy was to evaluate the feasibility of performing a 10 $MW_e$ pilot-scale using a novel aminosilicone based $CO_2$ capture solvent (GAP-$1_m$/ TEG) by conducting the following tasks.

(i) **Technology Gap Analysis.** For each of the key process components, the information and testing required before commercialization (i.e. technology gaps) were identified and R&D directions were proposed to close the gaps. Solvent management was identified as the major gap to be addressed before pursuing a 10 $MW_e$ pilot demonstration.

(ii) **Environmental, Health, and Safety (EH&S) Assessment.** Learnings from 0.5 $MW_e$ pilot were incorporated in the previously completed EH&S assessments (bench-scale and 0.5 MWe pilot), and strategies were identified to minimizing any negative impact of the process in a 10 $MW_e$ pilot.

(iii) **Techno-economic Analysis** The pilot-scale engineering data obtained for the GAP-$1_m$ / TEG solvent with the steam stripper column (SSC) desorber were used to update the $CO_2$ capture process models in collaboration with West Virginia University. A techno-economic analysis was performed for a 550 MW coal fired power plant. The 1st year $CO_2$ removal cost for the aminosilicone-based carbon-capture process was evaluated at \$52.9/tonne $CO_2$. This is a 20% reduction compared to MEA, primarily due to lower overall capital cost. Further reduction in $CO_2$ capture cost is expected by lowering the manufacturing cost of the solvent, implementing flowsheet optimization and/or implementing the next generation aminosilicone solvent with improved stability and increased $CO_2$ working capacity.

(iv) **Solvent Manufacturability and Scale-up Study.** A manufacturer with the capacity and infrastructure capable of making the quantities anticipated for a large scale demo pilot was identified. Solvent samples were successfully qualified based on the initial $CO_2$ capture efficiency (2 $kW_e$ bench scale demo), and accelerated solvent degradation performance (thermal, hydrothermal, and oxidative degradation).

While the current GAP-$1_m$/TEG technology has many positive attributes, there are areas for improvements to enable its widespread deployment and testing in a 10 $MW_e$ pilot. Based on our process and economic models, and recent experiments performed in our laboratory, four attributes have been identified that will significantly reduce the cost of $CO_2$ capture for the aminosilicone solvents: a) increased $CO_2$ working capacity, b) improved solvent stability, c) lower solvent viscosity, and d) optimized heat of reaction. It is proposed that future R&D directions would include the design and demonstration of advanced aminosilicone solvents with the above attributes to meet the $CO_2$ cost target of 40 \$/t$CO_2$ at a 90% $CO_2$ capture efficiency with 95% $CO_2$ purity.

# 2 GE Aminosilicone Technology

The proposed technology is to use an aminosilicone-based solvent for $CO_2$-capture from the flue gas of a pulverized coal power plant. In previous GE Global Research work, as part of a prior DOE project (DE-NT0005310) an aminosilicone solvent was identified that demonstrates superior performance for $CO_2$ capture. This material consists of an aminosilicone oligomer known as GAP (3-aminopropyl end-capped polydimethylsiloxanes [PDMS]). It was found that the best performance was for a material where the average value for x is 1. The structure of this material, known as GAP-1 (1,5-Bis(3-aminopropyl 1,1,3,3,5,5-hexamethyl trisiloxane)), is shown in **Figure 1**.

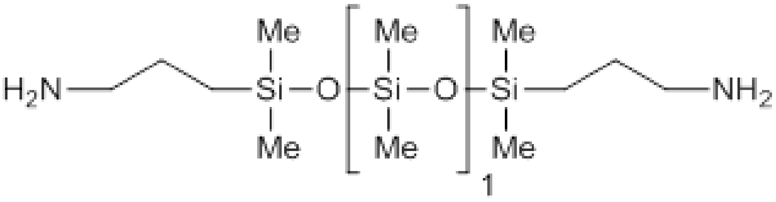


**Figure 1.** GAP-1 (1,5-Bis(3-aminopropyl) 1,1,3,3,5,5-hexamethyl trisiloxane).

GAP-1 readily reacts with $CO_2$ to form a carbamate (**Figure 2**).

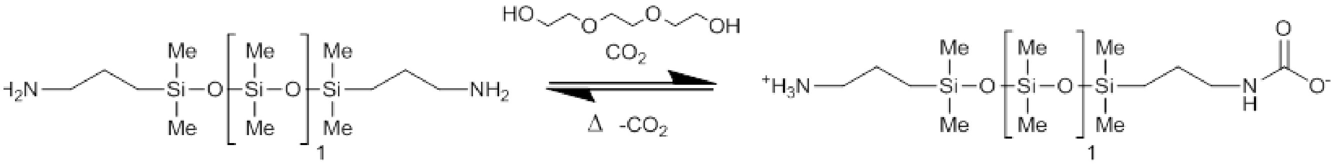


**Figure 2.** GAP-1 material reacting with $CO_2$

The GAP-1 synthesized for this project is actually a statistical mixture of GAP molecules with x values of 0 to 3, and will be distinguished from pure GAP-1 by the subscript “m” (GAP-$1_m$). GAP-$1_m$ consists of 40 wt.% GAP-0, 33 wt.% GAP-1, 19% GAP-2, and 8% GAP-3, as determined by $^1H$ NMR, with the average molecular weight being that of GAP-1. At elevated temperatures $CO_2$ is reversibly desorbed from GAP-$1_m$, permitting reuse of the $CO_2$ capture solvent. However, the viscosity of GAP-1$_m$ increases significantly upon absorption of $CO_2$, and can solidify at high $CO_2$ loadings. In order to mitigate these issues, it was found that a suitable $CO_2$ capture solvent could be produced by diluting GAP-1$_m$ in a co-solvent. Using triethylene glycol (TEG) as a co-solvent, a $CO_2$ capture solvent comprised of 60% (by wt.) GAP-1$_m$ with 40% TEG demonstrated improved thermal stability and volatility relative to MEA with a similar capacity for $CO_2$. The use of a co-solvent ensures that the viscosity of the aminosilicone-based solvent is acceptable even at high $CO_2$ loadings, and inhibits solidification of the aminosilicone.

GAP-1$_m$/TEG exhibits a number of desirable properties as a $CO_2$ capture solvent when compared to MEA. **Figure 3** shows the vapor pressure of both MEA and GAP-1$_m$. As shown, both GAP-1$_m$ and TEG are significantly less volatile than MEA. This lower volatility simplifies $CO_2$ desorption and potentially reduces the solvent loss in both clean flue gas and $CO_2$ streams.

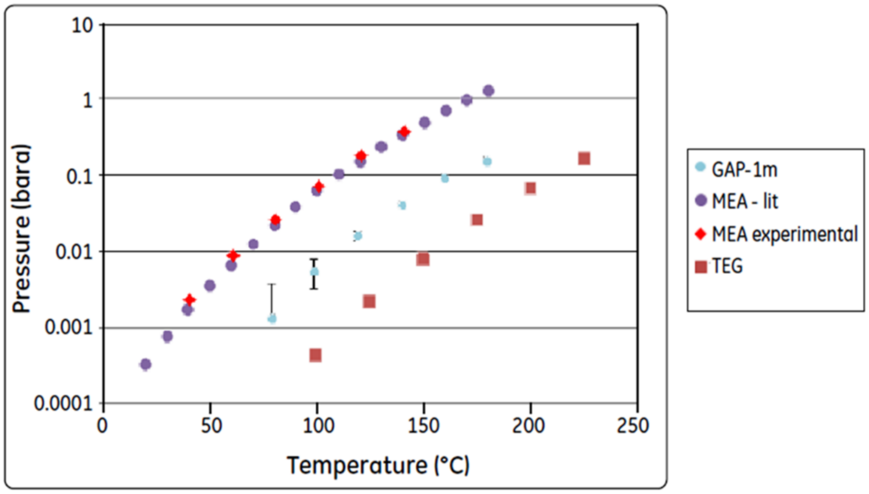


**Figure 3.** **Vapor Pressure**: MEA vs. GAP-1$_m$/TEG solvent

Thermal stability tests were performed in prior DOE funded projects, in which GAP-1$_m$ (lean solvent) was heated at temperatures from 120 to 160°C for over 80 days, in the presence of air. **Figure 4** shows the results when compared to MEA. At 120 °C, it was observed by GC that there was no detectable degradation of the material. At 150°C, lean aminosilicone solvent exhibits one order of magnitude lower thermal degradation rate than MEA.

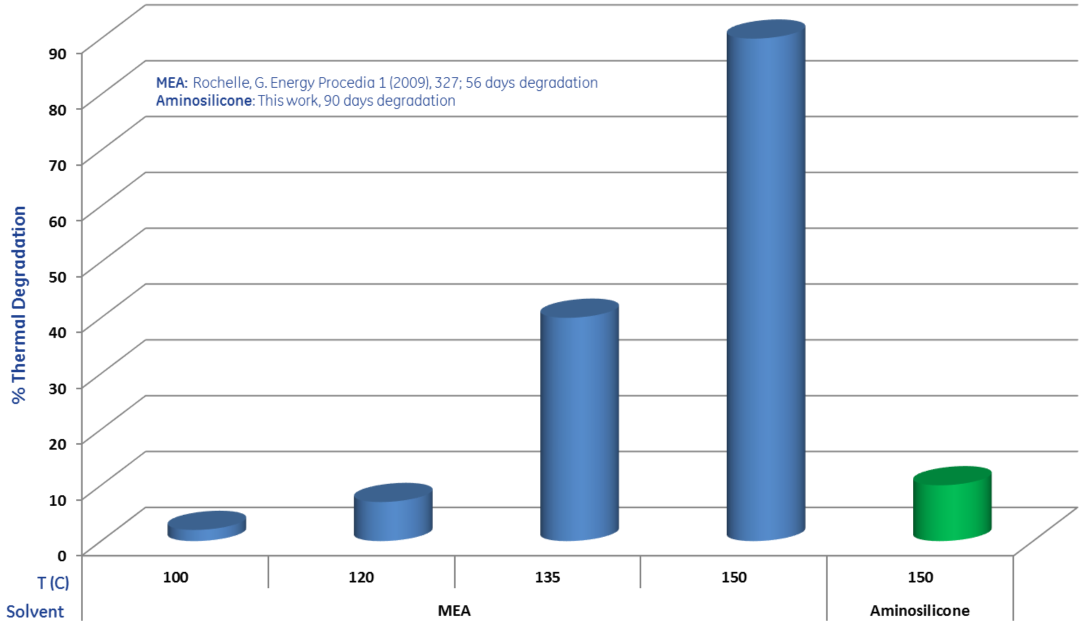


**Figure 4.** **Thermal Degradation:** MEA vs. GAP-$1_m$/TEG solvent (lean)

More recent studies were completed looking at the effects of water and $CO_2$ on thermal degradation. It was found that high concentration of carbon dioxide results in elevated thermal degradation rates. This is shown in **Figure 5**. Solvent that is fully loaded with $CO_2$ (the blue curves), shows a higher rate of thermal degradation over a range of temperatures, than the partially loaded samples (the green curves). Additionally, it was determined that the addition of water (at 5-10 wt.%) decreased the rate of thermal degradation for both the 100% loaded solvent and the 25% loaded solvent.

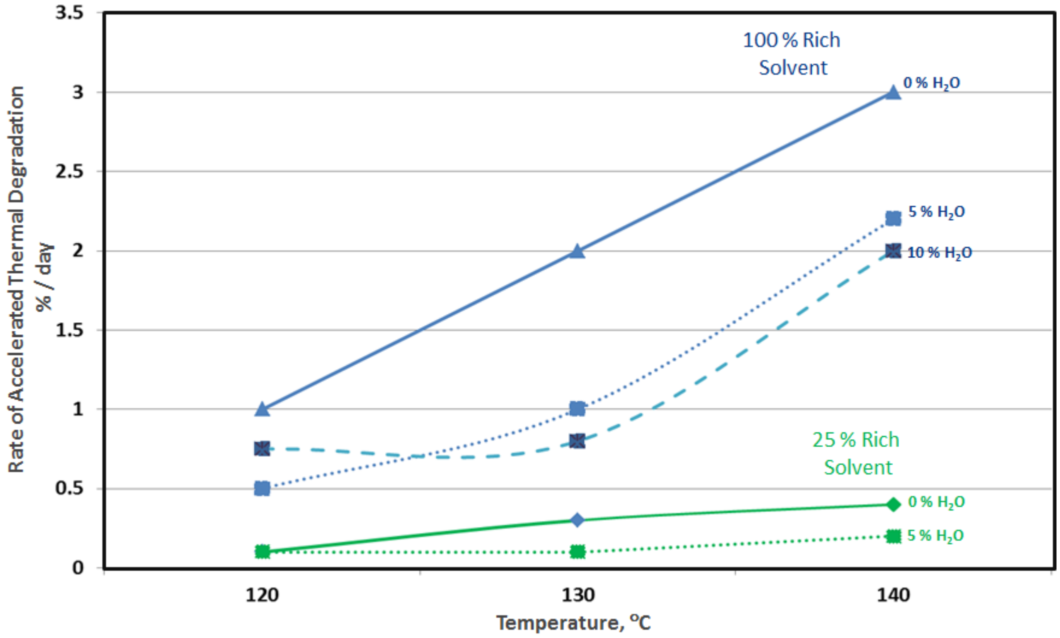


**Figure 5.** **Thermal Degradation:** GAP-$1_m$/TEG solvent (rich)
Rate of thermal degradation as a function of temperature, percent $CO_2$ loading, and water loading (2 kW bench scale process)

In order to better understand why $CO_2$ would promote thermal degradation, and why water would inhibit it, various analytical techniques were used to determine the products of thermal degradation. The route for thermal degradation identified is shown in **Figure 6**.

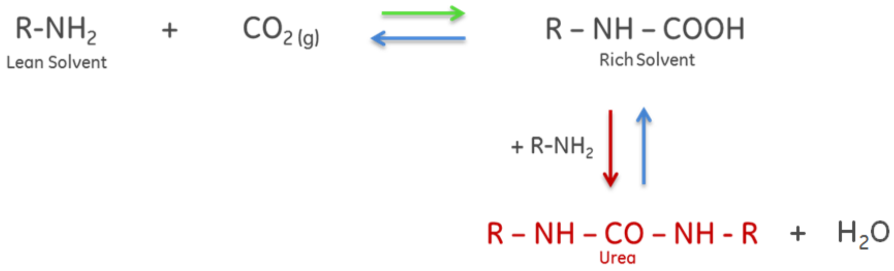


**Figure 6.** **Thermal Degradation of GAP-$1_m$/TEG solvent (rich):** Proposed Mechanism

Lean aminosilicone solvent can react with $CO_2$ to form a carbamate ($CO_2$-rich solvent). The carbamate molecule can then react with a $CO_2$-lean molecule in a side reaction to form urea and water, where two amine groups are inactive in the urea form. Increasing the concentration of $CO_2$-rich solvent pushes the equilibrium of the side reaction to favor the formation of urea, therefore increasing the rate of thermal degradation of the solvent. However, water is also a product of the side reaction. So adding water to the solvent should help push the equilibrium of the side reaction back to favoring the non-urea form. In summary, we found that the rate of thermal degradation of the rich solvent is proportional to temperature, $CO_2$ content of the solvent leaving the desorber and inversely proportional to water content as described below.

$$Rate\ of\ thermal\ degradation \sim \frac{T \times \%CO_{2,lean}}{\%\,H_2O}$$

Finally, corrosivity studies conducted in our bench scale system [DE-FE0007502] have shown that GAP-$1_m$/TEG is significantly less corrosive than MEA under the absorber and rich/lean heat exchanger conditions, decreasing capital costs by using less expensive materials of construction (**Figure 7**).

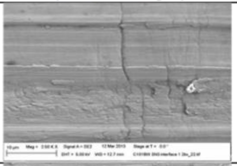
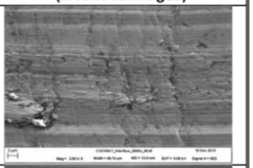
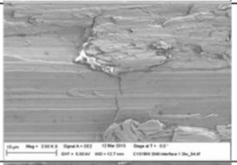
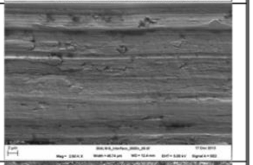
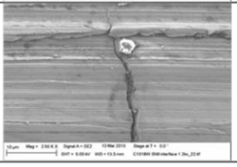
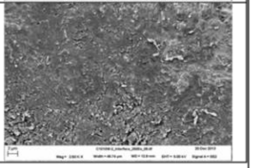
| Location / Metal Type | Conditions | Unexposed samples (interface images) | Exposed samples (interface images) | Corrosion Rate (μm/yr) |
|---|---|---|---|---|
| Lean Storage / C1018 | ~380 hours at ~34 °C and ~6138 hours at ~25 °C |  |  | 1.27 |
| Absorber Sump / C1018 | ~389 hours at ~52 °C and ~6138 hours at ~25 °C |  |  | 0.47 |
| Desorber / C1018 | ~388hours at ~145 °C and ~6138 hours at ~25 °C |  |  | 2188 |

**Figure 7.** **GAP-$1_m$/TEG Corrosivity**

Corrosion rates measured in the bench scale demo (2 $kW_e$)

# 3 Host Evaluation

We evaluated the system changes that would be required to demonstrate the GAP-$1_m$/TEG solvent in a typical aqueous amine pilot plant. As shown in the previous session, GAP-$1_m$/TEG solvent has higher viscosity (30 – 150 cP), and higher heat of absorption than a typical aqueous amine. On the other hand, our experience at NCCC showed that no special system modifications were required to accommodate the testing of the non-aqueous GAP-$1_m$/TEG solvent with the regenerator column as long as the water content was higher than 10 wt.%. We expect that a typical large demo plant such as the facility at the Technology Center at Mongstad (TCM), or the Shand Carbon Capture Test Facility (Estevan, SK) could be utilized to test the GAP-$1_m$ / TEG working solution as long as the following conditions are met:

(a) Absorber column is fitted with an intercooler to reject heat and maintain temperatures below 70 $^{o}$C. As experienced at NCCC, higher amounts of water (> 10 wt.%) in the working solution lowered the absorber temperature due to evaporative cooling decreasing the cooling duty of the intercooler.

(b) All the gaskets and seals in direct contact with the working solution are compatible with the GAP-$1_m$ / TEG solvent.

(c) The pilot unit should feature a precise water management system consisting of efficient wash water towers, separators, mist separators and total condensers. Performance of the system is more sensitive to small changes in water content than a typical aqueous system.

(d) Any waste water resulted in the process should be collected in transfer vessels and disposed off-site.

(e) Water content in the working solution should be maintained above 10 wt.% to ensure lower viscosity working solution.

(f) All heat exchangers (lean cooler, rich-lean) and pumps should be verified that they can handle higher viscosity working solutions. Water content above 10 wt.% significantly lowers the viscosity and density of the working solution, hence improving both heat and mass transfer coefficient in the heat exchangers and absorber column, respectively.

# 4 Techno-economic Analysis

## 4.1 Process Description

A supercritical pulverized coal (PC) plant and $CO_2$-separation unit based on mono-ethanol amine (MEA) is described in Case 12 of the DOE Bituminous Baseline Study.[1]

A simplified block diagram of the power plant and $CO_2$-separation system is shown in **Figure 8**. The pulverized coal boiler generates steam, which is sent to the steam turbines. The flue gas is sent through a selective catalytic reduction (SCR) unit to reduce nitrogen oxides ($NO_X$), a bag house to remove fly ash, and a flue gas desulfurizer (FGD) to remove sulfur dioxide. The flue gas is then sent through the carbon dioxide separation unit before being vented to the stack.

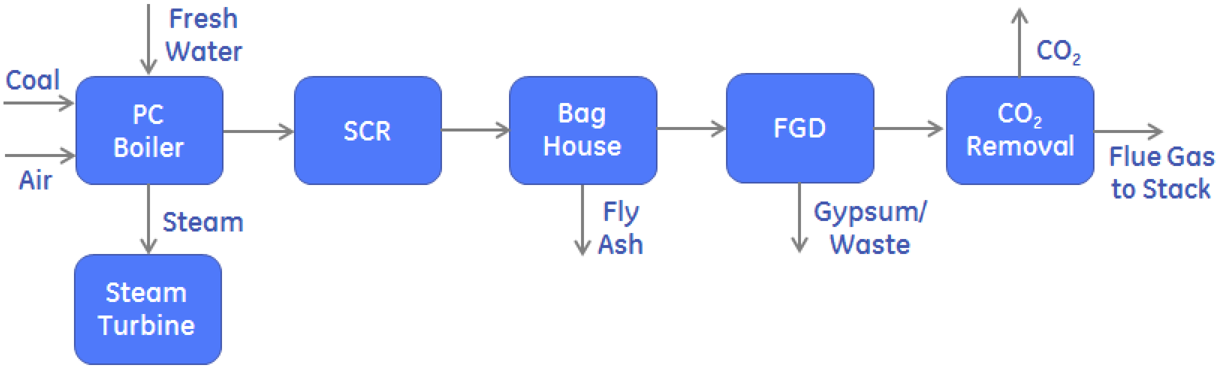


**Figure 8.** Coal-fired power plant block diagram with $CO_2$ removal

The MEA and GAP-$1_m$/TEG $CO_2$ separation units utilize four key processes, $CO_2$ absorption, $CO_2$ desorption, sorbent handling, and $CO_2$ compression.

The flue gas from the power plant is processed in a direct contact cooler to reduce the temperature to 40 °C (104 °F) and then enters the absorber. **Figure 9** shows the process for the aminosilicone case. The lean sorbent enters the absorber at 40 °C (104 °F) and captures most of the $CO_2$ from the flue gas. The rich sorbent leaves the absorber. The $CO_2$ absorption increases the temperature of the sorbent. The absorber is operated at 40-82 °C (104-180 °F) and at atmospheric pressure. The rich sorbent from the absorber is fed to the rich-lean heat exchanger and heated before being fed to the desorber (stripper) for separation of the absorbed $CO_2$. A 11.1 °C (20 °F) approach is assumed for this rich-lean heat exchanger. This is defined as the hot fluid outlet temperature minus the cold fluid inlet temperature. The lean sorbent from the desorber is passed through the other side of the rich-lean heat exchanger.

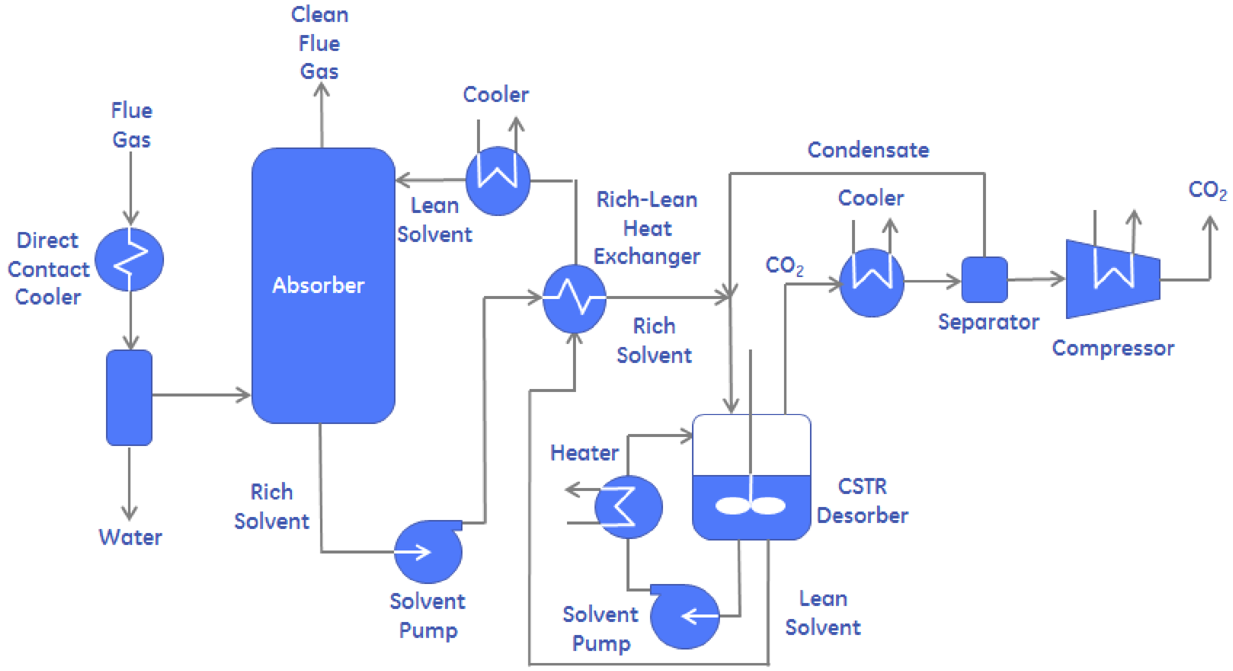


**Figure 9.** Aminosilicone-based $CO_2$ separation sub-system with CSTR desorber

For the aminosilicone solvent baseline case (Case A, described below), the desorber operates at 140 °C (284 °F) and 4.3 atm (63 psia). For the sensitivity studies, the desorber conditions were varied from 130 to 140 °C (266 to 284 °F) and from 1.4 to 4.3 atm (20 to 63 psia). These results are presented in subsequent sections. For the MEA baseline case, the desorber reboiler conditions are about 116 °C (241 °F) and 1.6 atm (24 psia). For both systems, steam is supplied to the desorber to provide heat, which releases $CO_2$ from the rich sorbent. Steam is supplied from the medium- to low-pressure steam turbine crossover pipe of the steam turbine in the power plant sub-system. Steam conditions were selected based on best efficiency of the power plant and the removal cost of $CO_2$ from the overall system. The hot vapor from the top of the desorber consisting primarily of $CO_2$ is cooled in a heat exchanger utilizing water. The stream then flows to a separator where the vapor and entrained liquid are separated. The $CO_2$ gas is removed from the separator and then delivered to the $CO_2$ product compressor. The liquid from the bottom of the separator is returned back to the desorber. The lean sorbent from the desorber is pumped through the rich-lean heat exchanger to the absorber. The lean sorbent is cooled further before being fed to the absorber in order to increase the loading of $CO_2$ in the absorber.

## 4.2 Power Plant Modeling

A model of a supercritical PC plant was built in Thermoflow, a thermodynamic design tool which includes cost estimation methods for conventional coal power plants. The Thermoflow model interacted with the carbon-capture model by exchanging flue gas, process steam, and water at the boundaries between the two systems. Capital costs, operating costs, and net power output were rolled up at a plant level.

The modeling process began by calibrating to Case 11 from the Bituminous Baseline Study. Gas and steam flows, pressures and temperatures throughout the plant, along with exhaust composition, auxiliary loads, and net plant output were closely matched to Case 11 to create a calibration point for the model in Thermoflow. By matching to Case 11 it was possible to replicate efficiency levels on all of the major equipment in the power block, including pumps, fans, steam turbine sections, the boiler, and environmental equipment. These efficiencies were then held fixed as the model was updated to include $CO_2$-capture, thus ensuring consistency between the DOE report and the analysis with carbon capture. It was also possible to tune the cost model in Thermoflow to achieve a good match for overall capital costs with Case 11 from the Bituminous Baseline Study. The cost breakdown in Thermoflow's cost estimation tool is not at the same level of detail as in the Bituminous Baseline Study, so when calibrating the plant capital costs it was necessary to calibrate only on the full plant level rather than on a component level.

**Figure 10** shows a simplified block diagram of the power block, which is applicable to both the model with $CO_2$ capture and without. Detailed process flow information for each stream in **Figure 10** is shown in **Table 1** for the model without $CO_2$ capture. This model is intended to be a close match with Case 11 from the Bituminous Baseline Study.

Power plant modeling was conducted in Thermoflow for a number of cases. As described above, the first case was similar to Case 11 in the DOE Bituminous Baseline Study which is for a supercritical PC plant without $CO_2$ capture. Secondly, a Thermoflow model was built for a scaled up system for 550 MW net power with a $CO_2$-capture system added. For this case, the power plant model was built in Thermoflow and the carbon-capture island was modeled in Aspen Plus and Aspen Capital Cost Estimator. The scaled-up model is Case H which will be discussed in the next sections.

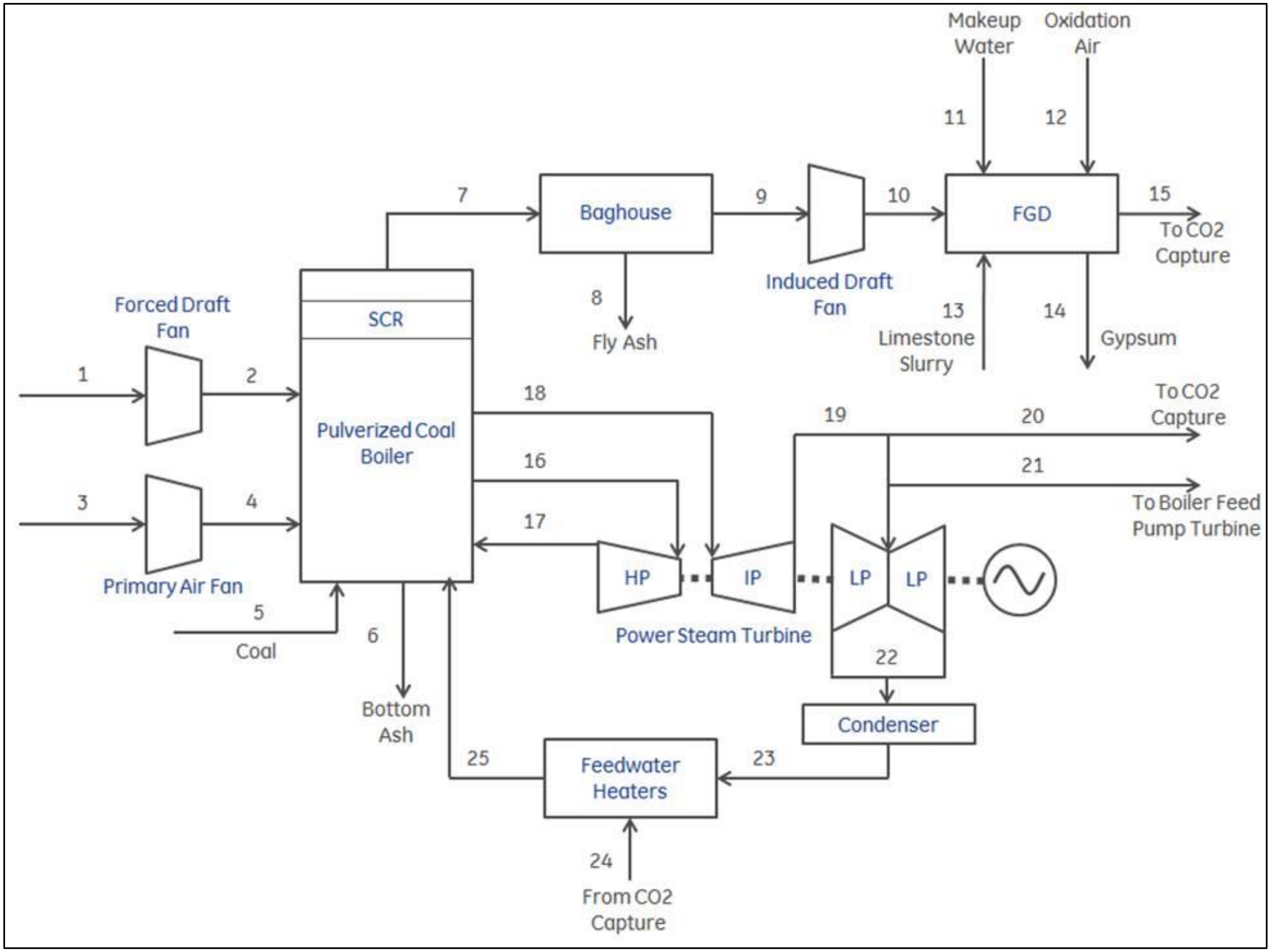


**Figure 10.** Block flow diagram for power plant

**Table 1**. Stream table for power plant case without $CO_2$ capture (comparable to Case 11)[2]

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|
| V-L Mole Fraction | | | | | | | |
| Ar | 0.0093 | 0.0093 | 0.0093 | 0.0093 | 0.0000 | 0.0000 | 0.0088 |
| $CO_2$ | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0000 | 0.0000 | 0.1485 |
| $H_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $H_2O$ | 0.0101 | 0.0101 | 0.0101 | 0.0101 | 0.0000 | 0.0000 | 0.0893 |
| $N_2$ | 0.7729 | 0.7729 | 0.7729 | 0.7729 | 0.0000 | 0.0000 | 0.7310 |
| $O_2$ | 0.2074 | 0.2074 | 0.2074 | 0.2074 | 0.0000 | 0.0000 | 0.0202 |
| $SO_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0022 |
| Total | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 0.0000 | 0.0000 | 1.0000 |
| | | | | | | | |
| V-L Flowrate (lbmol/hr) | 106,097 | 106,097 | 32,592 | 32,592 | - | - | 146,883 |
| V-L Flowrate (lb/hr) | 3,061,401 | 3,061,401 | 940,431 | 940,431 | - | - | 4,371,358 |
| Solids Flowrate (lb/hr) | - | - | - | - | 410,264 | 8,142 | 32,568.79 |
| | | | | | | | |
| Temperature (°F) | 59 | 65 | 59 | 77 | 59 | - | 342 |
| Pressure (psia) | 14.7 | 15.1 | 14.7 | 16.2 | 14.7 | - | 14.3 |
| Enthalpy (Btu/lbm) | -4.3 | -3.0 | -4.3 | 0.1 | - | - | 69.2 |
| Density ($lb/ft^3$) | 0.076 | 0.078 | 0.076 | 0.081 | - | - | 0.047 |
| V-L Molecular Weight | 28.85 | 28.85 | 28.85 | 28.85 | - | - | 29.76 |

|  | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
|---|---|---|---|---|---|---|---|
| V-L Mole Fraction |  |  |  |  |  |  |  |
| Ar | 0.0000 | 0.0088 | 0.0088 | 0.0000 | 0.0093 | 0.0000 | 0.0000 |
| $CO_2$ | 0.0000 | 0.1485 | 0.1485 | 0.0000 | 0.0003 | 0.0000 | 0.0004 |
| $H_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $H_2O$ | 0.0000 | 0.0893 | 0.0893 | 1.0000 | 0.0101 | 1.0000 | 0.9996 |
| $N_2$ | 0.0000 | 0.7310 | 0.7310 | 0.0000 | 0.7729 | 0.0000 | 0.0000 |
| $O_2$ | 0.0000 | 0.0202 | 0.0202 | 0.0000 | 0.2074 | 0.0000 | 0.0000 |
| $SO_2$ | 0.0000 | 0.0022 | 0.0022 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| Total | 0.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
|  |  |  |  |  |  |  |  |
| V-L Flowrate (lbmol/hr) | - | 146,883 | 146,883 | 15,884 | 2,284 | 8,483 | 348 |
| V-L Flowrate (lb/hr) | - | 4,371,358 | 4,371,358 | 286,236 | 65,916 | 152,864 | 6,264 |
| Solids Flowrate (lb/hr) | 32,569 | - | - | - | - | 33,832 | 56,664 |
|  |  |  |  |  |  |  |  |
| Temperature (°F) | - | 342 | 362.9 | 59 | 59 | 59 | 0 |
| Pressure (psia) | - | 13.84 | 15.06 | 14.7 | 14.7 | 14.7 | 0.0 |
| Enthalpy (Btu/lbm) | - | 69.2 | 74.7 | 27.1 | -4.3 | - | - |
| Density ($lb/ft^3$) | - | 0.046 | 0.048 | 62.379 | 0.076 | - | - |
| V-L Molecular Weight | - | 29.76 | 29.76 | 18.02 | 28.85 | - | 18.03 |

|  | 15 | 16 | 17 | 18 | 19 | 20 | 21 |
|---|---|---|---|---|---|---|---|
| V-L Mole Fraction |  |  |  |  |  |  |  |
| Ar | 0.0081 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $CO_2$ | 0.1372 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $H_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $H_2O$ | 0.1575 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| $N_2$ | 0.6767 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $O_2$ | 0.0203 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $SO_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| Total | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
|  |  |  |  |  |  |  |  |
| V-L Flowrate (lbmol/hr) | 161,275 | 203,480 | 168,736 | 168,736 | 152,819 | - | 12,899 |
| V-L Flowrate (lb/hr) | 4,646,871 | 3,666,712 | 3,040,619 | 3,040,619 | 2,753,799 | - | 232,437 |
| Solids Flowrate (lb/hr) | - | - | - | - | - | - | - |
|  |  |  |  |  |  |  |  |
| Temperature (°F) | 132 | 1100 | 664 | 1100 | 688 | - | 688 |
| Pressure (psia) | 14.7 | 3514.7 | 693.7 | 655.8 | 134.9 | - | 134.9 |
| Enthalpy (Btu/lbm) | 14.8 | 1495.0 | 1323.7 | 1570.5 | 1371.4 | - | 1371.4 |
| Density (lb/ft$^3$) | 0.063 | 4.319 | 1.141 | 0.722 | 0.200 | - | 0.200 |
| V-L Molecular Weight | 28.81 | 18.02 | 18.02 | 18.02 | 18.02 | - | 18.02 |

|  | 22 | 23 | 24 | 25 |
|---|---|---|---|---|
| V-L Mole Fraction |  |  |  |  |
| Ar | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $CO_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $H_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $H_2O$ | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| $N_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $O_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $SO_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| Total | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
|  |  |  |  |  |
| V-L Flowrate (lbmol/hr) | 114,800 | 154,153 | - | 203,480 |
| V-L Flowrate (lb/hr) | 2,068,688 | 2,777,829 | - | 3,666,712 |
| Solids Flowrate (lb/hr) | - | - | - | - |
|  |  |  |  |  |
| Temperature (°F) | 101 | 104 | - | 557 |
| Pressure (psia) | 1.0 | 264.2 | - | 4185.2 |
| Enthalpy (Btu/lbm) | 1016.3 | 72.3 | - | 552.9 |
| Density (lb/ft$^3$) | 0.003 | 61.999 | - | 47.687 |
| V-L Molecular Weight | 18.02 | 18.02 | - | 18.02 |

**Table 2** summarizes the power output from the power plant, without $CO_2$ capture, along with materials consumed during normal operation. It includes a detailed summary of auxiliary loads and how they combine with the steam turbine power to impact the total plant net-power output and efficiency. Auxiliary loads required only minor tuning in order to conform to the results from DOE Case 11.[2]

**Table 2**. Power summary for case without $CO_2$ capture (comparable to DOE Case 11)

| **POWER SUMMARY (Gross Power at Generator Terminals, kWe)** | |
|---|---|
| Steam Turbine Power | 580,418 |
| **Total (Steam Turbine) Power, kWe** | **580,418** |
| **Auxiliary Load Summary, kWe** | |
| Boiler Fuel Delivery | 3,216 |
| Ash Handling | 529 |
| Primary Air Fans | 1,358 |
| Forced Draft Fans | 1,524 |
| Induced Draft Fans | 7,444 |
| Baghouse (ESP) | 70 |
| Wet FGD | 5,536 |
| Carbon-Capture Process | - |
| $CO_2$ Compression | - |
| Miscellaneous BOP | 289 |
| Condensate Pumps | 953 |
| Circulating Water Pumps | 3,889 |
| Cooling Tower Fans | 3,284 |
| Transformer Losses | 1,820 |
| BFP Booster Pump | 498 |
| **Total Auxiliaries, kWe** | **30,411** |
| **Net Power, kWe** | **550,008** |
| Net Plant Efficiency (HHV) | 39.2% |
| Net Plant Heat Rate, (Btu/kWh) | 8,702 |
| **Condenser Cooling duty, ($10^6$ Btu/hr)** | 2,212 |
| **Consumables** | |
| As-Received Coal Feed, (lb/hr) | 410,264 |
| Limestone Sorbent Feed, (lb/hr) | 33,833 |
| Thermal Input (kWt) | 1,402,678 |
| Raw Water Consumption (gpm) | 6,740 |

The Thermoflow model includes a cost estimation tool. The results from this are summarized in **Table 3**. The cost estimates for the model without carbon capture were tuned in order to line up with the results from Case 11 in the economic updates (June 2011 Basis) for the Bituminous Baseline Study.[2] The factors that were applied in order to achieve this match were held constant for further analysis of cases with $CO_2$ capture.

**Table 3.** Equipment cost summary for case without $CO_2$ capture (comparable to DOE Case 11).[2]

| | $ | $/kW |
|---|---|---|
| **Specialized Equipment** | **$ 503,571,680** | **$ 912** |
| **Boiler** | **$ 190,948,513** | **$ 346** |
| Furnace | $ 81,914,520 | $ 148 |
| Convective Elements | $ 55,081,043 | $ 100 |
| Additional Waterwall | $ 5,734,579 | $ 10 |
| Soot Blowers | $ 4,858,259 | $ 9 |
| Desuperheaters and Controls | $ 8,363,538 | $ 15 |
| Air and Flue Gas Ducts | $ 5,955,797 | $ 11 |
| Coal Pulverizers and Feeders | $ 19,589,477 | $ 35 |
| FD Fan, PA Fan, ID Fan | $ 3,079,953 | $ 5.6 |
| Structural Steel, Ladders, Walkways | $ 2,481,073 | $ 4.5 |
| Rotary Air Heaters | $ 3,887,829 | $ 7.0 |
| | $ - | $ - |
| **Steam Turbine** | **$ 112,162,148** | **$ 203** |
| | | |
| **Feedwater Heaters** | **$ 9,790,217** | **$ 18** |
| Feedwater Heater 1 | $ 706,216 | $ 1.3 |
| Feedwater Heater 2 | $ 677,982 | $ 1.2 |
| Feedwater Heater 3 | $ 631,536 | $ 1.1 |
| Feedwater Heater 4 | $ 813,651 | $ 1.5 |
| Feedwater Heater 5-DA | $ 954,821 | $ 1.7 |
| Feedwater Heater 6 (6A,6B) | $ 1,665,926 | $ 3.0 |
| Feedwater Heater 7 (7A,7B) | $ 2,205,182 | $ 4.0 |
| Feedwater Heater 8 (8A,8B) | $ 2,135,025 | $ 3.9 |
| | | |
| **Water Cooled Condensers** | **$ 4,703,533** | **$ 8.5** |
| Main Condenser | $ 4,138,816 | $ 7.5 |
| Feed Pump Turbine Condenser | $ 565,023 | $ 1.0 |
| | | |
| **Particulate and Mercury Control** | **$ 22,139,295** | **$ 40** |
| | | |
| **Flue Gas Desulfurization** | **$ 87,523,161** | **$ 159** |
| | | |
| **Nitrogen Oxide Control (SCR)** | **$ 39,389,787** | **$ 71** |
| | | |

| | $ | $/kW |
|---|---|---|
| **Stack** | **$ 9,447,807** | **$ 17** |
| | | |
| **Continuous Emissions Monitoring System** | **$ 627,299** | **$ 1.1** |
| | | |
| **Distributed Control System** | **$ 1,675,191** | **$ 3.0** |
| | | |
| **Transmission Voltage Equipment** | **$ 15,090,301** | **$ 27** |
| Transformers | $ 13,353,578 | $ 24 |
| Circuit Breakers | $ 1,018,812 | $ 1.8 |
| Miscellaneous Equipment | $ 718,644 | $ 1.3 |
| | | |
| **Generating Voltage Equipment** | **$ 10,074,427** | **$ 18** |
| Generator Buswork | $ 5,234,596 | $ 9 |
| Circuit Breakers | $ 4,359,515 | $ 7.9 |
| Miscellaneous Equipment | $ 479,706 | $ 0.9 |

| | | |
|---|---|---|
| **Other Equipment** | **$ 126,556,231** | **$ 229** |
| **Pumps** | **$ 12,782,669** | **$ 23** |
| Boiler Feed Pump (+ Turbine) | $ 8,445,190 | $ 15 |
| Boiler Feed Booster Pump | $ 130,955 | $ 0.2 |
| Condenser C.W. Pump | $ 2,290,345 | $ 4.1 |
| Condensate Forwarding Pump | $ 599,474 | $ 1.1 |
| Condenser Vacuum Pump | $ 373,495 | $ 0.7 |
| Aux Cooling Water Pump (Closed Loop) | $ 40,050 | $ 0.1 |
| Treated Water Pump | $ 6,783 | $ 0.01 |
| Diesel Fire Pump | $ 172,876 | $ 0.3 |
| Jockey Fire Pump | $ 5,182 | $ 0.01 |
| Demin Water Pump | $ 13,419 | $ 0.02 |
| Raw Water Pumps | $ 28,232 | $ 0.1 |
| Aux Cooling Water Pump (Open Loop) | $ 40,050 | $ 0.1 |
| Startup Boiler Feed Pump | $ 637,239 | $ 1.2 |
| | | |
| **Tanks** | **$ 960,883** | **$ 1.7** |
| Hydrous Ammonia | $ 160,595 | $ 0.3 |
| Demin Water | $ 104,252 | $ 0.2 |
| Raw Water | $ 340,440 | $ 0.6 |
| | $ | $/kW |
| Neutralized Water | $ 78,037 | $ 0.1 |
| Acid Storage | $ 32,620 | $ 0.1 |

|  | $ | $/kW |
|---|---|---|
| Caustic Storage | $ 32,620 | $ 0.1 |
| Dedicated Fire Protection Water Storage | $ 212,355 | $ 0.4 |
|  | $ - | $ - |
| **Cooling Tower** | **$ 10,215,077** | **$ 19** |
|  |  |  |
| **Auxiliary Cooling Water Heat Exchanger** | **$ 138,904** | **$ 0.3** |
|  |  |  |
| **Steam Turbine Crane** | **$ 1,984,621** | **$ 3.6** |
|  |  |  |
| **Station Instrument Air Compressors** | **$ 816,256** | **$ 1.5** |
|  |  |  |
| **General Plant Instrumentation** | **$ 430,632** | **$ 0.8** |
|  |  |  |
| **Medium Voltage Equipment** | **$ 6,408,794** | **$ 12** |
| Transformers | $ 908,452 | $ 1.6 |
| Circuit Breakers | $ 344,459 | $ 0.6 |
| Switchgear | $ 1,805,415 | $ 3.3 |
| Motor Control Centers | $ 3,044,880 | $ 5.5 |
| Miscellaneous | $ 305,221 | $ 0.6 |
|  |  |  |
| **Low Voltage Equipment** | **$ 1,577,221** | **$ 2.9** |
| Transformers | $ 550,622 | $ 1.0 |
| Circuit Breakers | $ 460,216 | $ 0.8 |
| Motor Control Centers | $ 491,003 | $ 0.9 |
| Miscellaneous | $ 751,898 | $ 1.4 |
|  |  |  |
| **Coal Handling Equipment** | **$ 62,983,114** | **$ 114** |
|  |  |  |
| **Ash Handling Equipment** | **$ 22,231,445** | **$ 40** |
|  |  |  |
| **Miscellaneous Equipment** | **$ 6,026,614** | **$ 11** |

| **Civil** | **$ 82,771,128** | **$ 150** |
|---|---|---|
| **Site Work** | $ 17,302,872 | $ 31 |
| **Excavation and Backfill** | $ 4,839,333 | $ 9 |
| **Concrete** | $ 59,554,161 | $ 108 |
| **Roads Parking and Walkways** | $ 1,074,761 | $ 1.9 |

| Mechanical | $ 249,878,964 | $ 453 |
|---|---|---|
| On Site Transportation and Rigging | $ 8,948,256 | $ 16 |
| Equipment Erection and Assembly | $ 179,486,985 | $ 325 |
| Piping | $ 59,145,791 | $ 107 |
| Steel | $ 2,297,932 | $ 4.2 |

| Electrical Assembly and Wiring | $ 22,045,205 | $ 40 |
|---|---|---|
| Controls | $ 13,696,410 | $ 25 |
| Assembly and Wiring | $ 8,348,796 | $ 15 |

| Buildings and Structures | $ 20,288,854 | $ 37 |
|---|---|---|
| Boiler House and Turbine Hall | $ 18,282,573 | $ 33 |
| Administration Control Room, Machine Shop, Warehouse | $ 1,979,771 | $ 3.6 |
| Guard House | $ 26,510 | $ 0.05 |

| Engineering and Plant Startup | $ 52,908,687 | $ 96 |
|---|---|---|
| Engineering | $ 43,097,130 | $ 78 |
| Start Up | $ 9,811,557 | $ 18 |

| Totals | | |
|---|---|---|
| **Subtotal Contractor's Internal Cost** | **$ 1,058,020,749** | **$ 1,917** |
| Contractors Soft & Misc Costs | $ 200,206,199 | $ 363 |
| **Subtotal Contractor's Price** | **$ 1,258,226,948** | **$ 2,279** |
| Owner's Soft and Misc Costs | $ 267,642,586 | $ 485 |
| **Total Owner's Cost** | **$ 1,525,869,535** | **$ 2,764** |

Details about consumable materials are also available from the Thermoflow model. These were used with unit cost values from the economic updates (June 2011 Basis) for the Bituminous Baseline Study in order to calculate annual costs of consumables and fuel. The fixed operating costs and maintenance material costs were not independently calculated by the power block model and were therefore assumed equal to the values in DOE Case 11 to avoid inconsistency. The annual cost figures are summarized in **Table 4**.

**Table 4.** Annual cost summary for case without $CO_2$ capture (comparable to DOE Case 11)[2]

| | | | Annual Cost | Annual Unit Cost |
|---|---|---|---|---|
| | | | $ | $/kWh-net |
| **Fixed Operating Costs** | | | **$ 38,828,811** | **$ 0.00806** |
| **Maintenance Material Costs** | | | $ 10,945,892 | $ 0.00227 |
| | Consumption / day | Unit Cost | | |
| Water (/1000 gallons) | 3,293 | 1.67 | $ 1,706,242 | $ 0.00035 |
| Chemicals | | | | |
| MU & WT Chem.(lbs) | 15,939 | 0.27 | $ 1,335,191 | $ 0.00028 |
| Limestone (ton) | 478 | 33.48 | $ 4,961,323 | $ 0.00103 |
| Ammonia (19% $NH_3$) ton | 74 | 330 | $ 7,589,915 | $ 0.00158 |
| **Subtotal Chemicals** | | | $ 13,886,429 | $ 0.00288 |
| Other | | | | |
| SCR Catalyst ($m^3$) | 0.31 | 5775.94 | $ 556,513 | $ 0.00012 |
| **Subtotal Other** | | | $ 556,513 | $ 0.00012 |
| Waste Disposal | | | | |
| Total Ash (ton) | 478 | 25.11 | $ 3,720,271 | $ 0.00077 |
| **Subtotal Waste Disposal** | | | $ 3,720,271 | $ 0.00077 |
| **Total Variable Operating Costs** | | | **$ 19,869,457** | **$ 0.00412** |
| Fuel (ton) | 4923 | 68.60 | **$ 104,780,439** | **$ 0.02175** |

**Table 5** details the energy flows in and out of the control volume in the power block model, and confirms that the model achieves a proper energy balance.

**Table 5.** Energy balance for case without $CO_2$ capture (comparable to DOE Case 11)[2]

| | HHV | Sensible + Latent Heat | Power | Total |
|---|---|---|---|---|
| Heat In (MMBtu/hr) | | | | |
| Coal | 4797 | | | 4797 |
| Ambient Air | | 53.3 | | 53.3 |
| FGD Water | | 22.0 | | 22.0 |
| FGD Oxidation Air | | 3.8 | | 3.8 |
| Totals | 4797 | 79 | | 4876 |
| Heat Out (MMBtu/hr) | | | | |
| Bottom Ash | | 4.4 | | 4.4 |
| Fly Ash + FGD Ash | | 1.7 | | 1.7 |
| Flue Gas | | 611 | | 611 |
| Unburned Carbon | | 13.3 | | 13.3 |
| Boiler Losses | | 42.1 | | 42.1 |
| Fuel Delivery Losses | | 2.2 | | 2.2 |
| Main Condenser | | 1970 | | 1970 |
| BFPT Condenser | | 230 | | 230 |
| Steam Piping Losses | | 11.1 | | 11.1 |
| ST/Generator Mech/Elec/Gear Losses | | 22.7 | | 22.7 |
| BFPT Mech Losses | | 0.7 | | 0.7 |
| Pumps Mech/Elec Losses | | 2.4 | | 2.4 |
| Fans Mech/Elec Losses | | 3.8 | | 3.8 |
| FGD Energy Losses | | 31.7 | | 31.7 |
| Misc Losses and Auxiliaries | | 52.6 | | 52.6 |
| Net Power | | | 1877 | 1877 |
| Totals | 0 | 2999 | 1877 | 4876 |

**Table 6** summarizes the pieces of equipment which contribute to the total water consumption in the power block model.

**Table 6.** Water consumption for case without $CO_2$ capture (comparable to DOE Case 11)[2]

| Water Use | Water Consumption (gpm) |
|---|---|
| Carbon-Capture Process | |
| FGD Makeup | 573 |
| Cooling Tower | 3,558 |
| **Total** | **4,130** |

## 4.3 $CO_2$-Capture System ASPEN Plus Model Development

An ASPEN Plus model was developed for a supercritical commercial-scale process with aminosilicone-based solvent. The base case chosen was similar to Case 11 in the DOE-NETL study. Models were developed for a number of different $CO_2$-capture cases with varying absorber and desorber operating conditions. In order to compare the different cases of the carbon-capture island, the flue gas flow rate was fixed to match the Case 11 from the DOE NETL study which produces 550 MW net power without $CO_2$ capture. Comparing these cases facilitated final selection of the best case that had the lowest overall removal cost of $CO_2$. The best case was then scaled up to 550 MW net power with $CO_2$ capture. Further, two more cases were modeled starting from the scaled-up best case to further optimize the power plant and the carbon-capture island integration. The details of the selected cases are explained in the subsequent sections. The overview of the model is presented in **Figure 11**.

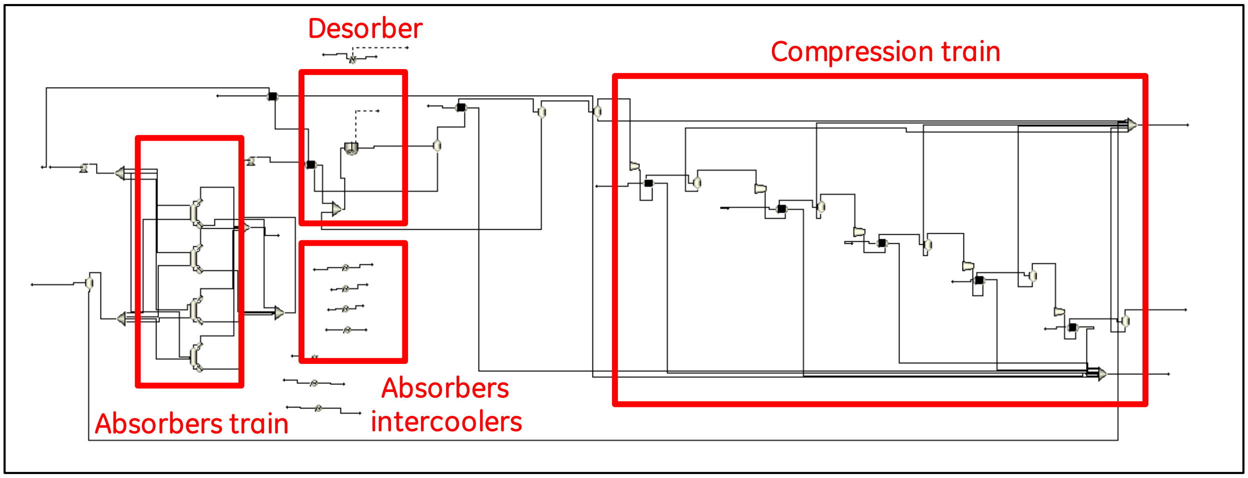


**Figure 11.** Aspen Plus model for $CO_2$ separation sub-system

Each part of the process will be discussed below.

### 4.3.1 Absorber Design

The $CO_2$-capture process was designed for a supercritical PC power plant, and the best case was scaled up to achieve 550 MW of net power with $CO_2$ capture. Flue gas enters the post-combustion $CO_2$-capture island from the coal power plant. The flue gas flow rate and composition were determined from the results of the power plant model using Thermoflow. The flue gas is cooled to 40 °C in a direct contact cooler, where condensed water is removed and sent to a waste water treatment plant. The absorber train consists of 4 units, and flue gas is evenly split among each of the columns. The flow sheet from the ASPEN Plus model of the absorber train is shown in **Figure 12**.

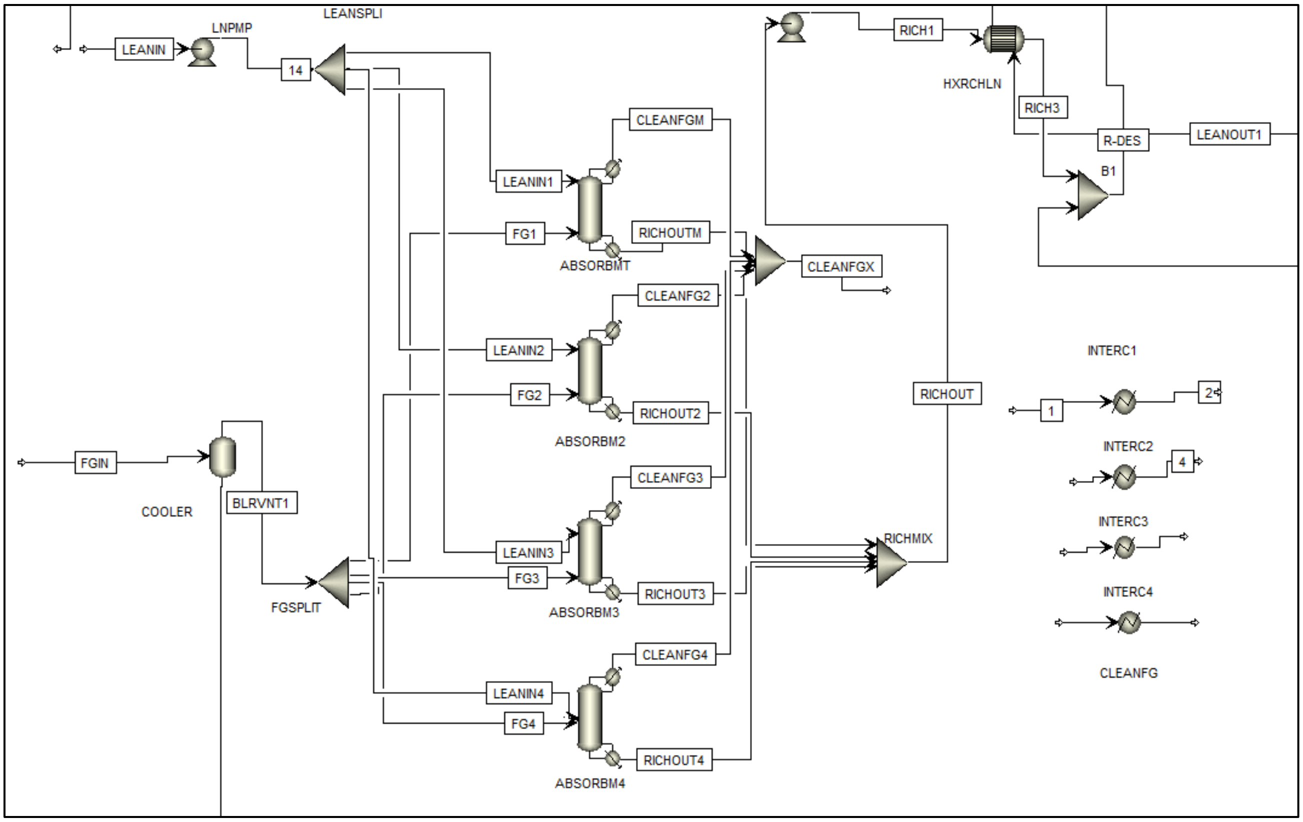


**Figure 12.** Aspen Plus flow sheet for the absorber train portion of the carbon-capture process

The absorbers are designed as RadFrac unit operations in Aspen Plus, where mass transfer is modeled based on rate-based calculations and chemical reactions are assumed to be in equilibrium. These assumptions were made based on bench-scale experiments conducted in the prior award (DE-FE0007502).

During the last cooperative agreement, an ASPEN Plus model for the bench-scale process was developed, and the packing type used in the model for the absorber corresponded to the actual packing used in the bench-scale process. Because there is a range of choices for packing type for commercial-scale processes, sensitivity analysis was conducted with respect to packing type in order to understand its effect on system performance. This analysis was conducted at a fixed lean solvent flow rate to the absorber train, and the change in $CO_2$ capture was determined.

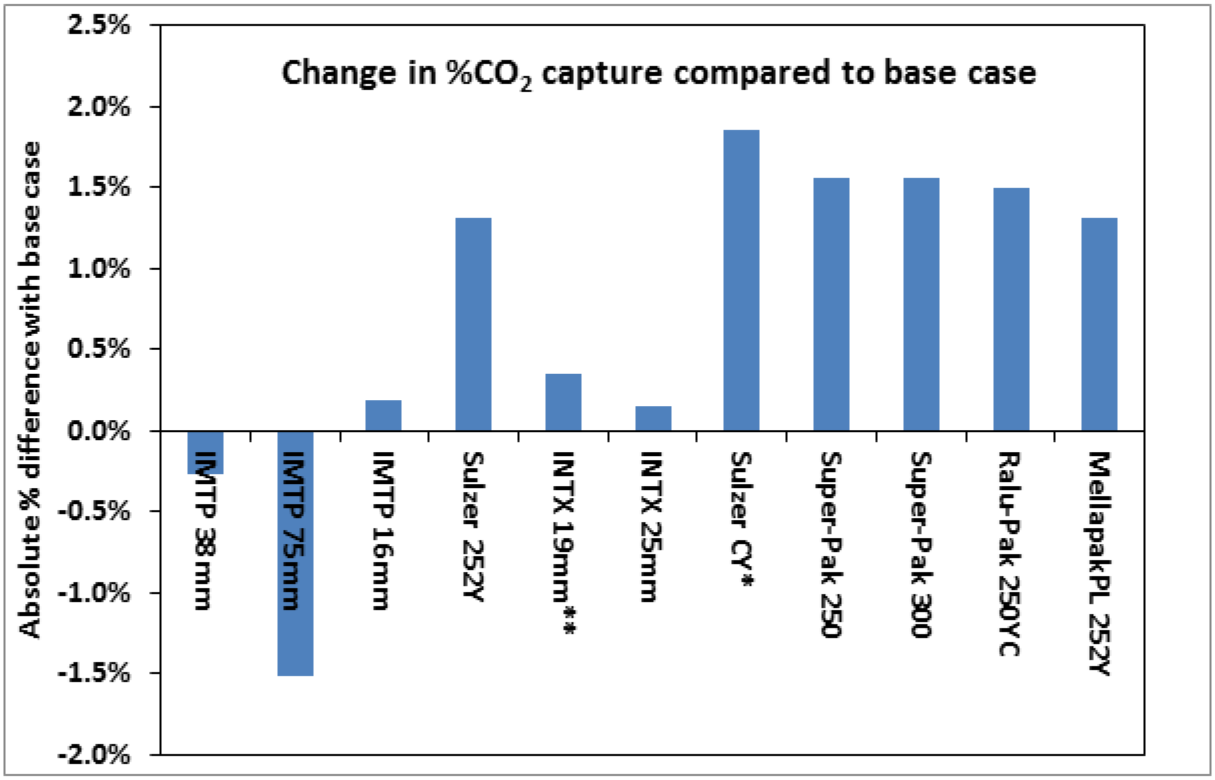


**Figure 13.** Effect of packing type on percent of $CO_2$ captured

It can be seen that, overall, structured packing offers higher performance compared to random packing for this system. The best case shown provides ~2% improvement in capture efficiency compared to the base case. The packing type which is available at the NCCC is Mellapak Plus 252Y, and therefore this packing was selected for further analysis. Also, this packing is commercially available in carbon steel (CS), which is significantly less expensive than stainless steel (SS). Because of the aminosilicone's lower corrosivity relative to other solvents, carbon steel packing may be used.

#### 4.3.1.1 *Packing Height Sensitivity Analysis*

The sensitivity analysis with respect to packing height was conducted for Mellapak Plus 252Y structured packing, and the results are presented in **Figure 14**. It can be seen the reduction of packing height from 95 ft to 50 ft reduces the absolute value of $CO_2$ capture by ~0.6%, and therefore the lean solvent flow rate would need to be increased slightly to obtain 90% capture. The height of the packing was selected to be 50 ft, because the capital cost of the absorber train offsets the cost of a small lean-solvent flow rate increase. Diameter of each absorber was optimized to avoid flooding, and it was determined to be 33 ft for the final cases.

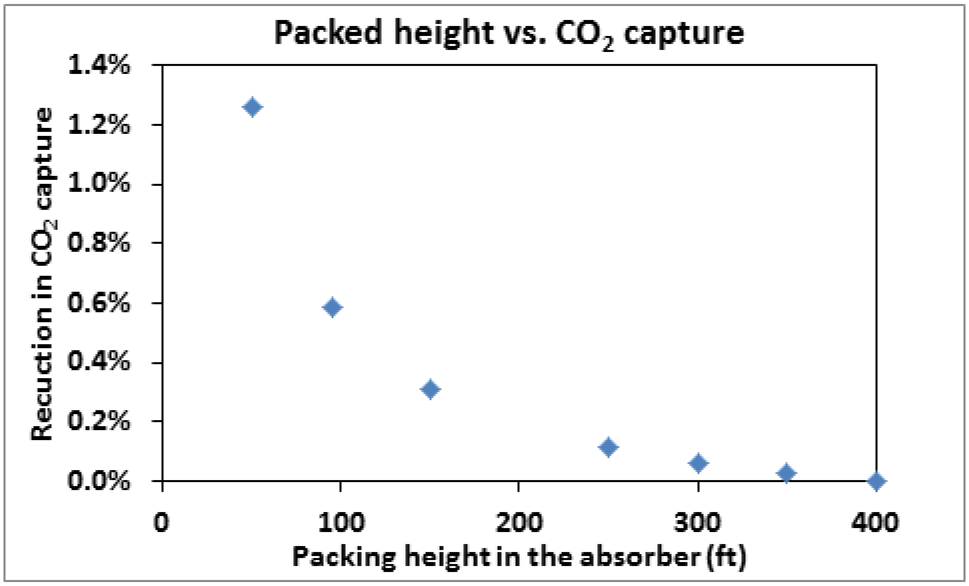


**Figure 14.** The effect of packing height on $CO_2$ capture

### 4.3.2 CSTR Desorber Design

It was previously shown that the aminosilicone-based solvent has significantly lower vapor pressure compared to MEA, and this property facilitates operating the desorption process at higher temperatures and pressures without significant solvent losses. This advantageous property also enables the desorption of $CO_2$ to be accomplished in a continuous stirred-tank reactor (CSTR) versus a distillation column, which reduces the CAPEX of the desorber system by ~50%. Among other advantages are easier operation and maintenance and smaller footprint.

The desorber system includes a recirculation loop with a high-pressure pump and heat exchanger to provide sufficient heat transfer surface area and increase liquid/gas interfacial area. The ASPEN Plus model flow diagram for the desorber is presented below in **Figure 15**. For each of the cases considered below, recirculation loop pump and heat exchanger sizes were calculated and used for capital cost estimation.

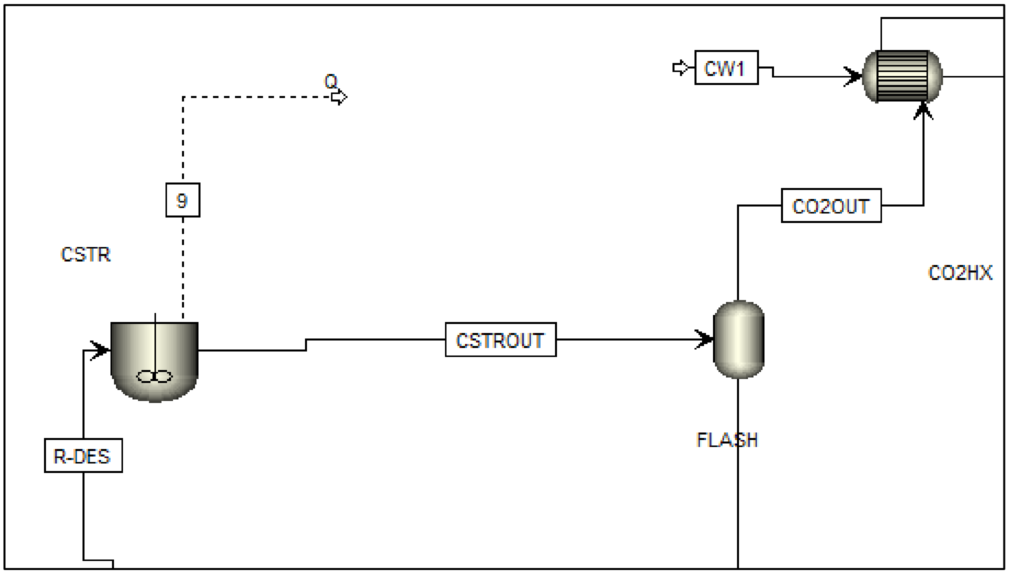


**Figure 15.** The desorber section of the ASPEN Plus flow sheet

The main design parameters for the desorber are temperature, pressure, and residence time. The current optimized desorber operates at a temperature of 130 °C, pressure of 63 psia, and residence time of 11 minutes. The residence time was selected based on a sensitivity analysis which showed that $CO_2$ desorption approached equilibrium at 11 minutes. The volume of the desorber is calculated based on this residence time.

The values used for the overall heat transfer coefficients for the desorber jacket and recirculation loop heat exchanger were selected based on a literature search and prior calculations, and are presented in **Table 7**.

**Table 7.** The heat transfer coefficients used in the desorber model

| *Type of heat transfer unit* | *Overall heat transfer coefficient U (Btu/hr·ft$^2$·F)* |
|---|---|
| Jacketed vessels: steam to organics, SS wall, average | 100 |
| Shell and Tube heat exchanger: steam to light organics, average | 185 |

The volume of the desorber is calculated based on a residence time of 11 minutes. The amount of heat which can be transferred through the desorber jacket can be calculated based on the following equation:

$$Q_{reactor} = U * A * LMTD$$

The total heat required for the desorber system is calculated by the ASPEN Plus model, and the heat duty for the recirculation loop heat exchanger is also determined. Based on these values, the appropriate size for heat exchanger and number of cycles/minute are calculated. The results for each of the aminosilicone-based cases studied for the carbon capture system are presented below in **Table 8**.

**Table 8.** Size of desorber and recirculation loop for different carbon capture cases

| | Desorber CSTR | | Recirculation loop | |
|---|---|---|---|---|
| | Total height, ft | Diameter, ft | HEX area, ft$^2$ | Number of cycles/min |
| Case A | 70 | 33.0 | 10,128 | 0.25 |
| Case B | 53 | 33.0 | 10,214 | 0.34 |
| Case C | 38 | 33.0 | 10,452 | 0.50 |
| Case D | 37 | 33.0 | 10,432 | 0.51 |
| Case E | 44 | 33.0 | 9,649 | 0.20 |
| Case H | 54 | 33.0 | 12,511 | 0.20 |

### 4.3.3 Rich-Lean Heat Exchanger

In order to recover as much heat as possible from the hot lean solvent stream leaving the desorber, a rich-lean heat exchanger will be utilized to preheat the rich cold solvent leaving the absorber train. In current simulations, the rich-lean heat exchanger is modeled as a shell and tube unit with a constant value of the overall heat transfer coefficient of 75 Btu/hr·ft$^2$·F. This value was previously estimated from heat transfer film coefficients based on known physical properties and design assumptions. In the current system, this unit represents ~25% of the total equipment cost for the $CO_2$-capture process. Therefore, additional work will be done in the future to find the optimal design for this heat exchanger, to increase the value of the overall heat transfer coefficient, which will reduce the CAPEX of the $CO_2$-capture system.

<u>Heat Transfer Coefficient</u>

The overall heat transfer coefficient for shell and tube heat exchangers can be calculated from the equation below.[3]

$$U_o = \frac{1}{\frac{1}{h_o} + R_{do} + \frac{xA_o}{k_w A_{wm}} + \left(\frac{1}{h_i} + R_{di}\right) A_o/A_i} \tag{1}$$

where $h_0$ and $h_i$ are individual film heat-transfer coefficients, $R_{do}$ and $R_{di}$ are fouling resistances; and $(xA_0/k_wA_{wm})$ is wall resistance.

Two separate methods were used to calculate individual film heat-transfer coefficients for tube and shell sides.

Shell-Side Individual Film Heat-Transfer Coefficient

Shell-side heat-transfer coefficient for an ideal tube bank $h_k$ can be determined as following.[3]

$$h_k = j_k c \frac{W}{S_m} \left(\frac{k}{c\mu}\right)^{2/3} \left(\frac{\mu_b}{\mu_w}\right)^{0.14} \quad (2)$$

where $j_k$ is the factor determined from the correlation for j-factor for and ideal tube bank (**Figure 16**), c is specific heat, k is the thermal conductivity, $\mu_b$ is bulk viscosity of the solvent, $\mu_w$ is viscosity evaluated at the mean surface temperature, W is mass flow rate, and $S_m$ is one cross-flow section.

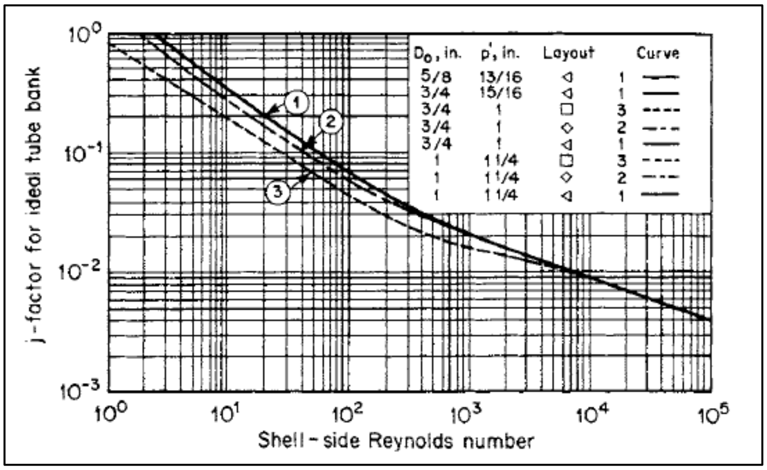


**Figure 16.** Correlation of j f actor for ideal tube bank

The shell side Reynolds number can be determined as following.

$$(N_{Re})_s = D_o W / \mu_b S_m \quad (3)$$

Steps for calculation of shell-side heat transfer coefficient are described below.

1) Identify assumptions for these calculations:
    a. Reynolds number on the shell side for MEA and GAP-$1_m$/TEG system is the same, and equals 1,000.
    b. Ratio of bulk-to-wall viscosity is assumed to be 10. Due to the higher temperature of the wall surface versus bulk, the viscosity will be lower at the surface. The estimated value has little impact on the heat transfer coefficient

due to the small exponent in Equation 2. Ten was chosen as a conservative estimate.

    c. Tube diameter is 1.5 inch.

2) Calculate ratio of $W/S_m$ from Equation 3.
3) Find $j_k$ value from the plot in **Figure 16**.
4) Substitute physical properties of the solvent, value of $j_k$, and the value of $W/S_m$ into the equation 2 to find $h_o$.

Tube-Side Individual Film Heat-Transfer Coefficient

The tube side heat transfer coefficient for circular tubes can be determined from the following Nusselt number correlation for laminar flow.[4]

$$Nu = 1.86(Re\text{Pr})^{0.33}(\frac{d}{L})^{0.33}(\frac{\mu_{wall}}{\mu_{bulk}})^{0.14} \qquad (4)$$

Also, Nusselt number can be correlated to the heat transfer coefficient h through the following expression.[5]

$$Nu = \frac{hd}{12k} \qquad (5)$$

Below are the steps for the calculation of the tube-side heat transfer coefficient.

1) Identify assumption for these calculations:
    a. Reynolds number on the tube side for MEA and GAP-$1_m$/TEG system is the same, and it equals 1,000 (laminar flow). This number was selected as a moderate value corresponding to a flow of ~ 10 ft/sec.
    b. Tube diameter is 1.5 in.
2) Calculate Prandtl number for each solvent system.
3) Calculate Nusselt number from Equation 4.
4) Calculate $h_i$ from Equation 5.

### Overall Heat-Transfer Coefficient

The overall heat transfer coefficient can be calculated from Equation 1, and below are the steps for calculations.

1) Identify assumptions for these calculations:
    a. Thickness of the pipe wall is 0.25 in.
    b. Pipe material is carbon steel.
    c. Fouling coefficient is 5,000 $W/m^2 \cdot K$

2) Use Equation 1 to determine overall heat transfer coefficient, U.

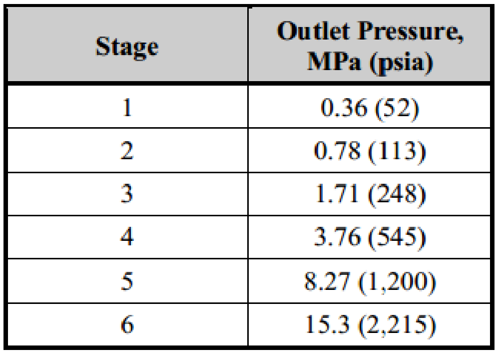
These calculations were used to determine the overall heat transfer coefficients for a 30/70 MEA/water system and to compare it to the 60/40 GAP-$1_m$/TEG system. The values of overall heat transfer coefficient for 60/40 GAP-$1_m$/TEG and 30/70 MEA/water are 75 and 93 $Btu/(hr \cdot ft^2 \cdot F)$, respectively.

It has to be noted that this value of U is specific to the assumptions made and considered conditions. Due to the high viscosity of the rich GAP-$1_m$/TEG solvent, turbulent flow might be a challenge for the tube side of the heat exchanger, and pressure drop would also need to be considered for the final design. So, a velocity in the laminar regime was chosen. To increase the overall heat transfer, shell-side Reynolds number can be potentially increased.

### Compression Train

The purpose of the compression train it to deliver a high-purity $CO_2$ stream at 2215 psia for transportation and storage. The discharge pressures at each stage are presented in **Table 9**.

**Table 9.** The outlet pressures at each stage in the compression train



| Stage | Outlet Pressure, MPa (psia) |
|---|---|
| 1 | 0.36 (52) |
| 2 | 0.78 (113) |
| 3 | 1.71 (248) |
| 4 | 3.76 (545) |
| 5 | 8.27 (1,200) |
| 6 | 15.3 (2,215) |

Since the desorber operates at 63 psia in the aminosilicone-based process, the first stage of the compression train can be removed, significantly reducing the cost of the compression train. The pressurized gas stream is cooled to 40 °C after each compressor with cooling water and all liquid condensate is removed in a vapor/liquid flash separator. Cooling water is supplied from the power plant cooling tower system. The compressors at each stage have a polytropic efficiency of 86% and mechanical efficiency of 98%.

The final $CO_2$ stream has to satisfy the conceptual design limits for enhanced oil recovery as listed in Exhibit 2-1 of the NETL QGESS titled "$CO_2$ Impurity Design Parameters". [6] **Table 10** shows the required specifications for the product $CO_2$ stream and the composition of the $CO_2$ stream for the aminosilicone base-case model.

**Table 10.** Case H $CO_2$ stream outlet composition as compared to EOR specifications

| Component | Unit | Enhanced Oil Recovery specification | | CASE H |
|---|---|---|---|---|
| | | Conceptual design | Range in Literature | |
| $CO_2$ | Vol % (min) | 95 | 90-99.8 | 99.39 |
| $H_2O$ | $ppm_v$ | 500 | 20-650 | 812 |
| $N_2$ | Vol% | 1 | 0.01-2 | <0.01 |
| $O_2$ | Vol% | 0.001 | 0.001-1.3 | <0.001 |
| Ar | Vol% | 1 | 0.01-1 | 0 |

It can be seen that final high pressure $CO_2$ stream generated by the aminosilicone-based process has slightly higher water amount than the EOR specifications. In future work the amount of cooling will be increased in order to match specification limits.

Multiple cases were considered for technical and economic analysis of the CSTR, and below is the summary table of all cases with specific conditions (**Table 11**)

**Table 11:**. Summary of major cases considered for the aminosilicone-based $CO_2$ separation system

| | *Absorber intercoolers (Y/N)* | *Number of absorbers* | *Intercooler load (each)* | *Desorber T,°F* | *Desorber P (psia)* | *Number of desorbers* | *Absorber packing type* | *Packing material* | *Sulfur in FG (ppm)* |
|---|---|---|---|---|---|---|---|---|---|
| Case A | N | 4 | NA | 284 °F | 63 | 2 | Rachig rings | CS | 5 |
| Case B | Y | 4 | 30 MW | 284 °F | 63 | 2 | Rachig rings | CS | 5 |
| Case C | Y | 4 | 60 MW | 284 °F | 63 | 2 | Rachig rings | CS | 5 |
| Case D | Y | 4 | 60 MW | 284 °F | 63 | 2 | MellapakPL 252Y | CS | 5 |
| Case E | Y | 4 | 60 MW | 266 °F | 63 | 2 | MellapakPL 252Y | CS | 5 |
| Case F | Y | 3 | 80 MW | 266 °F | 63 | 2 | MellapakPL 252Y | CS | 5 |
| Case G | Y | 3 | 80 MW | 266 °F | 63 | 2 | MellapakPL 252Y | CS | 5 |
| Case G | Y | 3 | 80 MW | 266 $^{o}$F | 63 | 2 | MellapakPL 252Y | CS | 5 |

Case G was scaled up to 552 MW net power including the $CO_2$-capture island to generate Case H.

## 4.4 J23 Model

Aspen model developed for the CSTR desorber and low water content working solution was further modified to capture the system performance for the steam stripper column (SSC) under higher water content. First, properties of GAP-1$_m$ – TEG – $H_2O$ system with water content up to 10 wt.% were measured and modelled. Model was then validated wetted wall column (WWC), bench scale system (2 kW) and pilot scale (0.5 MWe) data. The updated model was denoted J23.

### 4.4.1 Property Evaluation and Modelling

#### 4.4.1.1 *Viscosity*

The viscosity model is developed using the Andrade model, which is built into the Aspen Plus user interface, as a starting point. The model equations are given by:[7]

$$\ln(\mu_{mix}) = \sum_i w_i \ln(\mu_i) + \sum_i \sum_{j \neq i} (k_{ij} w_i w_j + m_{ij} w_i^2 w_j^2) \tag{6}$$

$$k_{ij} = a_{ij} + \frac{b_{ij}}{T} \tag{7}$$

$$m_{ij} = c_{ij} + \frac{d_{ij}}{T} \tag{8}$$

The term $\mu_i$ represents the viscosity of pure component *i*, which is calculated as:

$$\ln(\mu_i) = a_i + \frac{b_i}{T} + c_i \ln(T) \tag{9}$$

where the terms $a_i$, $b_i$, and $c_i$ are component dependent fitting parameters. The terms $a_{ij}$, $b_{ij}$, $c_{ij}$, and $d_{ij}$ are binary interaction fitting parameters. The weight fraction of component *i* is represented by $w_i$. The components of interest for this model development are GAP-$1_m$, GAP-$1_m$ carbamate, TEG, and $H_2O$. The pure component viscosities of TEG and $H_2O$ are known as a function of temperature, so values provided by the Aspen Plus databank are used to calibrate the parameters for Eq. 6 for these components. For GAP-$1_m$, the parameters of this equation are calibrated to fit pure component data provided as part of this work. The parameters for this model are given in **Table 12** and the comparison between model and experimental data for GAP-$1_m$ viscosity is given in **Figure 17**.

**Table 12.** Pure component viscosity model parameters for GAP-$1_m$ (viscosity calculated in cP)

| Parameter | Value |
|---|---|
| A | -43.724 |
| B | 4391.75 |
| C | 5.345 |

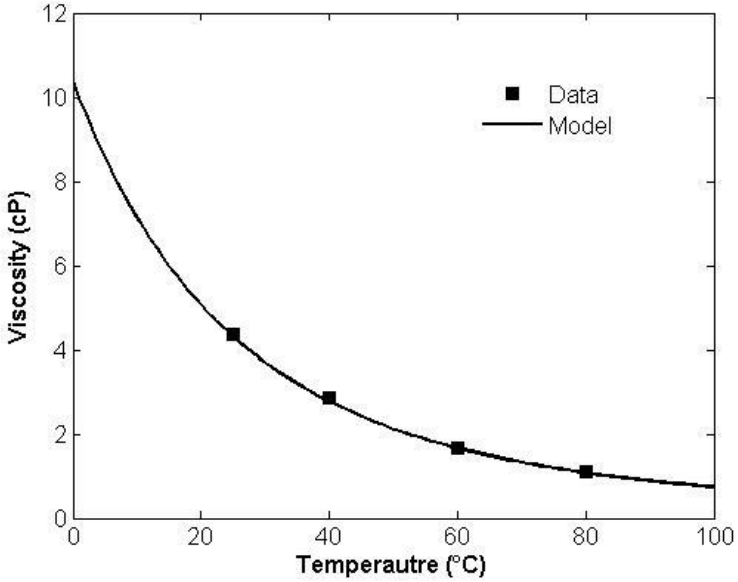


**Figure 17.** Comparison of pure component GAP-$1_m$ viscosity data to model predictions

Due to the large number of parameters available in this model, a model selection methodology in which the Akaike Information Criterion (AIC)[8] is used as the model selection metric. The quantity is defined as:

$$AIC = Nln\left(\frac{SSE}{N}\right) + 2k \tag{10}$$

where *N* is the number of data used in the parameter regression, *k* is the number of parameters fit for a given model, and *SSE* is the sum of squared error for the model and data comparison. The objective is to choose a model that minimizes the *AIC*, essentially providing a trade-off between the quality of the model fit and its complexity in terms of the number of parameters included. In this methodology, parameters are added to the model incrementally until the value of *AIC* starts to increase when further adding parameters. The final model form is given in Eq. 11 and the values of the parameters included are given in **Table 13**.

$$\begin{aligned} ln(\mu_{mix}) = {} & w_{GAP}\ln(\mu_{GAP}) + w_{TEG}\ln(\mu_{TEG}) + w_{H_2O}\ln\left(\mu_{H_2O}\right) + w_{GAPC}\left(\mathrm{a} + \frac{b}{T}\right) \\ & + w_{GAP}w_{TEG}\left(c + \frac{d}{T}\right) + ew_{GAP}w_{GAPC} + fw_{GAP}w_{H_2O} + gw_{TEG}w_{H_2O} \\ & + hw_{GAPC}w_{TEG} + w_{GAPC}w_{H2O}\left(i + \frac{j}{T}\right) + kw_{GAP}^2w_{TEG}^2 \\ & + +w_{GAPC}^2w_{H2O}^2\left(l + \frac{m}{T}\right) \end{aligned} \tag{11}$$

**Table 13.** Values of parameters included in viscosity model (viscosity calculated in cP)

| Parameter | Value |
|---|---|
| A | -12.9988 |
| B | 7627.65 |
| C | -3.61486 |
| D | 2129.73 |
| E | -1.41403 |
| F | 7.42995 |
| G | 0.550119 |
| H | -2.23113 |
| I | 40.0024 |
| J | -20467.2 |
| K | 5.34504 |
| L | -363.437 |
| M | 154357 |

Note that since the pure component viscosity of GAP-$1_m$ carbamate is unknown, its parameters are incorporated as fitting parameters for this model. A parity plot of the viscosity model fit is given in **Figure 18**.

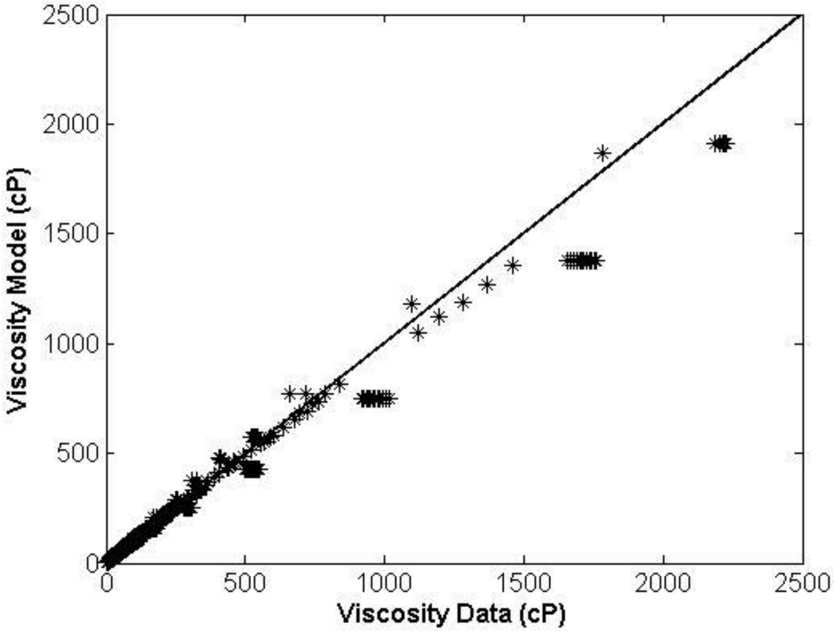


**Figure 18.** Parity plot for viscosity model fit. A total of 2064 data are incorporated into model regression, with a correlation of $\boldsymbol{R^2 = 0.984}$.

**Figure 19** shows the prediction of the solution viscosity as a function of temperature and composition. For this plot the relative weight percentages of $H_2O$ ($w^*_{H_2O}$) and GAP-1$_m$ carbamate ($w^*_{GAPC}$) are defined such that the actual composition ($w_i$) may be calculated as:

$$w_{H_2O} = w^*_{H_2O} \tag{12}$$

$$w_{TEG} = 0.40 \tag{13}$$

$$w_{GAPC} = w^*_{GAPC}\left(1 - \left(w_{TEG} + w_{H_2O}\right)\right) \tag{14}$$

$$w_{GAP} = 1 - (w_{H_2O} + w_{TEG} + w_{GAPC}) \tag{15}$$

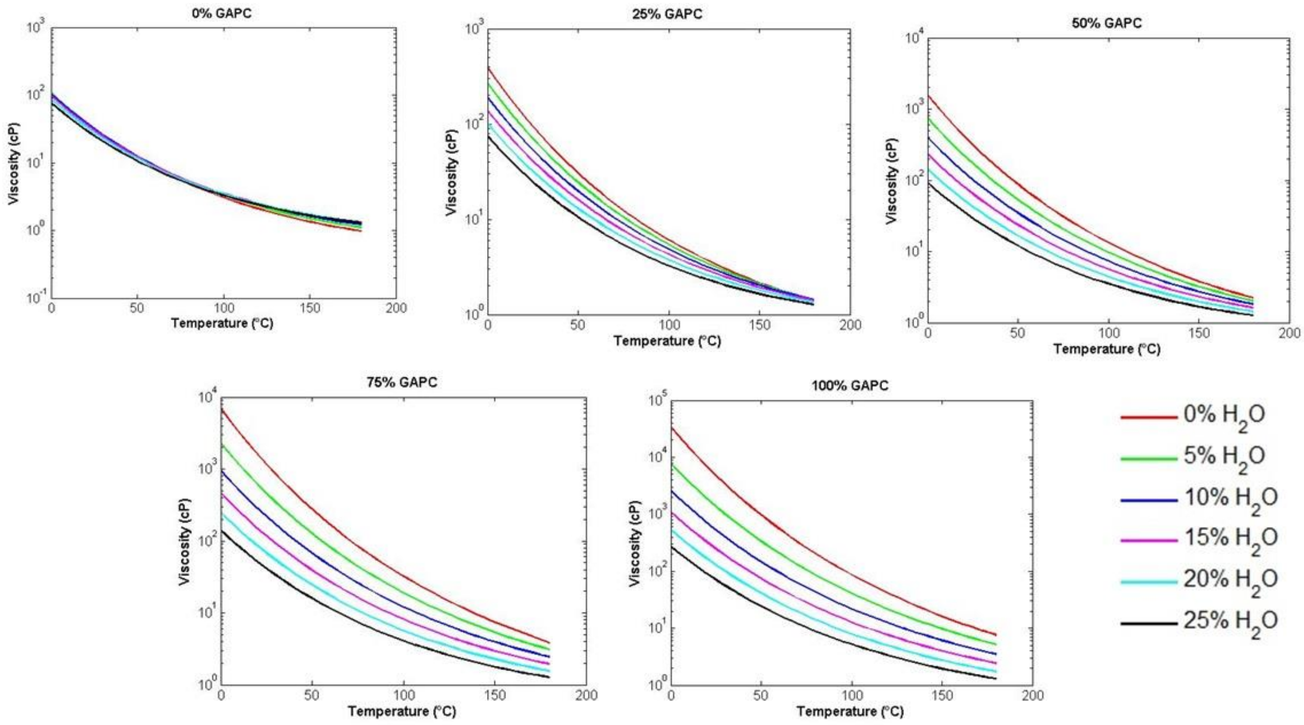


**Figure 19.** Solution viscosity as a function of temperature and solvent composition

#### 4.4.1.2 *Vapor Pressure*

The pure component vapor pressure of GAP-1$_m$ is fit to experimental data, using the Aspen Plus model as a starting point, which is given in the form:

$$P^*_{GAP} = \exp\left(a_1 + \frac{a_2}{T + a_3} + a_4 T + a_5 \ln(T) + a_6 T^{a_7}\right) \tag{16}$$

Due to the small number of data available for developing the GAP-1$_m$ vapor pressure model, only two parameters are included in the final model. The values of the parameters for the GAP-1$_m$ vapor pressure model are given in **Table 14** and the comparison of the model to the experimental data is given in **Figure 20**.

**Table 14.** Parameter values for GAP-1$_m$ vapor pressure model (calculated in bar)

| Parameter | Value |
|---|---|
| $a_1$ | 13.642 |
| $a_2$ | -7435.9 |

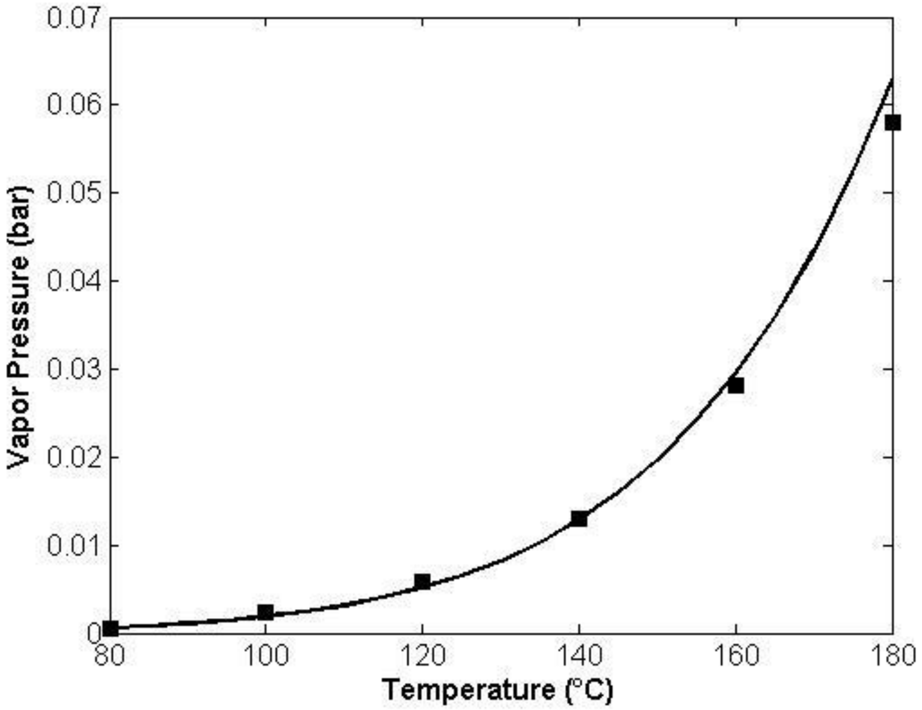


**Figure 20.** Fit of GAP-$1_m$ vapor pressure model to experimental data

### 4.4.1.3 *Density/Molar Volume*

A molar volume model for the GAP-$1_m$ - GAP-$1_m$ carbamate - TEG is proposed of the form:

$$V_{sln} = \sum_i x_i V_i + \sum_{j \neq i} \sum_i x_i x_j V_{ij}^* \tag{17}$$

$$V_i = a_i + \frac{b_i}{T} + c_i \ln(T) \tag{18}$$

where $x_i$ and $V_i$ are the mole fraction and molar volume of species *i*, $a_i$ - $c_i$ are the adjustable parameters for the pure component molar volume terms, and $V_{ij}^*$ is a binary pair interaction term. As for the viscosity, the molar volume of TEG is known and the terms for Eq. 18 are determined from the Aspen Plus databank. A few data points for density are given for fitting the parameters of the molar volume model, noting that molar volume is related to density by:

$$\rho_{sln} = \frac{MW_{sln}}{V_{sln}} \tag{19}$$

The density data available are given in **Table 15**.

**Table 15.** Density data available for developing molar volume model

| Data No. | T(°C) | $w_{GAP}$ | $w_{TEG}$ | $w_{GAPC}$ | $\rho_{sln}$ (g/mL) |
|---|---|---|---|---|---|
| 1 | 25 | 0.6 | 0.4 | 0 | 1.0216 |
| 2 | 25 | 0.42 | 0.391 | 0.189 | 1.0422 |
| 3 | 25 | 0.24 | 0.382 | 0.378 | 1.0606 |
| 4 | 25 | 0 | 0.37 | 0.63 | 1.0843 |
| 5 | 40 | 0.6 | 0.4 | 0 | 1.0109 |
| 6 | 40 | 0 | 0.37 | 0.63 | 1.0721 |
| 7 | 60 | 0.6 | 0.4 | 0 | 0.9963 |
| 8 | 60 | 0 | 0.37 | 0.63 | 1.0569 |
| 9 | 80 | 0.6 | 0.4 | 0 | 0.9828 |
| 10 | 80 | 0 | 0.37 | 0.63 | 1.0451 |

Since eight of the ten data are for a binary system (TEG and either GAP-$1_m$ or GAP-$1_m$ carbamate), the pure component molar volume values are determined directly from Eq. 17, with the term containing $V_{ij}^*$ assumed to be zero. For the data in which the weight fraction of GAP-$1_m$ carbamate is 0, the model given by Eq. 17 reduces, for a single data point, as:

$$V_{data} = x_{GAP}V_{GAP} + x_{TEG}V_{TEG} \tag{20}$$

since the molar volume of TEG is known, the value of the GAP-$1_m$ molar volume may be calculated directly. If the pure component molar volume (Eq. 18) is truncated to two terms, the values of the parameters $a_{GAP}$ and $b_{GAP}$ may be calculated directly with a linear fit of all values of $V_{GAP}$ calculated for the data in which $x_{GAPC}$ is 0. An analogous procedure is performed for determining the parameters for GAP-1$_m$ carbamate, in which the data in which $x_{GAP} = 0$ are considered. The calculation of the molar volume model parameters is illustrated in **Figure 21** and the values of the parameters are tabulated in **Table 16**.

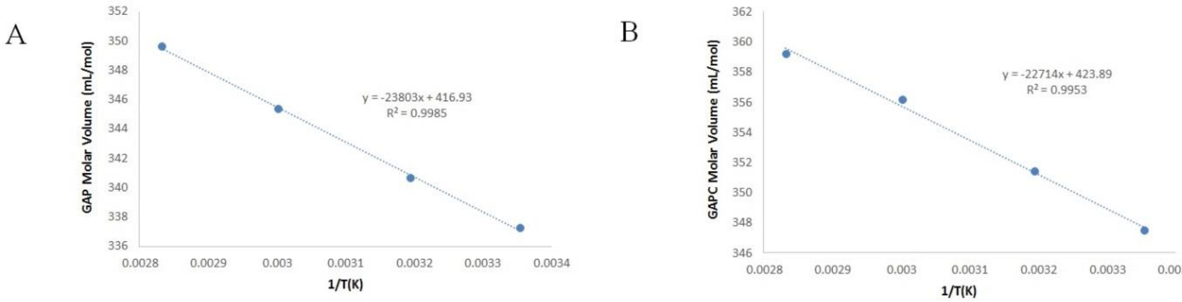


**Figure 21.** Calculation of model parameters for pure component molar volume for (A) GAP-1$_m$ and (B) GAP-1$_m$ carbamate

**Table 16.** Values of parameters for molar volume model

| Parameter | Value |
|---|---|
| $a_{GAP}$ | 416.93 |
| $b_{GAP}$ | -23803 |
| $a_{GAPC}$ | 423.89 |
| $b_{GAPC}$ | -22714 |

This model is also shown to be accurate for the two data points for the ternary GAP1$_m$-GAP1$_m$ carbamate -TEG system, although they are not directly included in the model development. Due to the small number of data available for determining the model parameters, the term $V_{ij}^{*}$ is assumed to be zero. Although no data are given for solutions containing water, the molar volume of water is incorporated into the model using the equation:

$$V_{mix} = x_{H_2O}V_{H_2O} + (1 - x_{H_2O})V_{sln} \tag{21}$$

where $V_{mix}$ is the overall molar volume and $V_{sln}$ is the molar volume of the GAP1$_m$-GAP1$_m$ carbamate -TEG system, as defined in Eq. 17. The molar volume of water is calculated in the form outlined in Eq. 18, and the coefficients are determined from the information in the Aspen Plus databank.

### 4.4.2 Thermodynamic Model

The thermodynamic model used for this system assumes that the system speciation may be represented by a single equilibrium reaction, given as:

$$GAP1m + CO_2 \leftrightarrow GAP1m\ carbamate \tag{22}$$

For fitting the thermodynamic model, experimental data are given in terms of temperature (T), initial $CO_2$ weight fraction ($W_{TOT}$), and $CO_2$ partial pressure ($P_{CO_2}$). For computational efficiency, $W_{TOT}$ is treated as the dependent variable for the regression analysis, so that the objective function used in the parameter regression is:

$$\min_{\tilde{\theta}} f(\tilde{\theta}) = \sum_i [W_{TOT,i} - W^*_{TOT,i}(\tilde{\theta})]^2 \tag{23}$$

where $\tilde{\theta}$ is the set of parameters included in the model regression and $W^*_{TOT,i}(\tilde{\theta})$ is the calculated value of the initial $CO_2$ weight fraction. The model parameters are included in the calculation of the molarity basis equilibrium constant ($K^*_{eq}$) and the Henry constant of $CO_2$ ($H_{CO_2}$), which are given by:

$$H_{CO_2} = \exp\left(H_1 + \frac{H_2}{T}\right) \tag{24}$$

$$K^*_{eq} = \exp\left(K^*_1 + \frac{K^*_2}{T}\right) = \frac{[GAPC]}{[GAP][CO_2]} \tag{25}$$

$$\tilde{\theta} = [K^*_1\ K^*_2\ H_1\ H_2] \tag{26}$$

The final mole fraction of $CO_2$, after the equilibrium reaction is taken into consideration, is determined by the physical equilibrium relationship:

$$x_{CO_2} = \frac{P_{CO_2}}{H_{CO_2}} \tag{27}$$

The molarity of CO2 in solution after reaction is calculated as:

$$[CO_2] = \frac{x_{CO_2}}{1 - x_{CO_2}} * \frac{N_{GAP,o} + N_{TEG,0}}{V_{sln}} \tag{28}$$

where $N_{GAP,o}$ and $N_{TEG,0}$ are the initial molar amounts of GAP-1m and TEG in the solution into which CO2 is loaded, and $V_{sln}$ is the initial volume of solution. The molarity of GAP-1m carbamate is then calculated as:

$$[GAPC] = \frac{N_{GAP,0}}{V_{sln}} \left(1 - \frac{1}{K_{eq}^*[CO_2] + 1}\right) \tag{29}$$

The model prediction of the CO2 weight fraction is:

$$W_{TOT,i}^*(\tilde{\theta}) = \frac{MW_{CO_2} V_{sln}([GAPC] + [CO_2])}{100 + MW_{CO_2} V_{sln}([GAPC] + [CO_2])} \tag{30}$$

where $MW_{CO_2}$ is the molecular weight of CO2.

The optimal set of parameter values is given as:

$$\tilde{\theta}^T = \begin{bmatrix} K_1^* \\ K_2^* \\ H_1 \\ H_2 \end{bmatrix}^* = \begin{bmatrix} -25.0312 \\ 10480 \\ 8.09002 \\ -1400 \end{bmatrix} \tag{31}$$

The parity plot of model and data values of the CO2 weight fraction is given in **Figure 22**. A total of 41 data points are included in the regression, and the resulting correlation coefficient between the model and data fit is $R^2 \approx 0.974$.

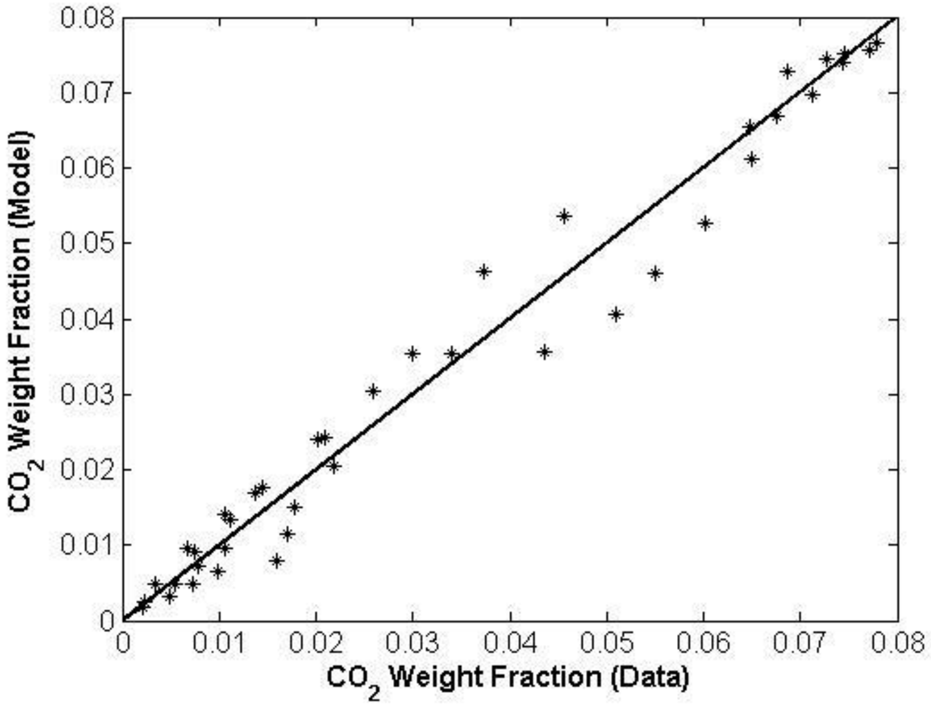


**Figure 22.** Parity plot of VLE data considered for thermodynamic model regression

### 4.4.3 Process model development

The process model for the high-viscosity solvent is developed using the following models for mass transfer coefficients[9] and interfacial area[10]:

$$k_G = D_G C_G \left(\frac{a}{d_H}\right)^{0.5} {Sc_G}^{0.333} \left(\frac{u_G \rho_G}{a \mu_G}\right)^{0.75} \sqrt{\frac{1}{\varepsilon - h_L}} \tag{32}$$

$$k_L = C_L \left(\frac{\rho_L g}{\mu_L}\right)^{0.167} \left(\frac{D_L}{d_H}\right)^{0.5} \left(\frac{u_L}{a}\right)^{0.333} \tag{33}$$

$$a_e = A_1 \left[\frac{\rho_L}{\sigma} g^{1/3} \left(\frac{u_L A}{L_P}\right)^{4/3}\right]^{A_2} \tag{34}$$

where $k_i$ is the liquid side mass transfer coefficients, $D_i$ the Diffusivity, $Sc_i$ the Schmidt number, $u_i$ the velocity, $\rho_i$ gas density, $\mu_i$ the viscosity, $a$ the packing specific area, $\varepsilon$ the packing void fraction, $h_L$ the absorber holdup, $d_H$ the packing hydraulic diameter, $\sigma$ the surface tension, $\frac{A}{L_P}$ denotes the wetted perimeter. The subscripts G and L indicates the gas and liquid phases. The parameters $C_L$, $C_G$, $A_1$ and $A_2$ are regressed simultaneously using a methodology previously applied to a MEA-$H_2O$-$CO_2$ system[11]. Wetted wall column and bench scale data (2 kW continuous operation) are simultaneously considered in the regression. It can be noted that the GE bench-scale experiments studied several solvent and gas flowrates in a system comprising of an absorber and a CSTR for solvent regeneration. The process models were developed in Aspen Plus™ V8.4 while the optimizations were performed using the FOQUS[10] framework.

The objective function for the optimization problem was:

$$obj = \sum_{i=1}^{n} \left[\left(\frac{F_{i,model} - F_{i,exp}}{F_{i,exp}}\right)^2 + \left(\frac{C_{i,model} - C_{i,exp}}{C_{i,exp}}\right)^2\right] \tag{35}$$

where $F$ denotes the wetted wall column flux and $C$ the bench-scale $CO_2$ capture ratio.

Random samples were drawn from the bench scale experimental data to be used for the parameter estimation. Remaining samples from the bench scale experiments were used for validation. The parity plots of model and data of the bench-scale $CO_2$ capture ratio, and the model and normalized Flux in the wetted wall column are given in **Figure 23** and **Figure 24**. Model errors are found to be within ±20%. While improvements in the model error could be achieved by further development of the model, especially for the bench scale results, the model was considered to be good enough considering the error in the experimental data and results from the validation studies of the bench scale model presented later in this document.

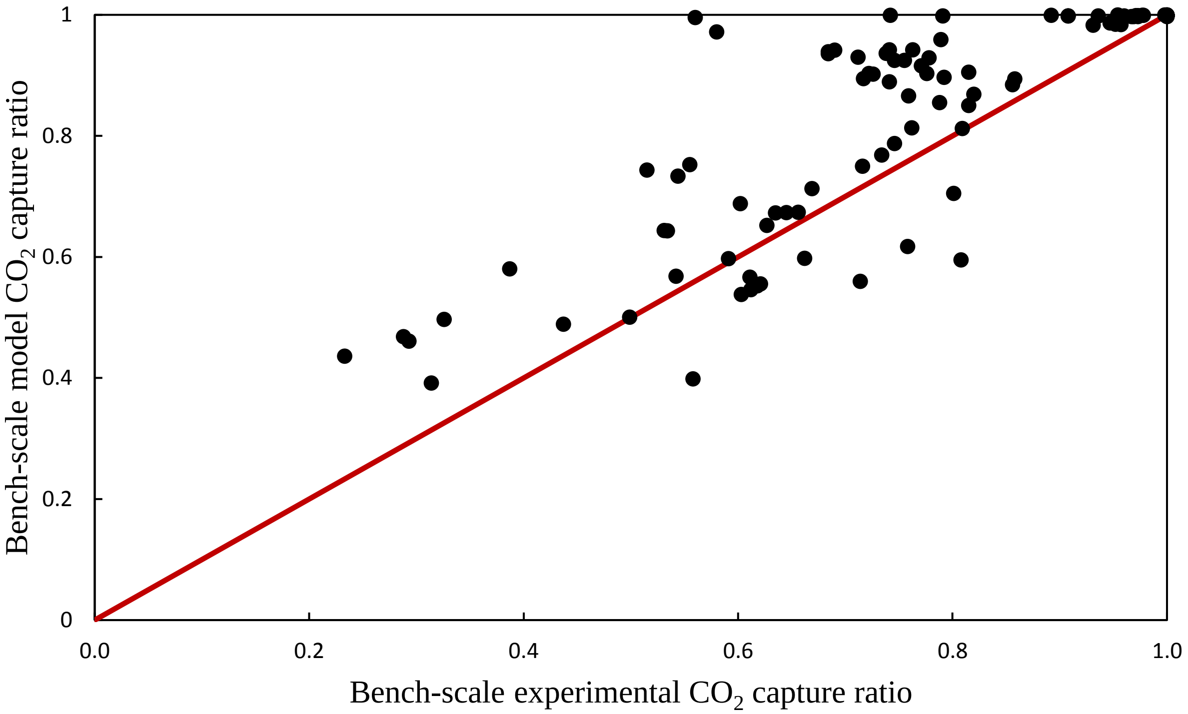


**Figure 23.** Parity plot of $CO_2$ capture: Bench Scale (2 kW) vs. model

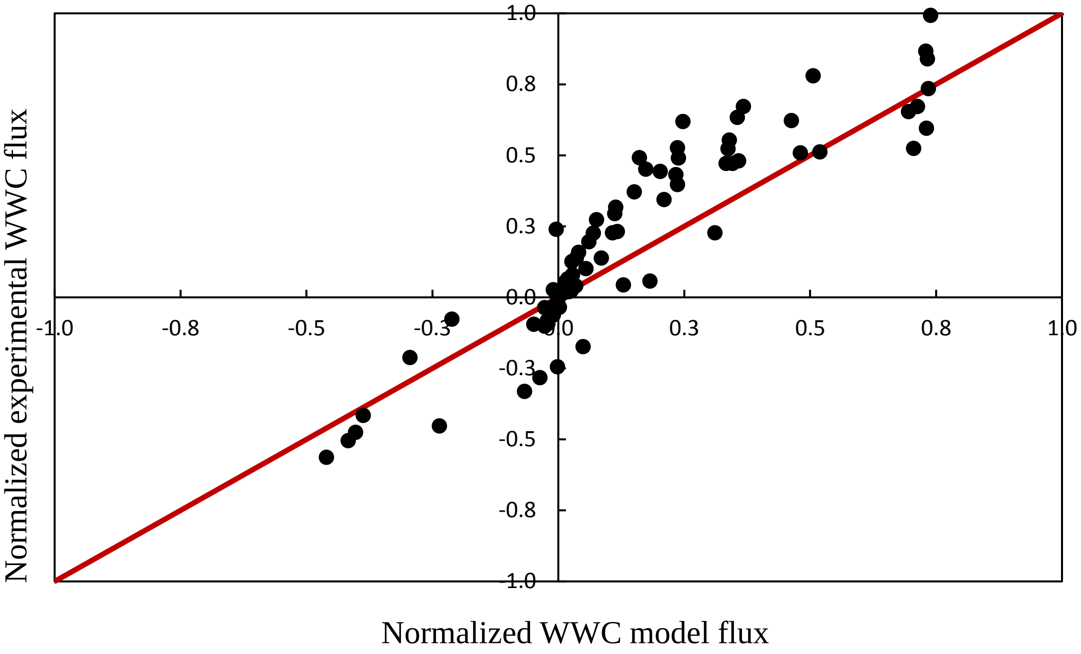


**Figure 24.** Parity plot of wetted wall column normalized $CO_2$ flux

### 4.4.4 Bench-scale validation

**Figure 25** presents the parity plot for $CO_2$ capture where the data that are not utilized in the regression are considered.

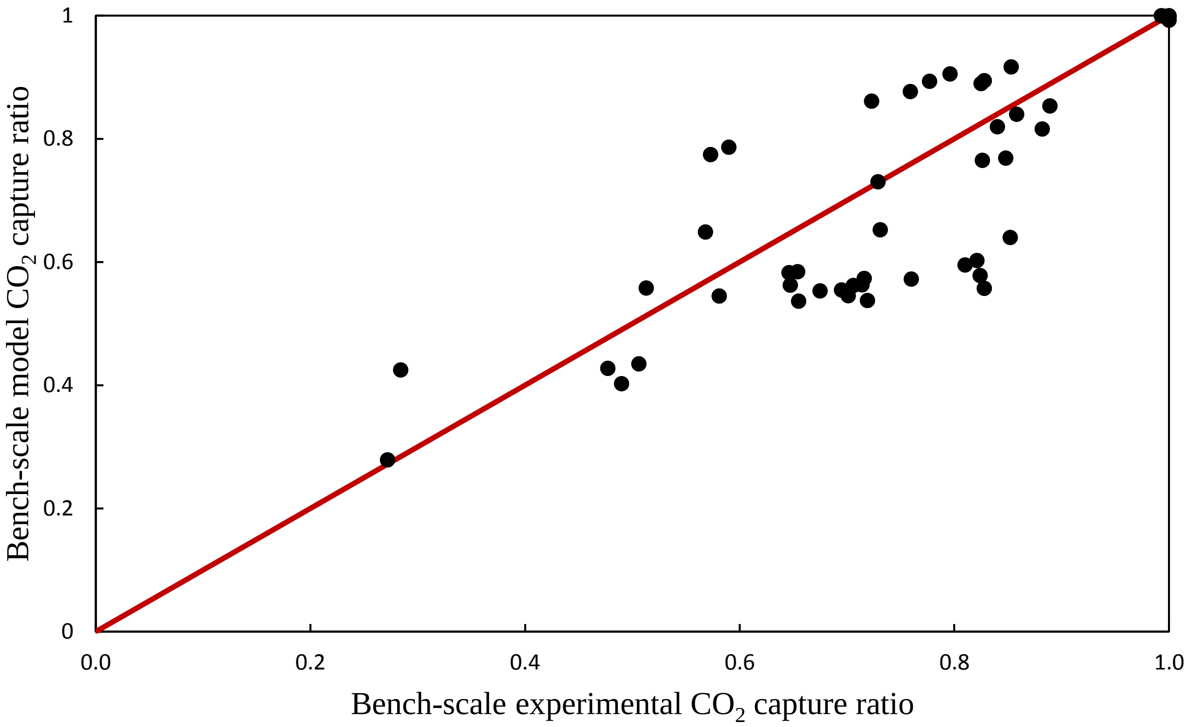


**Figure 25.** Parity plot of the bench-scale $CO_2$ capture ratio

The solvent regeneration was also validated using the bench-scale data, using the implemented CSTR model, which used the equilibrium constants derived from the thermodynamic model. The parity plot for the lean solvent $CO_2$ loading from the CSTR is presented in **Figure 26**.

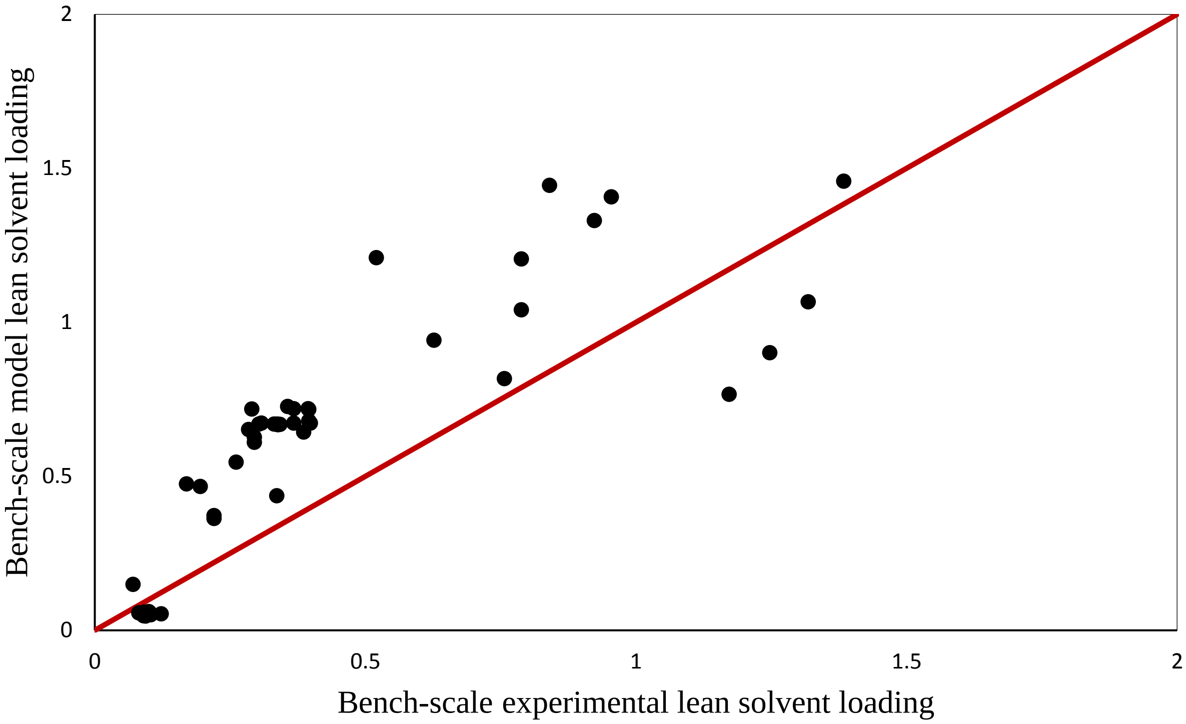


**Figure 26.** Parity plot of the bench-scale lean solvent $CO_2$ loading

### 4.4.5 J23 Model: 0.5 MWe Pilot Validation

The model described in 3.4.1 – 3.4.5 (denoted as J23 model) was scaled-up to 0.5 $MW_e$, and the results were compared with the dataset obtained during the 0.5 $MW_e$ pilot demo performed at NCCC under DOE contract DE-FE0013755. **Figure 27** shows comparison of % $CO_2$ capture in the absorber. The $CO_2$ desorption rate in the steam stripper column is compared in **Figure 28**, in which about 50% of the cases are outside of the desired error bound of 10%. However, when the steam stripper column model was evaluated independently by considering the rich-solvent data as the input, the results improved significantly (**Figure 29**). It is conceivable that the errors from the absorber model gets propagated to the stripper performance, amplifying the errors observed for the overall integrated absorber - desorber.

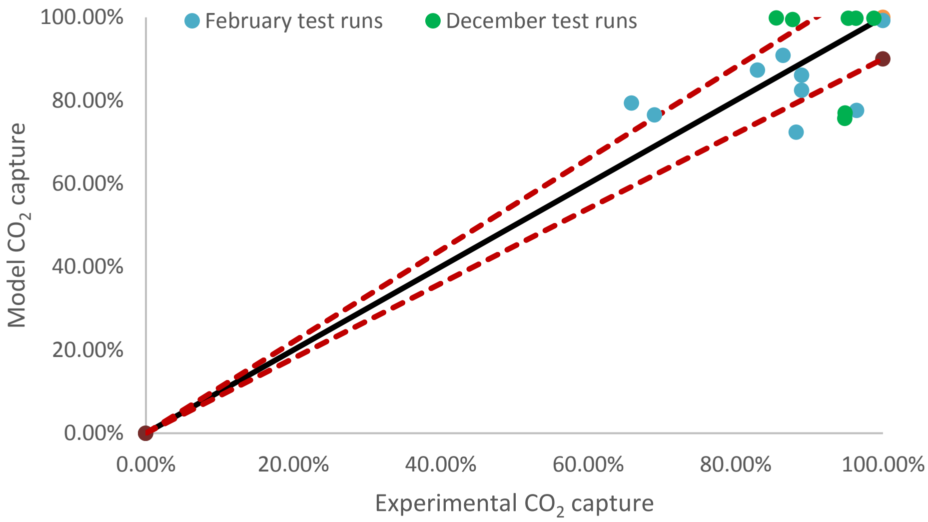


**Figure 27.** $CO_2$ Capture Efficiency (absorber): Experimental vs. J23 model (0.5 $MW_e$ scale)

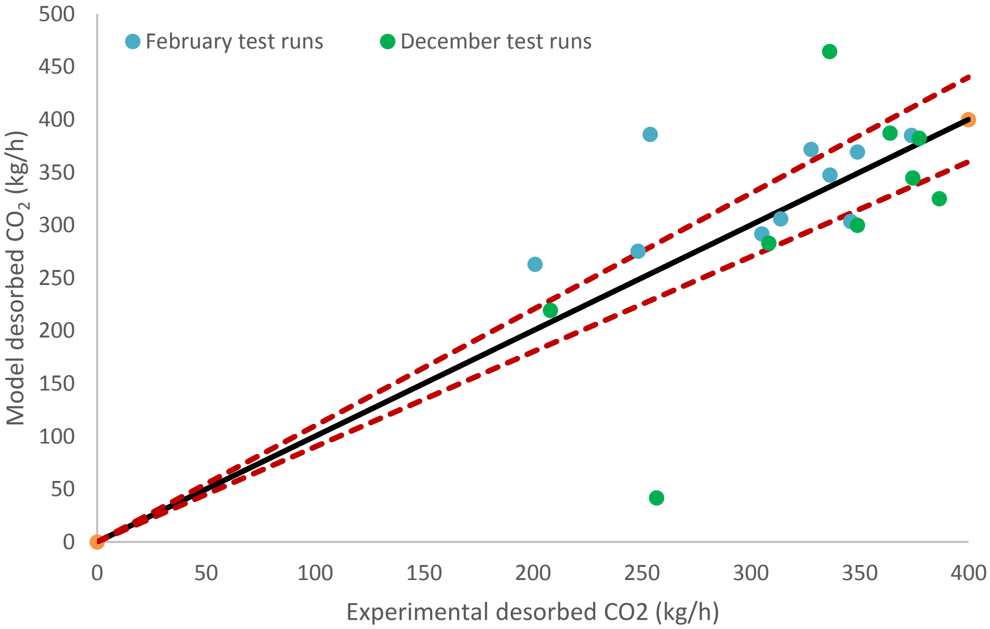


**Figure 28.** $CO_2$ Capture Efficiency (absorber and steam stripper): Experimental vs. J23 model (0.5 $MW_e$ scale)

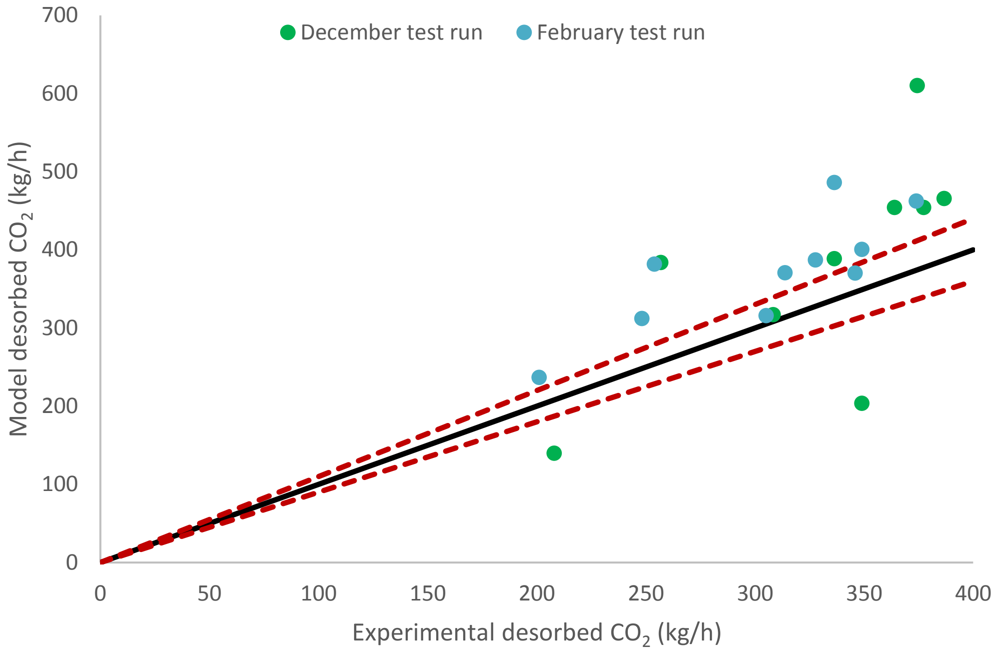


**Figure 29.** $CO_2$ Capture Efficiency (steam stripper only): Experimental vs. J23 model (0.5 $MW_e$ scale)

**Figure 30** and **Figure 31** compare the experimental data of the temperature profile in the absorber and stripper, respectively, with the results obtained from the provided J23 model. It can be noted that the there is considerable discrepancy in the absorber temperature profile mainly because of specifying the intercooler heat removal as the uniform heat loss throughout the absorber.

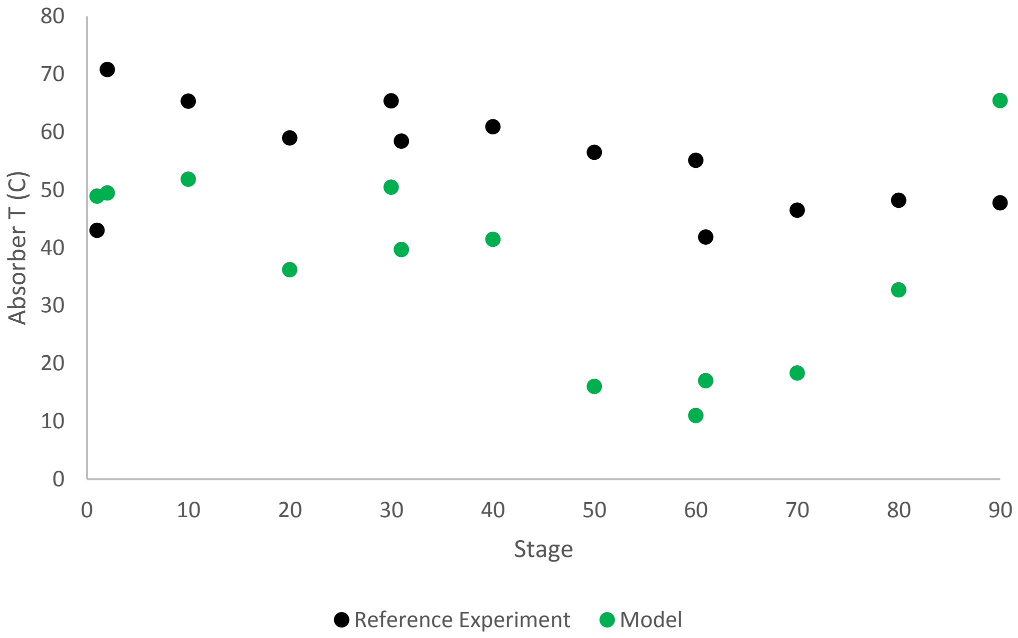


**Figure 30.** Absorber temperature profile: Experimental vs. J23 model (0.5 $MW_e$ scale)

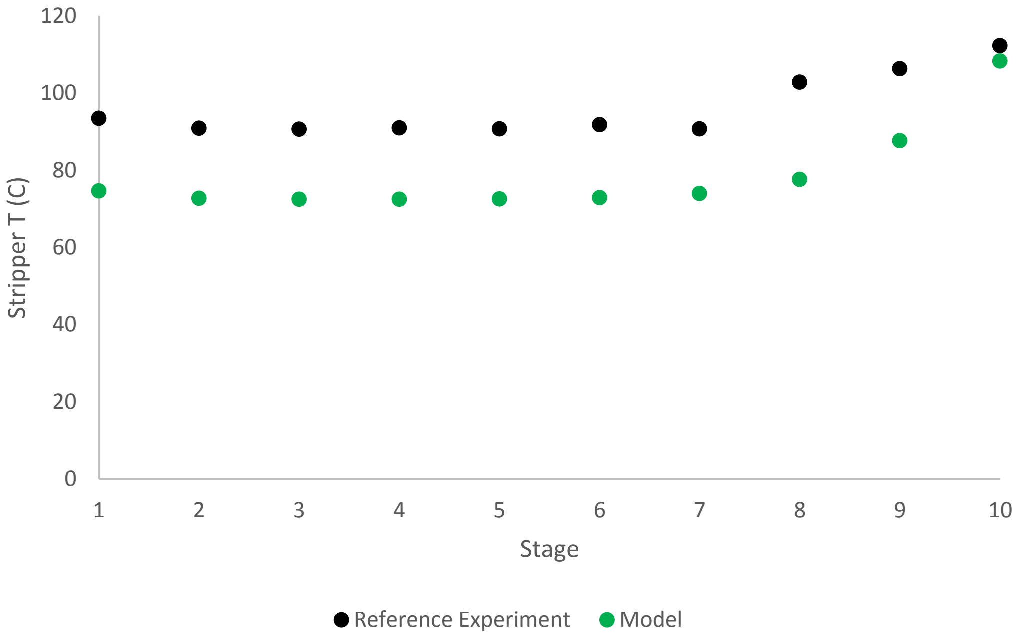


**Figure 31.** Steam stripper temperature profile: Experimental vs. J23 model (0.5 $MW_e$ scale)

## 4.5 J24 Model

### 4.5.1 J24 Model: 0.5 $MW_e$ Validation

The following modifications have been implemented in the J23 model to improve its ability to model the data recorded at 0.5 $MW_e$ Demo:

- The reboiler was modeled using Aspen plus™ built-in option for a reboiler with the heat duty calculated from the steam flowrate and conditions.
- The resolution of the stripper was increased to 40 stages.
- The lean/rich heat exchanger was modeled by specifying the lean solvent outlet temperature.
- Intercoolers were implemented for the absorber.

The new model was denoted J24. Overall the results improved over the J23 model. **Figure 32** shows the results for the absorber using J24 model. Fidelity of the model was considerably improved for $CO_2$ capture efficiency using the either integrated J24 absorber-stripper (**Figure 33**) or the stripper mode (**Figure 34**).

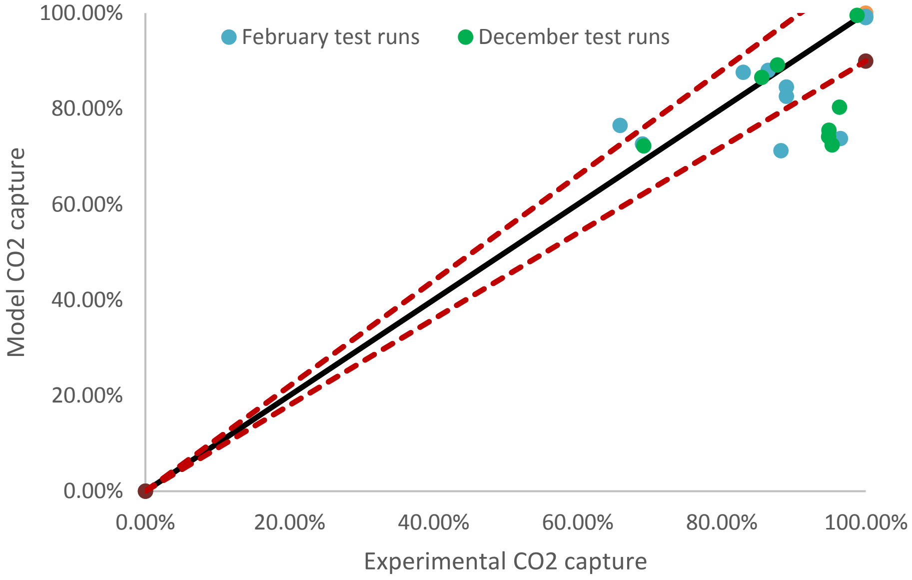


**Figure 32.** $CO_2$ capture Efficiency (absorber): 0.5 MWe Demo vs J24 model (0.5 $MW_e$ scale)

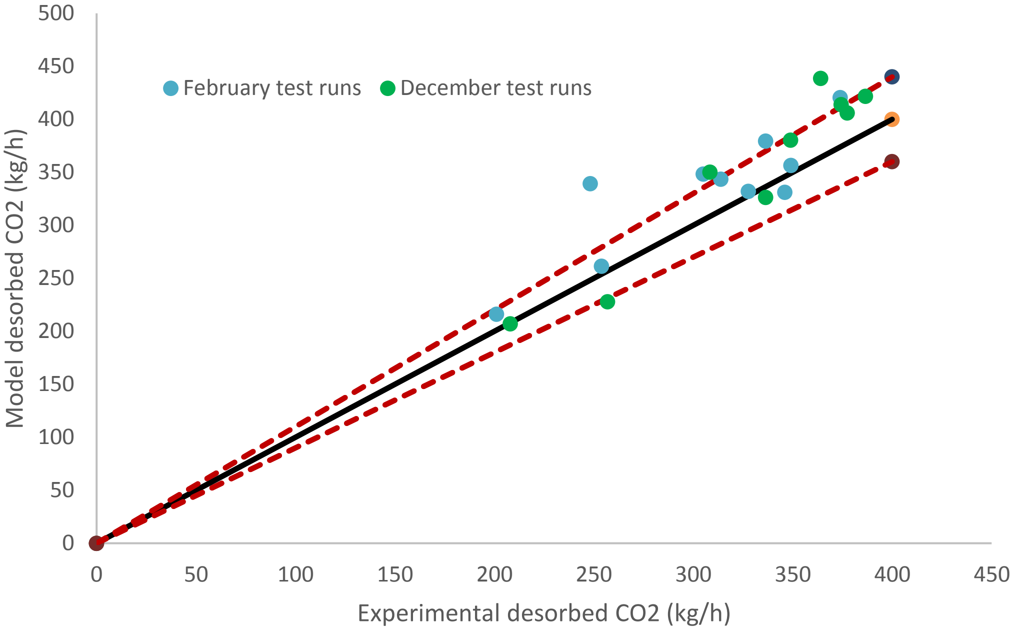


**Figure 33.** $CO_2$ Capture Efficiency (absorber and steam stripper): Experimental vs. J24 model (0.5 $MW_e$ scale)

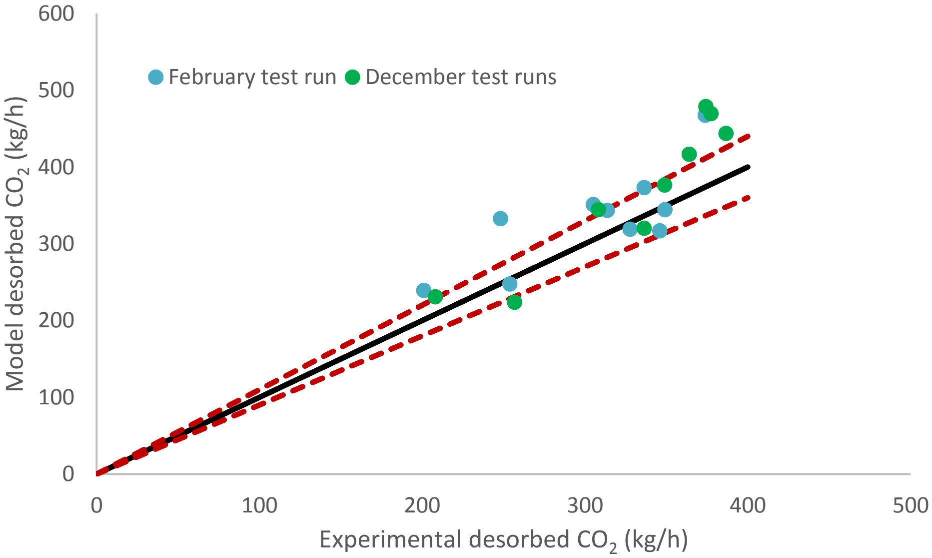


**Figure 34.** $CO_2$ Capture Efficiency (steam stripper only): Experimental vs. J24 model (0.5 $MW_e$ scale)

Comparison of the temperature profiles obtained by the updated model is presented in **Figure 35** and **Figure 36** for the absorber and stripper, respectively. It is noticed that the intercooler implementation considerably improved the absorber results. The stripper temperature profile also matches better than before.

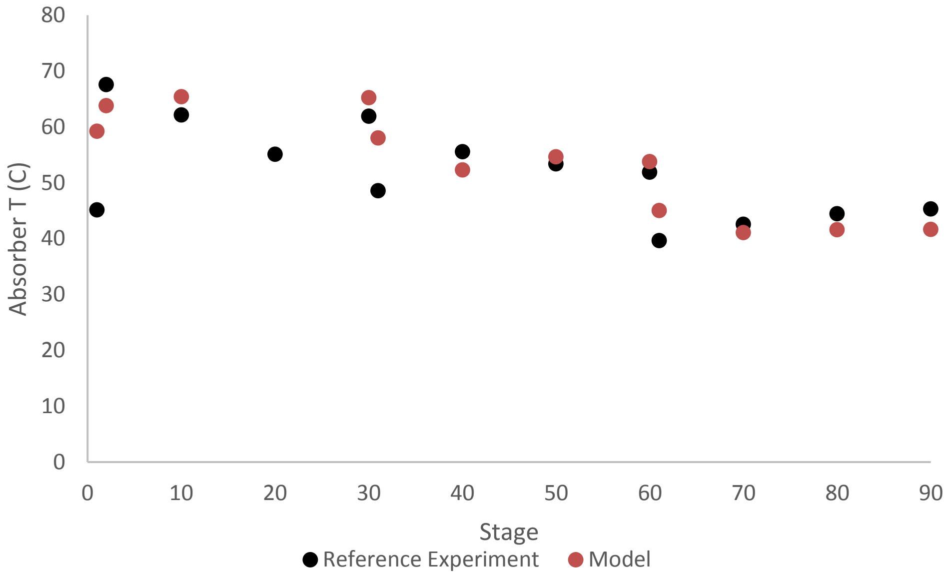


**Figure 35.** Absorber temperature profile: Experimental data vs J24 model (0.5 $MW_e$ scale)

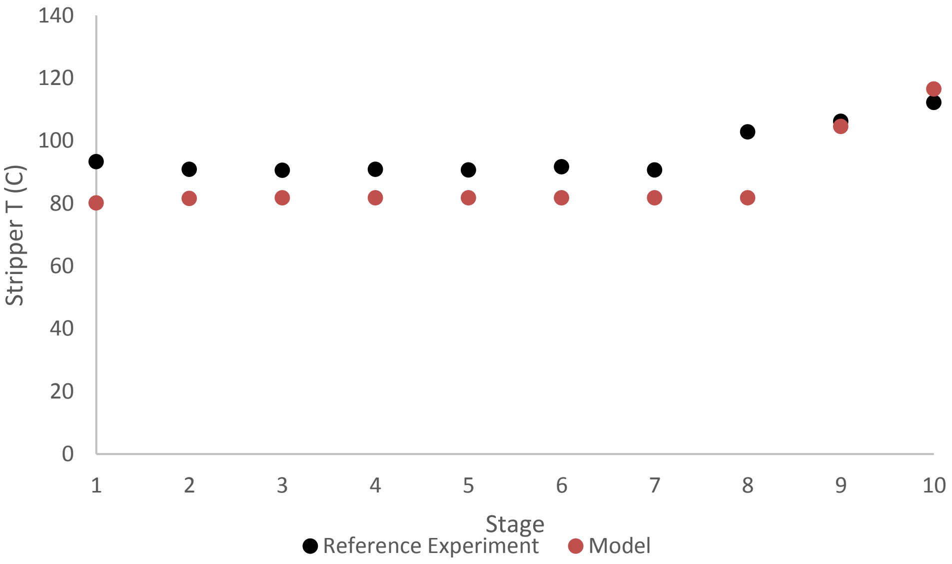


**Figure 36.** Steam stripper temperature profile: Experimental data vs J24 model (0.5 $MW_e$ scale)

In conclusion, J24 model describes well the performance of the absorber and steam stripping column measured during the 0.5 MWe pilot of the GAP-$1_m$/TEG solvent. J24 model fidelity can be further improved by incorporating properties (VLE, density, viscosity) for working solutions containing higher water content ($H_2O$ > 10 wt.%).

### 4.5.2 J24 Model at 550 MW with Steam Stripper column

J24 model was found to provide satisfactory accuracy for the test runs conducted at the National Carbon Capture Center (0.5 MW equivalent) as well as for the bench-scale runs at the GE Global Research, Niskayuna and wetted wall column experiments run by PNNL. It was decided to scale up the process to 550 MW equivalent utilizing the steam stripper column. The input flue gas and steam conditions were similar to Case 11 in the DOE-NETL study. The lean solvent flow rate was adjusted to achieve 90% $CO_2$ capture in a 550 MW equivalent plant.

A number of sensitivity studies was considered to evaluate system performance while varying the size/numbers of absorbers and desorbers, solvent composition (TEG % and $H_2O$%), intercooling and steam duty. These are listed in **Table 17**. Overall objective for these sensitivity studies was to identify optimal operating conditions by taking into account both the capital and operating costs. Since the maximum equivalent diameter of the absorbers/strippers is not known and is likely to vary depending on a number of factors, it was decided to perform sensitivity studies by changing the number of absorbers and strippers. Absorber and stripper sizes were adjusted accordingly to keep the flooding around 80%. In addition, concentration of $H_2O$ and TEG in the solvent, extent of intercooling, and $CO_2$ loading of the lean solvent were varied. Each case was designed for a $CO_2$ capture rate of 90% by adjusting the solvent flowrate. Reboiler duty was varied to obtain the desired $CO_2$ loading of the lean solvent.

Cases 1 and 2a capture the effect of different TEG content in the solvent. It can be observed that when the TEG content is higher, it results in lower flowrate of the solvent and lower reboiler duty. Case 2 is similar to Case 2a, but the number of absorbers was reduced from 4 to 3. The absorber diameter was increased by 21%. In Case 2b, the solvent flowrate through the intercoolers was increased to 2 times that of the base case, while maintaining its outlet temperature to the baseline value. This change resulted in a decrease in the solvent flowrate by about 22%. Case 3 reduced the $H_2O$ content in the lean solvent from 19% to 15%, thus increasing the total GAP-$1_m$ concentration in the solvent. This change reduced the solvent flowrate by another 3.5%. For evaluating the effect of intercooling at different compositions, the intercooler flowrates was doubled in Case 4 while the solvent composition remained the same as Case 1. The solvent flowrate decreased by about 12% in comparison to Case 18.

Since the solvent composition of Case 3 was found to yield the least solvent flowrate and reboiler duty, Cases 5-7a were run using the Case 20 solvent composition. In Cases 5-7, the intercooler flowrate was set to 2 times that of the base case. In Case 5, the number of strippers was reduced from 2 to 1 while keeping the stripper duty similar to Case 3. Effects of 10% higher and lower $CO_2$ loading in the lean solvent were studied in Cases 6 and 7, respectively. In Case 7a, the intercooler flowrate was reduced to 1.2 times that of the base case while everything else being similar to Case 7. This change resulted in higher liquid flowrate and reboiler duty than Case 7. It is observed that Case 7 has the least solvent flowrate and reboiler duty. **Figure 37** and **Figure 38** present the absorber and stripper temperature profile, respectively, for the base case and Case 7.

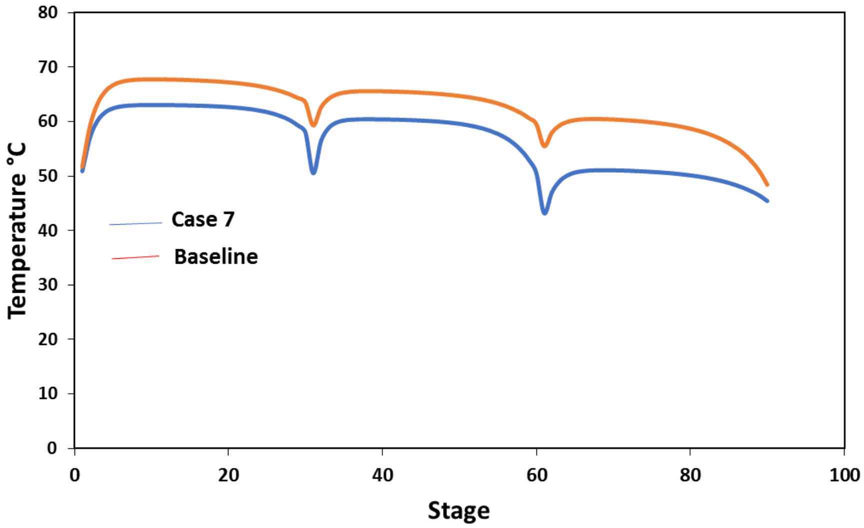


**Figure 37.** Absorber temperature profile

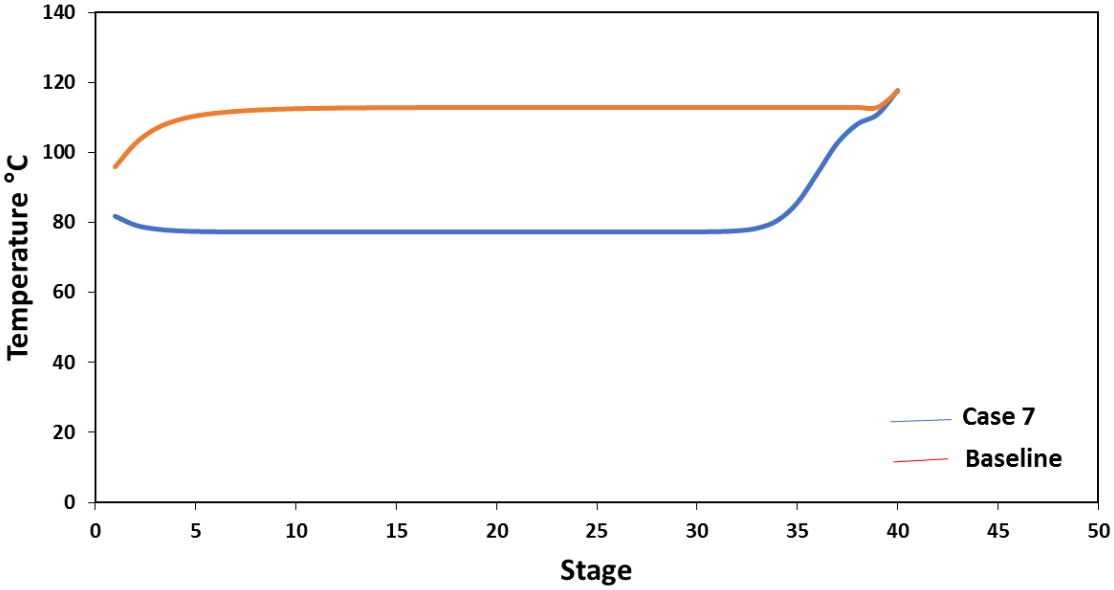


**Figure 38.** Stripper temperature profiles

**Table 17.** Case studies for the 550 MW Equivalent $CO_2$ Capture Plant

| case | # absorbers | Absorber D (m) | # strippers | Stripper D (m) | Inter-cooling | Solvent Composition (w%) | | | Liquid flow (kg/hr) | Total reboiler Q (GJ/hr) |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | **TEG** | **GAP-1$_m$** | **$H_2O$** | | |
| **Base** | 4 | 12.61 | 2 | 14.51 | baseline | 34 | 47 | 19 | 9323881 | 430.00 |
| **1** | 4 | 12.52 | 2 | 12.67 | baseline | 20 | 61 | 19 | 8502002 | 408.64 |
| **2a** | 4 | 11.97 | 2 | 12.11 | baseline | 15 | 66 | 19 | 8877418 | 411.62 |
| **2** | 3 | 14.51 | 2 | 14.68 | baseline | 15 | 66 | 19 | 9482472 | 422.08 |
| **2b** | 3 | 15.10 | 2 | 15.28 | 2 x baseline | 15 | 66 | 19 | 7367261 | 383.70 |
| **3** | 3 | 15.17 | 2 | 15.35 | 2 x baseline | 15 | 70 | 15 | 7089095 | 382.66 |
| **4** | 3 | 15.13 | 2 | 15.31 | 2 x baseline | 20 | 61 | 19 | 7467877 | 388.46 |
| **5** | 3 | 15.17 | 1 | 15.35 | 2 x baseline | 15 | 70 | 15 | 7089095 | 385.50 |
| **6** | 3 | 15.23 | 1 | 15.41 | 2 x baseline | 15 | 70 | 15 | 7269548 | 389.10 |
| **7** | 3 | 15.21 | 1 | 15.39 | 2 x baseline | 15 | 70 | 15 | 6815498 | 381.90 |
| **7a** | 3 | 15.21 | 1 | 15.39 | 1.2 x baseline | 15 | 70 | 15 | 8561687 | 418.60 |

## 4.6 Preliminary Cost Analysis for the 550 MW Cases with Steam Stripper Column

Based on the cases above, capital costs were calculated using Aspen Process Economic Analyzer (APEA) using the cost base of 2014 (1Q14) to select the best case for the steam stripper column. Operating costs were calculated by converting the total required duty for the reboiler and water coolers/condensers to electricity. The reboiler duty was converted to equivalent electricity consumption by first obtaining the equivalent steam consumption considering that reboiler steam is extracted from the IP/LP crossover. The cost of electricity was set to be 0.0775 $/kWh. Relative capital and operating costs are presented in **Table 18**. Case 7 yields the lowest capital and operating cost and it was selected for the comparison with the CSTR cases.

**Table 18.** GAP-$1_m$/TEG cases with SSC: Preliminary Cost Analysis

| Case | Capital Cost (US$) | Operating cost (US$/year) |
|---|---|---|
| **Base** | 1.00 | 1.00 |
| **1** | 1.00 | 0.79 |
| **2a** | 1.02 | 0.61 |
| **2** | 1.06 | 0.65 |
| **2b** | 1.06 | 0.57 |
| **3** | 1.05 | 0.56 |
| **4** | 1.05 | 0.57 |
| **5** | 0.96 | 0.56 |
| **6** | 0.99 | 0.58 |
| **7** | 0.96 | 0.56 |
| **7a** | 0.96 | 0.62 |

## 4.7 Integrated Power Plant with $CO_2$-Capture: Sensitivity Cases

A number of different process options were studied for the GAP-$1_m$/TEG solvent using both CSTR and SSC desorbers. **Table 19** lists the modifications that were made from Case A to Case L. Case L is the selected steam stripper case, as described in section 3.5 (case 7 from **Table 17**)

**Table 19.** List of major cases for $CO_2$ capture system using aminosilicones

| MEA | Base MEA (DOE Case 11 w CC and, Case 12) |
|---|---|
| **Aminosilicone Cases** | |
| Case A | 284 °F, 63 psia |
| Case B | Added Absorber Intercoolers |
| Case C | Increased Intercooling |
| Case D | Structured Packing |
| Case E | Reduced Desorber Temperature |
| Case F | Reduced Number of Absorbers |
| Case G | Reduced Absorber Diameter |
| **Scaled Up Aminosilicone Cases** | |
| Case H | Scaled to 550 MW Net / CSTR |
| Case I | Cooling Water Integration / CSTR |
| Case J | Waste Heat Recovery / CSTR |
| Case K | Low Pressure Desorption / CSTR |
| Case L | Low Pressure Desorption / SSC |

## 4.8 $CO_2$ Separation Unit Key Assumptions

The $CO_2$-seperation process model used the following design assumptions given in Case 11 of DOE NETL Bituminous Baseline Study.

(i) Composition of flue gas leaving the FGD (wet basis) is shown in **Table 20**.

**Table 20.** Flue gas composition leaving FGD

| | Volume % |
|---|---|
| $CO_2$ | 13.53 |
| $H_2O$ | 15.17 |
| $N_2$ | 68.9 |
| $O_2$ | 2.40 |
| | ppmv |
| SOx | 5-42 |
| NOx | 74 |

(ii) The flow rate of flue gas leaving the FGD (based on DOE Case 11 550 MW net supercritical PC plant): 4,713,221 lb/hr. The flow rate for the scaled-up cases varied due to differences in overall plant efficiency with the various $CO_2$-capture system configurations.

(iii) Pressure and temperature of flue gas leaving FGD: 14.8 psia and 135 °F

(iv) Conditions for LP steam available from power plant: 556 °F (base case, sensitivity was conducted with respect to steam conditions)

(v) Conditions for cooling water: feed = 60 °F, return = 80 °F with a minimum approach of 30 °F (sensitivity was conducted with respect to cooling water conditions)

(vi) $CO_2$ removal from flue gas: greater than 90%

(vii) $CO_2$ purity: greater than 95 vol%

(viii) $CO_2$ delivery pressure and temperature: 2,215 psia and 124 °F

### 4.8.1 MEA Baseline

The MEA and aminosilicone-based solvent baseline models are based on a typical temperature-swing sorbent separation process. The systems have four process variables that dominate the performance with a given sorbent and they are absorber temperature, desorber temperature, desorber pressure, and rich-lean heat exchanger approach temperature. The system models account for the major energy penalties for $CO_2$ separation, and they include the energy required:

(1) for vaporization of water

(2) to desorb the carbon dioxide (i.e., reaction energy)

(3) for sensible heating of the sorbent

The energy is supplied by feeding steam to the desorber unit. The models also account for $CO_2$-compression energy and auxiliary loads.

The sorbent-rich loading is defined as the weight % of $CO_2$ in the rich sorbent leaving the absorber column. The sorbent lean loading is defined as the weight % of $CO_2$ in the lean sorbent leaving the desorber column. The sorbent net loading is defined as the difference between the rich loading and the lean loading and was obtained from bench-scale experiments for the GAP-$1_m$/TEG system.

A detailed MEA Aspen Plus™ model that was built under this project was used to compare the results for this study.

The main features of the MEA model include an absorber, rich-lean heat exchanger, and a desorber. The same unit operations are important for the GAP-$1_m$/TEG system. The baseline MEA case is built from the description given in the Bituminous Baseline Study. **Figure 39** shows a comparison of the plant efficiency reported for Case 12 in the Bituminous Baseline Study with the plant efficiency calculated using GE Global Research's models for MEA and the power plant.

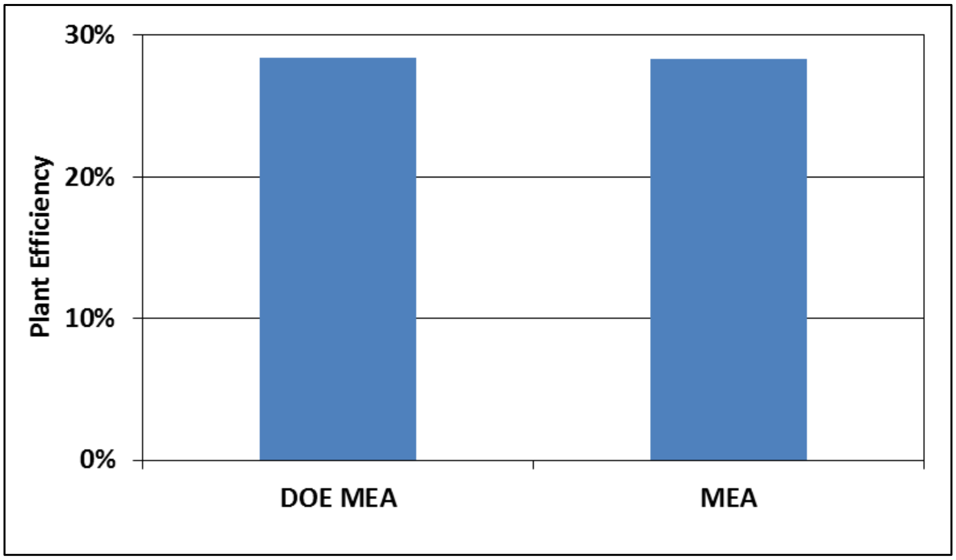


**Figure 39.** Comparison of estimated plant efficiency of $CO_2$ capture system using MEA vs. DOE estimated efficiency

### 4.8.2 GAP-$1_m$/TEG Integrated models

The $CO_2$-capture system block flow diagram scaled–up to 552 MW net power for Case H is presented on

**Figure 40** and the corresponding stream table is presented in **Table 21**.

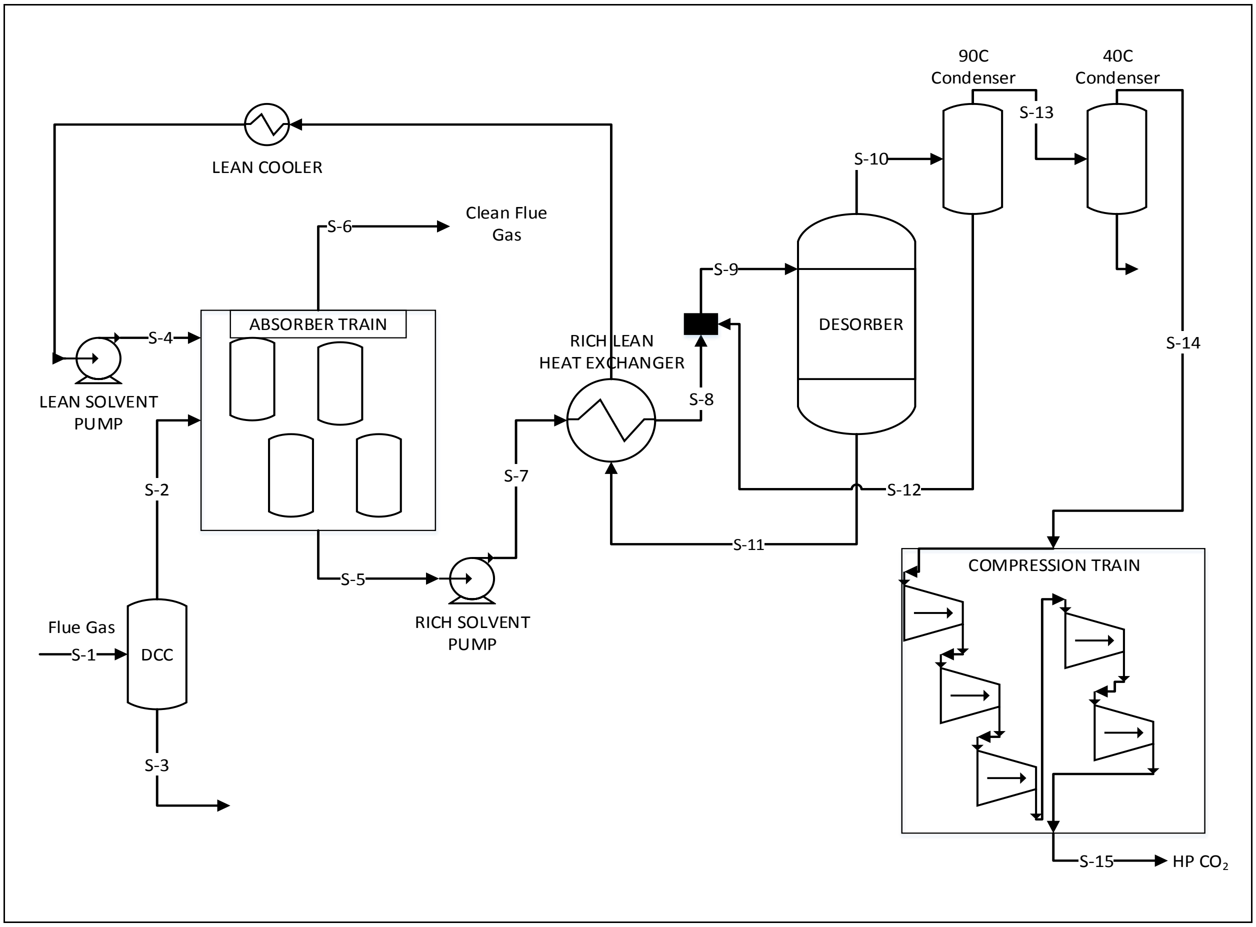


**Figure 40.** Block flow diagram of $CO_2$-capture system for Case H (see details in Table 19)

**Table 21.** Stream table for $CO_2$-capture system for Case H (see details in **Table 19**)

| **Stream Number** | **S-1** | **S-2** | **S-3** | **S-4** | **S-5** | **S-6** | **S-7** | **S-8** |
|---|---|---|---|---|---|---|---|---|
| Mole Fraction | | | | | | | | |
| $H_2O$ | 0.1517 | 0.0731 | 0.9999 | 0.2420 | 0.2820 | 0.0436 | 0.2820 | 0.2820 |
| $CO_2$ | 0.1353 | 0.1478 | 0.0001 | 0.0090 | 0.0007 | 0.0192 | 0.0007 | 0.0007 |
| $N_2$ | 0.6890 | 0.7528 | 0.0000 | 0.0001 | 0.0010 | 0.9057 | 0.0010 | 0.0010 |
| $O_2$ | 0.0240 | 0.0262 | 0.0000 | 0.0000 | 0.0000 | 0.0316 | 0.0000 | 0.0000 |
| GAP1 | 0.0000 | 0.0000 | 0.0000 | 0.2190 | 0.0215 | 0.0000 | 0.0215 | 0.0215 |
| GAP1CARB | 0.0000 | 0.0000 | 0.0000 | 0.0789 | 0.2631 | 0.0000 | 0.2631 | 0.2631 |
| TEG | 0.0000 | 0.0000 | 0.0000 | 0.4510 | 0.4317 | 0.0000 | 0.4317 | 0.4317 |
| Total | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| | | | | | | | | |
| Total Flow lbmol/hr | 212,156 | 194,164 | 17,992 | 136,228 | 142,321 | 161,256 | 142,321 | 142,321 |
| Total Flow lb/hr | 6,100,920 | 5,776,755 | 324,165 | 23,414,975 | 24,648,212 | 4,516,809 | 24,648,212 | 24,648,212 |
| | | | | | | | | |
| Temperature F | 135 | 104 | 104 | 104 | 122 | 128 | 123 | 240 |
| Pressure psia | 14.7 | 14.7 | 14.7 | 15 | 14.7 | 14.7 | 93 | 93 |
| Vapor Frac | 1 | 1 | 0 | 0 | 0 | 1 | 0 | 0 |
| | | | | | | | | |
| Enthalpy Btu/lb | -1329.5 | -1089.4 | -6791.9 | -2272.7 | -2407.9 | -264.7 | -2407.7 | -2350.2 |
| Density lb/cuft | 0.066 | 0.072 | 61.142 | 56.338 | 58.046 | 0.065 | 58.025 | 53.743 |
| Average MW | 28.757 | 29.752 | 18.017 | 171.881 | 173.187 | 28.010 | 173.187 | 173.187 |

| **Stream Number** | **S-9** | **S-10** | **S-11** | **S-12** | **S-13** | **S-14** | **S-15** |
|---|---|---|---|---|---|---|---|
| Mole Fraction | | | | | | | |
| $H_2O$ | 0.2853 | 0.1629 | 0.2574 | 0.8924 | 0.1444 | 0.0170 | 0.0008 |
| $CO_2$ | 0.0007 | 0.8299 | 0.0085 | 0.0020 | 0.8509 | 0.9778 | 0.9939 |
| $N_2$ | 0.0010 | 0.0044 | 0.0000 | 0.0000 | 0.0045 | 0.0052 | 0.0053 |
| $O_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| GAP1 | 0.0218 | 0.0018 | 0.2159 | 0.0689 | 0.0001 | 0.0000 | 0.0000 |
| GAP1CARB | 0.2618 | 0.0006 | 0.0757 | 0.0244 | 0.0000 | 0.0000 | 0.0000 |
| TEG | 0.4294 | 0.0003 | 0.4424 | 0.0122 | 0.0000 | 0.0000 | 0.0000 |
| Total | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| | | | | | | | |
| Total Flow lbmol/hr | 143,095 | 31,144 | 138,883 | 774 | 30,370 | 26,423 | 25,991 |
| Total Flow lb/hr | 24,686,221 | 1,259,768 | 23,426,717 | 38,009 | 1,221,759 | 1,148,988 | 1,141,107 |
| | | | | | | | |
| Temperature F | 240 | 266 | 266 | 194 | 194 | 104 | 124 |
| Pressure psia | 63 | 63 | 63 | 63 | 63 | 63 | 2215 |
| Vapor Frac | 0 | 1 | 0 | 0 | 1 | 1 | 1 |
| | | | | | | | |
| Enthalpy Btu/lb | -2352.1 | -3887.1 | -2202.7 | -3549.3 | -3927.6 | -3839.2 | -3822.1 |
| Density lb/cuft | 53.705 | 0.327 | 50.617 | 43.516 | 0.361 | 0.453 | 15.526 |
| Average MW | 172.517 | 40.450 | 168.680 | 49.124 | 40.229 | 43.484 | 43.904 |

The $CO_2$ capture process adds additional auxiliary load on coal power plants, and the main contributors are solvent pumps, $CO_2$ compressors, flue gas blowers, cooling water fans and pumps. **Table 22** shows the power summary for Case H of the $CO_2$-capture system. It should be noted that the main feed-gas blower is part of the power plant, and only the additional power to increase the flue gas pressure to the required inlet pressure of the $CO_2$-capture process is shown in **Table 22**. The cooling tower is also part of the power plant, and its operation and capital costs are included in the power plant island costs. Therefore, the table shows only the power for the cooling water pumps, which deliver water from the cooling tower to the $CO_2$-capture process. $CO_2$ separation auxiliaries include lean and rich solvent pumps.

**Table 22.** Power summary for Case H

| POWER SUMMARY | |
|---|---|
| AUXILIARY LOAD SUMMARY, kWe | |
| Feed Gas Blower | 911 |
| $CO_2$ Separation Auxiliaries | 2,098 |
| $CO_2$ Compression | 43,088 |
| Cooling Water Pumps | 6,866 |
| TOTAL AUXILIARIES, kWe | 52,963 |
| | |
| COOLING WATER, ton/hr | 45,600 |
| | |
| STEAM, ton/hr | 750 |

Detailed process flow information for each stream in Case H (Case G scaled to 550 MW net) is provided in **Table 23**. The stream numbers are in reference to the simplified block diagram in **Figure 40**, and are consistent with the numbering scheme shown for the case without $CO_2$ capture.

**Table 23.** Stream properties from power plant modeling of Case H. The stream numbers correspond to the block flow diagram shown in **Figure 40**.

| | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|
| V-L Mole Fraction | | | | | | | |
| Ar | 0.0093 | 0.0093 | 0.0093 | 0.0093 | 0.0000 | 0.0000 | 0.0088 |
| $CO_2$ | 0.0003 | 0.0003 | 0.0003 | 0.0003 | 0.0000 | 0.0000 | 0.1485 |
| $H_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $H_2O$ | 0.0101 | 0.0101 | 0.0101 | 0.0101 | 0.0000 | 0.0000 | 0.0893 |
| $N_2$ | 0.7729 | 0.7729 | 0.7729 | 0.7729 | 0.0000 | 0.0000 | 0.7310 |
| $O_2$ | 0.2074 | 0.2074 | 0.2074 | 0.2074 | 0.0000 | 0.0000 | 0.0202 |
| $SO_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0022 |
| Total | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 0.0000 | 0.0000 | 1.0000 |
| | | | | | | | |
| V-L Flowrate (lbmol/hr) | 139,244 | 139,244 | 42,774 | 42,774 | - | - | 192,772 |
| V-L Flowrate (lb/hr) | 4,017,852 | 4,017,852 | 1,234,242 | 1,234,242 | - | - | 5,737,068 |
| Solids Flowrate (lb/hr) | - | - | - | - | 538,439 | 10,686 | 42,744 |
| | | | | | | | |
| Temperature (°F) | 59 | 65 | 59 | 77 | 59 | - | 342 |
| Pressure (psia) | 14.7 | 15.1 | 14.7 | 16.2 | 14.7 | - | 14.3 |
| Enthalpy (Btu/lbm) | -4.3 | -3.0 | -4.3 | 0.1 | - | - | 69.2 |
| Density ($lb/ft^3$) | 0.076 | 0.078 | 0.076 | 0.081 | - | - | 0.047 |
| V-L Molecular Weight | 28.85 | 28.85 | 28.85 | 28.85 | - | - | 29.76 |

|  | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
|---|---|---|---|---|---|---|---|
| V-L Mole Fraction |  |  |  |  |  |  |  |
| Ar | 0.0000 | 0.0088 | 0.0088 | 0.0000 | 0.0093 | 0.0000 | 0.0000 |
| $CO_2$ | 0.0000 | 0.1485 | 0.1485 | 0.0000 | 0.0003 | 0.0000 | 0.0004 |
| $H_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $H_2O$ | 0.0000 | 0.0893 | 0.0893 | 1.0000 | 0.0101 | 1.0000 | 0.9996 |
| $N_2$ | 0.0000 | 0.7310 | 0.7310 | 0.0000 | 0.7729 | 0.0000 | 0.0000 |
| $O_2$ | 0.0000 | 0.0202 | 0.0202 | 0.0000 | 0.2074 | 0.0000 | 0.0000 |
| $SO_2$ | 0.0000 | 0.0022 | 0.0022 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| Total | 0.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
|  |  |  |  |  |  |  |  |
| V-L Flowrate (lbmol/hr) | - | 192,772 | 192,772 | 20,917 | 3,052 | 11,339 | 467 |
| V-L Flowrate (lb/hr) | - | 5,737,068 | 5,737,068 | 376,920 | 88,056 | 204,322 | 8,424 |
| Solids Flowrate (lb/hr) | 42,744 | - | - | - | - | 45,194 | 75,672 |
|  |  |  |  |  |  |  |  |
| Temperature (°F) | - | 342 | 362.9 | 59 | 59 | 59 | 0 |
| Pressure (psia) | - | 13.84 | 15.06 | 14.7 | 14.7 | 14.7 | 0.0 |
| Enthalpy (Btu/lbm) | - | 69.2 | 74.7 | 27.1 | -4.3 | - | - |
| Density (lb/ft$^3$) | - | 0.046 | 0.048 | 62.379 | 0.076 | - | - |
| V-L Molecular Weight | - | 29.76 | 29.76 | 18.02 | 28.85 | - | 18.03 |

| | 15 | 16 | 17 | 18 | 19 | 20 | 21 |
|---|---|---|---|---|---|---|---|
| V-L Mole Fraction | | | | | | | |
| Ar | 0.0081 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $CO_2$ | 0.1372 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $H_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $H_2O$ | 0.1577 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| $N_2$ | 0.6766 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $O_2$ | 0.0204 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $SO_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| Total | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| | | | | | | | |
| V-L Flowrate (lbmol/hr) | 211,766 | 266,843 | 221,783 | 221,783 | 197,442 | 83,241 | 197,442 |
| V-L Flowrate (lb/hr) | 6,100,922 | 4,808,520 | 3,996,538 | 3,996,538 | 3,557,905 | 1,500,000 | 413,566 |
| Solids Flowrate (lb/hr) | - | - | - | - | | - | - |
| | | | | | | | |
| Temperature (°F) | 132 | 1100 | 663 | 1100 | 531 | 528 | 531 |
| Pressure (psia) | 14.7 | 3514.7 | 693.7 | 655.8 | 60.0 | 54.1 | 60.0 |
| Enthalpy (Btu/lbm) | 14.9 | 1495.0 | 1323.2 | 1570.5 | 1298.3 | 1297.3 | 1298.3 |
| Density (lb/ft$^3$) | 0.063 | 4.319 | 1.143 | 0.722 | 0.103 | 0.093 | 0.103 |
| V-L Molecular Weight | 28.81 | 18.02 | 18.02 | 18.02 | 18.02 | 18.02 | 18.02 |

|  | 22 | 23 | 24 | 25 |
|---|---|---|---|---|
| V-L Mole Fraction |  |  |  |  |
| Ar | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $CO_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $H_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $H_2O$ | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| $N_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $O_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| $SO_2$ | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| Total | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
|  |  |  |  |  |
| V-L Flowrate (lbmol/hr) | 75,343 | 115,437 | 83,241 | 197,442 |
| V-L Flowrate (lb/hr) | 1,357,682 | 2,080,170 | 1,500,000 | 4,808,520 |
| Solids Flowrate (lb/hr) | - | - | - | - |
|  |  |  |  |  |
| Temperature ($^oF$) | 101 | 107 | 286 | 557 |
| Pressure (psia) | 1.0 | 258.5 | 133.6 | 4185.2 |
| Enthalpy (Btu/lbm) | 1023.5 | 75.2 | 255.5 | 552.9 |
| Density ($lb/ft^3$) | 0.003 | 61.959 | 57.758 | 47.687 |
| V-L Molecular Weight | 18.02 | 18.02 | 18.02 | 18.02 |

**Table 24** summarizes power output from the power plant along with materials consumed during normal operation for Case H. It includes a detailed summary of auxiliary loads and how they contribute with the steam turbine power and $CO_2$ capture and compression loads to impact the total plant net power output and efficiency.

**Table 24.** Power summary from power plant modeling of Case H (see details in Table 19)

| **POWER SUMMARY (Gross Power at Generator Terminals, kWe)** | |
|---|---|
| Steam Turbine Power | 647,695 |
| **Total (Steam Turbine) Power, kWe** | **647,695** |
| **Auxiliary Load Summary, kWe** | |
| Boiler Fuel Delivery | 4,221 |
| Ash handling | 694 |
| Primary Air Fans | 1,783 |
| Forced Draft Fans | 2,000 |
| Induced Draft Fans | 9,746 |
| Baghouse (ESP) | 91 |
| Wet FGD | 11,857 |
| $CO_2$ Island Auxiliaries | 9,875 |
| $CO_2$ Compression | 43,088 |
| Miscellaneous BOP | 118 |
| ST Auxiliaries | 446 |
| Condensate Pumps | 699 |
| Circulating Water Pumps | 3,142 |
| Cooling Tower Fans | 5,262 |
| Transformer Losses | 2,031 |
| BFP Booster Pump | 652 |
| **Total Auxiliaries, kWe** | **42,743** |
| **Net Power, kWe** | **551,989** |
| Net Plant Efficiency (HHV) | 30.0% |
| Net Plant Heat Rate, (Btu/kWh) | 10,383 |
| **Condenser Cooling duty, ($10^6$ Btu/hr)** | 3,544 |
| **Consumables** | |
| As-Received Coal Feed, (lb/hr) | 538,439 |
| Limestone Sorbent Feed, (lb/hr) | 45,180 |
| Thermal Input (kWt) | 1,840,906 |
| Raw Water Consumption (gpm) | 6,740 |

The net power for Case H is calculated to be ~552MW.

**Table 25** details the energy flows in and out of the control volume of the full power plant model with $CO_2$ capture.

**Table 25.** Energy balance from power plant modeling of Case H ((see details in Table 19)

| | HHV | Sensible + Latent Heat | Power | Total |
|---|---|---|---|---|
| Heat In (MMBtu/hr) | | | | |
| Coal | 6296 | | | 6296 |
| Ambient Air | | 69.9 | | 69.9 |
| FGD Water | | 29.0 | | 29.0 |
| FGD Oxidation Air | | 6.6 | | 6.6 |
| Totals | 6296 | 105 | | 6401 |
| Heat Out (MMBtu/hr) | | | | |
| Bottom Ash | | 5.8 | | 5.8 |
| Fly Ash + FGD Ash | | 2.3 | | 2.3 |
| Flue Gas | | 590 | | 590 |
| HP CO2 | | 139 | | 139 |
| Unburned Carbon | | 17.4 | | 17.4 |
| Boiler Losses | | 55.3 | | 55.3 |
| Fuel Delivery Losses | | 2.9 | | 2.9 |
| Main Condenser | | 3124 | | 3124 |
| BFPT Condenser | | 410 | | 410 |
| Steam Piping Losses | | 14.3 | | 14.3 |
| ST/Generator Mech/Elec/Gear Losses | | 25.0 | | 25.0 |
| BFPT Mech Losses | | 0.9 | | 0.9 |
| Pumps Mech/Elec Losses | | 3.0 | | 3.0 |
| Fans Mech/Elec Losses | | 5.0 | | 5.0 |
| FGD Energy Losses | | 42.0 | | 42.0 |
| Misc Losses and Auxiliaries | | 80.7 | | 80.7 |
| Net Power | | | 1884 | 1884 |
| Totals | 0 | 4517 | 1884 | 6401 |

**Table 26** shows the air emissions for Case H.

**Table 26.** Air emissions for Case H (see details in Table 19**)**

| | lb/MMBtu |
|---|---|
| | |
| $SO_2$ | ~0 |
| $NO_x$ | 0.3 |
| Particulates | ~0 |
| Hg | ~0 |
| $CO_2$ | 72.3 |

The carbon balance for Case H is shown in **Table 27**.

**Table 27.** Carbon balance for Case H (see details in Table 19)

| Carbon In, (lb/hr) | | Carbon Out (lb/hr) | |
|---|---|---|---|
| Coal | 343,255 | Stack Gas | 37,153 |
| Air ($CO_2$) | 667 | FGD Product | 2,216 |
| FGD Reagent | 5,436 | $CO_2$ Product | 309,989 |
| **Total** | **349,358** | **Total** | **349,358** |

The sulfur balance for Case H is shown in **Table 28**.

**Table 28.** Sulfur balance for Case H (see details in Table 19)

| Sulfur In, (lb/hr) | | Sulfur Out (lb/hr) | |
|---|---|---|---|
| Coal | 13,515 | FGD Product | 13,481 |
| | | Stack Gas | 0 |
| | | Waste Solvent | 34 |
| **Total** | **13,515** | **Total** | **13,515** |

**Table 29** summarizes the pieces of equipment which contribute to the total water consumption in the power plant model with $CO_2$ capture.

**Table 29.** Water consumption for power plant modeling of Case H (see details in Table 19)

| Water Use | Water Consumption (gpm) |
|---|---|
| | |
| FGD Makeup | 754 |
| Cooling Tower | 5,702 |
| **Total** | **6,456** |

**Figure 41** shows the plant efficiency for the different cases as compared to Case 12 in the DOE NETL Bituminous Baseline Study. The plant efficiency for Case G is 30.1% as compared to 28.4% for the case using MEA. After scaling up the power island and the carbon-capture island to 550 MW net power, two more cases were evaluated that utilized heat integration between the two islands. The efficiency of the best case was improved to 30.4% by utilizing the heat integration strategies. The plant efficiency for Case L is 30.4 %, due to decrease in CAPEX by 25% vs. Case K as the steam stripper column disrober brings about a higher working capacity and reduced desorption temperature and solvent degradation. **Figure 42** shows the energy penalty for each case.

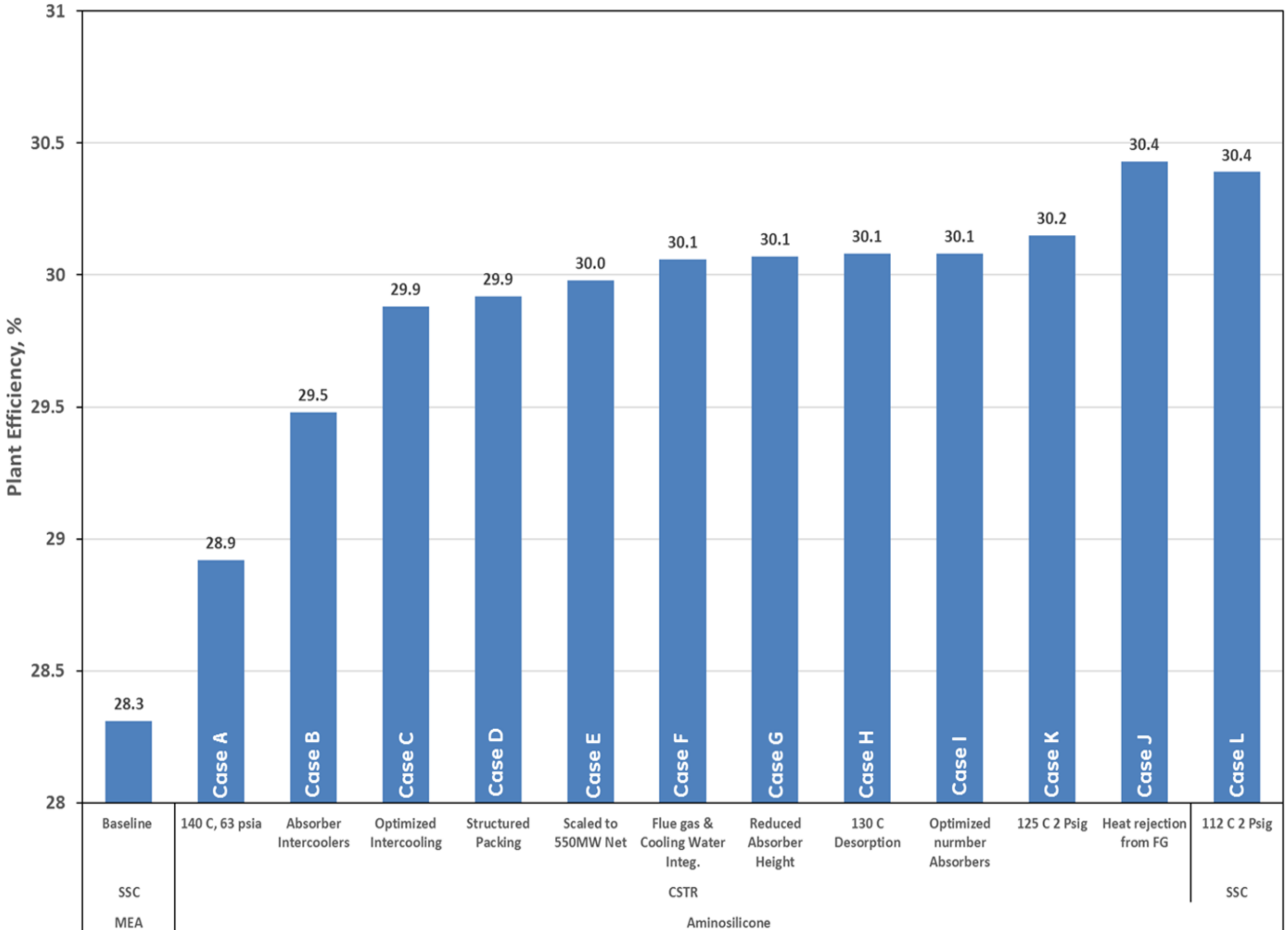


**Figure 41.** GAP-$1_m$/TEG Techno-economic analysis: Plant efficiency

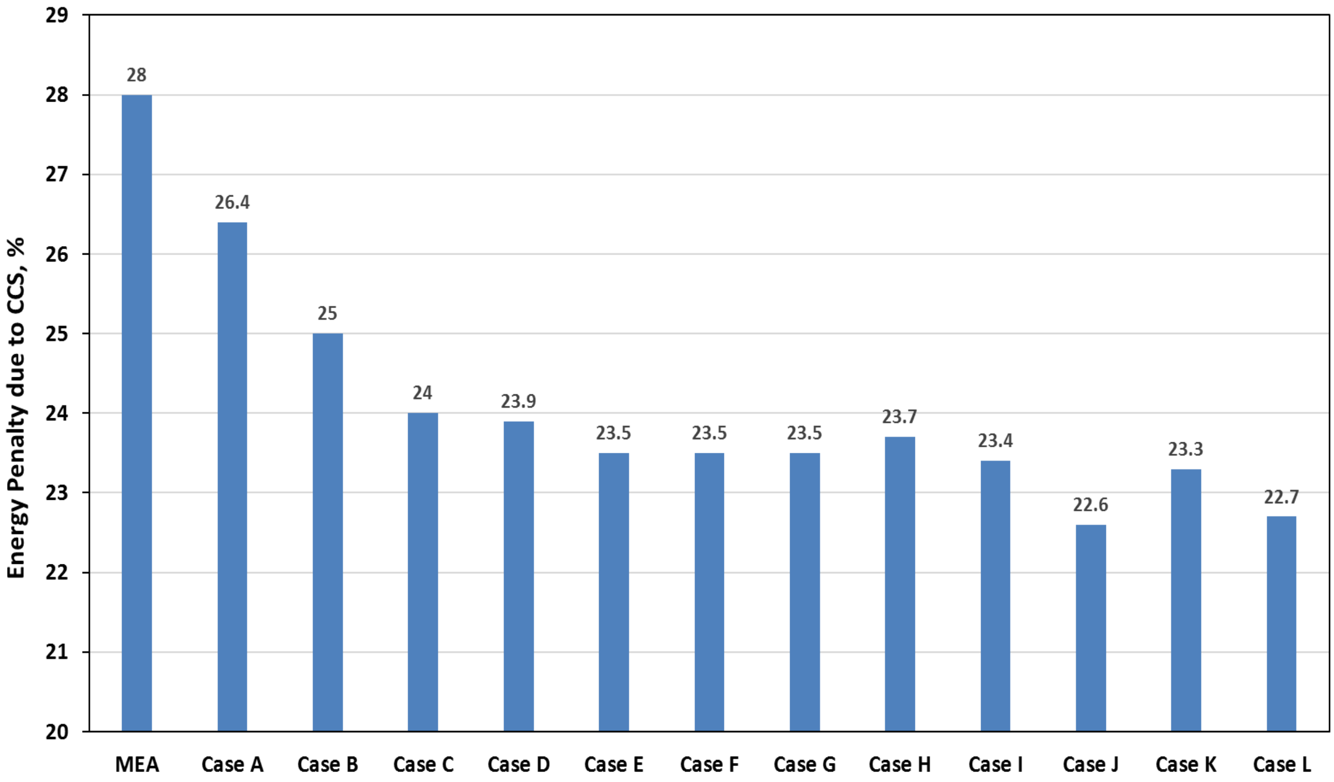


**Figure 42.** GAP-$1_m$/TEG Techno-economic analysis: Energy penalty due CO2 Capture Case details in Table 19.

### 4.8.3 Steam Reboiler Factor

One of the most important factors that determines the energy penalty using carbon capture is the steam penalty. A steam penalty factor in kWh/lb can be calculated based on the steam condition that is used in the carbon capture island. The energy penalty of carbon capture on a power plant is highly dependent on this factor and hence the steam extraction conditions. This factor was calculated by power plant modeling in Thermoflow and was estimated at 0.076 kWh/lb and 0.074 kWh/lb if steam is extracted at 571.4 °F/75 psia and 530.9 °F/60 psia for desorber operating temperatures of 284 °F and 266 °F, respectively. The effect of this factor can be seen in the plant efficiency in **Figure 42** between Case D and Case E.

After the power plant model was calibrated to Case 11, it was altered to allow for integration with the carbon capture process. One of the larger interactions between the power block and the carbon capture models is the export of process steam for use in the capture plant's desorber. Extracting such a large amount of steam has a significant impact on the design of the power cycle. In the model calibrated to Case 11, the low-pressure (LP) steam flow was sufficient to require a 4-flow low-pressure steam turbine. In the case with carbon capture almost half of the LP steam flow is diverted to the carbon-capture plant and thus only a 2-flow LP steam turbine is required. The selection of a 2-flow LP steam turbine over a 4-flow makes a large difference to steam turbine cost (~$60MM). Additionally, the selection of the crossover pressure is heavily influenced by the $CO_2$-capture process steam extraction. The desorber in the carbon-capture plant is designed to extract the maximum amount of heat from the process steam by condensing it to a saturated liquid. This sets a minimum steam pressure that can be utilized. If steam were extracted at too low of a pressure, it would not condense at the operating temperatures of the desorber, and a significantly larger extraction of steam would be required. Extracting steam above the minimum pressure doesn't yield significant cost savings, and is worse from a performance perspective, so the operating temperature of the desorber directly sets the optimum crossover pressure in the power block. Because of this, the desorber operating temperature was reduced from 284 °F to 266 °F (Case D to Case E) in order to allow an extraction of steam at a lower pressure, for an improvement in cycle efficiency. In this design, the steam side of the desorber operates at 54 psia, so the crossover pressure was selected to be 60 psia.

The condensate water returning from the desorber is still warm, but is only available at a low pressure. Returning the condensate to the condenser would be a waste of valuable heat, and would drive up the cooling tower duty. Alternatively, the condensate could be used for feedwater heating, either by passing it through the hot side of one or more feedwater heaters before returning it to the condenser, or by pumping the condensate to a high enough pressure to be admitted to the de-aerating feedwater heater. In this model it was selected to return the condensate to the de-aerating feedwater heater, but further optimization of this aspect of the design may be possible.

It is also important to consider an optimization of equipment affecting the flow of flue gases to the $CO_2$-capture equipment. Sulfur content in the exhaust gases has a detrimental effect on $CO_2$-capture hardware and solvents, so additional flue gas desulfurization equipment in the power block can be justified based on a reduction in maintenance and material costs for the $CO_2$-capture plant. Increasing the effectiveness of the flue gas desulfurization system comes at a cost of both increased capital costs and increased auxiliary loads. In the design of this plant the flue gas sulfur content was optimized in order to minimize the cost of $CO_2$-capture. Initially the flue gas desulfurization system was designed to leave 42 ppm of $SO_2$ in the flue gas. In order to decrease the amount of $SO_2$, the cost of flue gas desulfurization equipment increases significantly. The optimal point for minimized $CO_2$capture cost was found at 5 ppm of sulfur. **Figure 43** shows the cost and auxiliary load deltas that were found during the optimization of the flue gas desulfurization system.

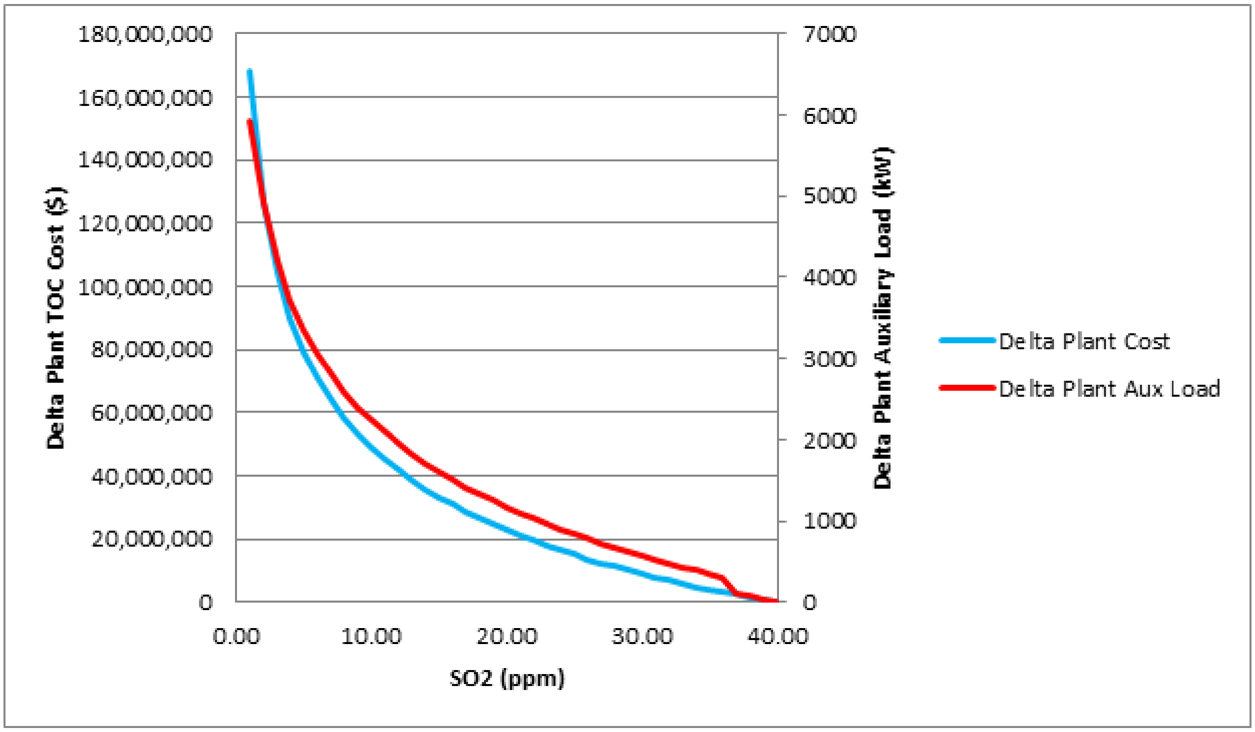


**Figure 43.** Flue gas desulfurization optimization

## 4.9 Economic Analysis

CAPEX estimations for the carbon-capture island were completed for MEA and the aminosilicone-based cases in order to calculate the first year COE, first year removal cost of $CO_2$, and first year avoided cost of $CO_2$. The annual costs were estimated as follows:

Annual cost includes the following items:

- Power Island – CAPEX, OPEX, and fuel - The estimated values were compared against DOE estimated values for Case 11 of the cost updates for the Bituminous Baseline Study. Further estimates were conducted for a power island that would be required for 550 MW net power with carbon capture using aminosilicone-based solvent.
- Capital recovery and other fixed charges- The recovery charges are dependent on the Capital Charge Factor (CCF). The CCF used in this study was chosen based on NETL's cost estimation methodology using the case for High risk IOU for five years.

- Cost of cooling water- The cost of cooling water from the Bituminous Baseline Study was used for the non-scaled cases. For the scaled-up cases, the increased cooling water demand increased cooling tower CAPEX and OPEX.
- $CO_2$ transport, storage and monitoring- \$10/tonne as provided by DOE in the cooperative agreement.
- Solvent cost- Solvent cost of \$20/lb was used in this study. This solvent cost is based off of the estimates made for solvent cost in the previous DOE award (DE-FE0007502). Further, a sensitivity analysis was conducted with respect to solvent cost, which is provided in the subsequent section.
- Fixed O&M costs- Estimated using a plant on stream factor of 310.25 days and a charge of \$875/day.
- Maintenance and material cost- Estimated using 1.6% of the material cost.

The details of the calculations are provided below

<u>Power Island – CAPEX, OPEX, and Fuel</u> – this cost is the same for all non-scaled cases. It can also be calculated using the expression below:

$$Power\ island\ cost = COE \cdot power\ generated$$

COE, which is used in this expression, is equal to 80.95 mils/kWh, from Case 11 COE w/o TS&M.

For the scaled-up cases, the cost was estimated using Thermoflow calculations.

<u>Capital Recovery and other Fixed Charges</u>

The capital recovery was calculated based on the following formula:

$$Capital\ recovery = Capital\ charge\ factor * installed\ CAPEX$$

The capital charge factor (CCF) value is selected based on several factors:

- Type of power plant financial structure (IOU vs. IPP)
- High risk or low risk finance structure
- Capital expenditure period: three years vs. five years.

**Table 30** reports capital charge factors for a variety of finance structures.

**Table 30.** Capital charge factors for various finance structures

| Finance Structure | High Risk IOU | | Low Risk IOU | |
|---|---|---|---|---|
| Capital Expenditure Period | Three Years | Five Years | Three Years | Five Years |
| Capital Charge Factor (CCF) | 0.111 | 0.124 | 0.105 | 0.116 |
| | | | | |
| Finance Structure | High Risk IPP | | Low Risk IPP | |
| Capital Expenditure Period | Three Years | Five Years | Three Years | Five Years |
| Capital Charge Factor (CCF) | 0.177 | 0.214 | 0.149 | 0.176 |

The value selected for the post-combustion $CO_2$-capture process is 12.4%, which corresponds to a high risk IOU structure with a five year capital expenditure period.

First year COE was calculated based on the following formula:

$$COE = \frac{total\ annual\ costs}{power\ generated}$$

First year removal cost for $CO_2$ was calculated using the expression below:

$$Removal\ cost\ \left(\frac{\$}{ton}\right) = \frac{COE_{with\ capture} - COE_{without\ capture}}{lb\ of\ CO2\ separted * power\ generated}$$

Total Cost of Cooling Water

The total cost of cooling water was determined based on the amount of cooling water required as predicted by the ASPEN Plus model for the carbon-capture process and the cost of cooling water.

$CO_2$ Transport, Storage, and Monitoring

This cost was calculated based on the amount of $CO_2$ separated and the cost of transportation, storage, and Monitoring (TS&M).

Maintenance Material Costs

The maintenance material costs were calculated from the formula below:

$$\begin{aligned} &Maintenance\ material\ costs \\ &\qquad = Equipment\ and\ material\ costs * Maintenance\ and\ material\ cost\ \% \end{aligned}$$

The first year removal cost of $CO_2$ was estimated for a supercritical power plant with carbon capture using MEA as a solvent. The results are shown in **Figure 44** as compared to Case 12 in the Bitimunous Baseline Study Cost Update.[2] The values are in good agreement with each other.

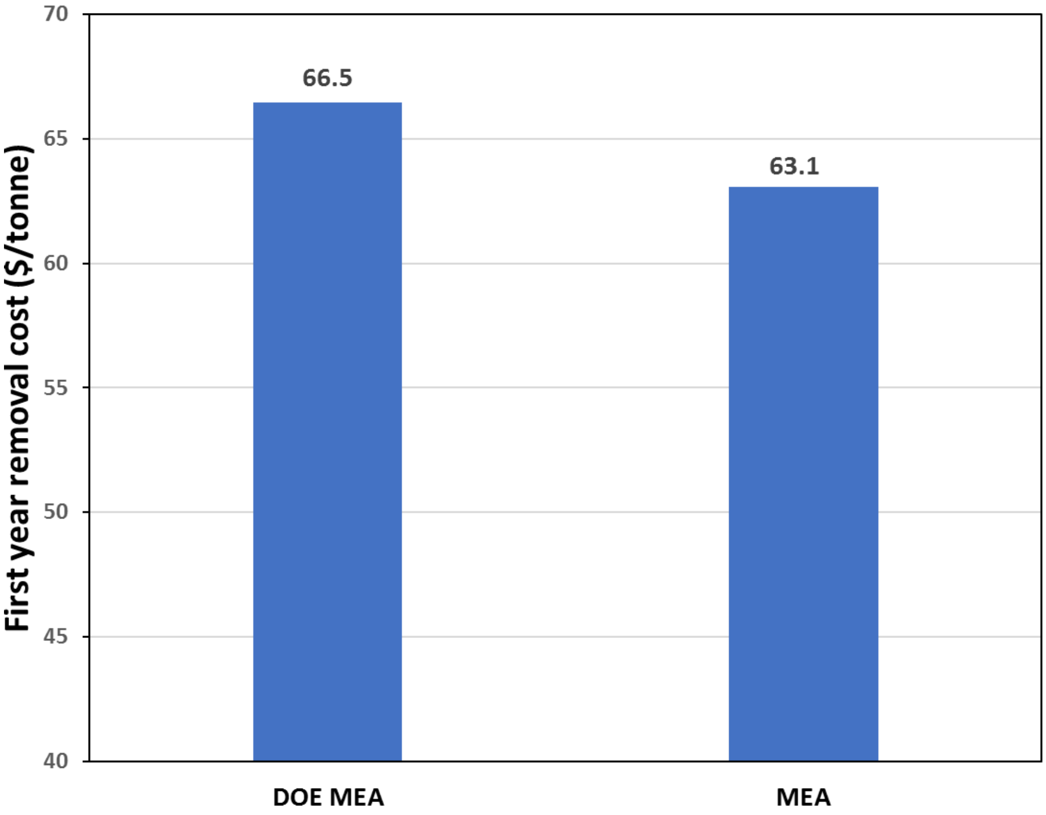


**Figure 44.** Comparison of first year removal cost of $CO_2$ using MEA vs. DOE estimated value[2]

The removal cost was estimated for a supercritical power plant using the aminosilicone-based material as a solvent for carbon capture. As mentioned earlier for the first few cases (Case A-G) the power plant island was taken as the same size as Case 11 in the Bituminous Baseline Study. This was done to determine the effect of different parameters of the carbon-capture island on process economics without changing the size and other variables of the power island. Once a best case was found for the conditions of the carbon-capture island, then the scale was adjusted to get to a 550 MW net power with carbon capture (shown as Case H-J). The cost summary for the power plant model with $CO_2$ capture (Case H) is shown in **Table 31**. The total cost of the power block increased by ~$333MM over the case without $CO_2$ capture.

**Table 31**. Equipment cost summary from power plant modeling of Case H
See details in Table 19

| | $ | $/kW |
|---|---|---|
| **Specialized Equipment** | **$ 609,811,487** | **$ 1,105** |
| **Boiler** | **$ 234,107,909** | **$ 424** |
| Furnace | $ 101,283,882 | $ 183 |
| Convective Elements | $ 65,610,249 | $ 119 |
| Additional Waterwall | $ 7,507,987 | $ 14 |
| Soot Blowers | $ 6,098,788 | $ 11 |
| Desuperheaters and Controls | $ 10,253,053 | $ 19 |
| Air and Flue Gas Ducts | $ 7,467,654 | $ 14 |
| Coal Pulverizers and Feeders | $ 24,580,927 | $ 45 |
| FD Fan, PA Fan, ID Fan | $ 3,878,047 | $ 7.0 |
| Structural Steel, Ladders, Walkways | $ 3,064,060 | $ 5.6 |
| Rotary Air Heaters | $ 4,363,261 | $ 7.9 |
| | | |
| **Steam Turbine** | **$ 89,908,464** | **$ 163** |
| | | |
| **Feedwater Heaters** | **$ 11,359,687** | **$ 21** |
| Feedwater Heater 1 | $ 542,457 | $ 1.0 |
| Feedwater Heater 2 | $ 527,972 | $ 1.0 |
| Feedwater Heater 3 | $ 527,728 | $ 1.0 |
| Feedwater Heater 4 | $ 537,078 | $ 1.0 |
| Feedwater Heater 5-DA | $ 895,946 | $ 1.6 |
| Feedwater Heater 6 (6A,6B) | $ 2,390,574 | $ 4.3 |
| Feedwater Heater 7 (7A,7B) | $ 2,764,842 | $ 5.0 |
| Feedwater Heater 8 (8A,8B) | $ 3,173,090 | $ 5.7 |
| | | |
| **Water Cooled Condensers** | **$ 3,201,005** | **$ 5.8** |
| Main Condenser | $ 2,467,013 | $ 4.5 |
| Feed Pump Turbine Condenser | $ 733,991 | $ 1.3 |
| | | |
| **Particulate and Mercury Control** | **$ 26,720,630** | **$ 48** |
| | | |
| **Flue Gas Desulfurization** | **$ 151,257,175** | **$ 274** |
| | $ | $/kW |
| **Nitrogen Oxide Control (SCR)** | **$ 52,211,298** | **$ 95** |
| | | |
| **Stack** | **$ 10,733,066** | **$ 19** |

| | | |
|---|---|---|
| | | |
| **Continuous Emissions Monitoring System** | **$ 627,300** | **$ 1.1** |
| | | |
| **Distributed Control System** | **$ 1,737,273** | **$ 3.1** |
| | | |
| **Transmission Voltage Equipment** | **$ 16,574,415** | **$ 30** |
| Transformers | $ 14,739,549 | $ 27 |
| Circuit Breakers | $ 1,045,579 | $ 1.9 |
| Miscellaneous Equipment | $ 789,287 | $ 1.4 |
| | | |
| **Generating Voltage Equipment** | **$ 11,373,267** | **$ 21** |
| Generator Buswork | $ 5,935,887 | $ 11 |
| Circuit Breakers | $ 4,895,854 | $ 8.9 |
| Miscellaneous Equipment | $ 541,526 | $ 1.0 |

| | | |
|---|---|---|
| **Other Equipment** | **$ 154,572,349** | **$ 280** |
| **Pumps** | **$ 15,195,073** | **$ 28** |
| Boiler Feed Pump (+ Turbine) | $ 11,234,334 | $ 20 |
| Boiler Feed Booster Pump | $ 173,367 | $ 0.3 |
| Condenser C.W. Pump | $ 1,858,945 | $ 3.4 |
| Condensate Forwarding Pump | $ 377,533 | $ 0.7 |
| Condenser Vacuum Pump | $ 398,799 | $ 0.7 |
| Aux Cooling Water Pump (Closed Loop) | $ 43,656 | $ 0.1 |
| Treated Water Pump | $ 7,199 | $ 0.01 |
| Diesel Fire Pump | $ 172,817 | $ 0.3 |
| Jockey Fire Pump | $ 5,182 | $ 0.01 |
| Demin Water Pump | $ 14,251 | $ 0.03 |
| Raw Water Pumps | $ 34,857 | $ 0.1 |
| Aux Cooling Water Pump (Open Loop) | $ 43,656 | $ 0.1 |
| Startup Boiler Feed Pump | $ 830,475 | $ 1.5 |
| | | |
| **Tanks** | **$ 1,052,452** | **$ 1.9** |
| Hydrous Ammonia | $ 168,509 | $ 0.3 |
| Demin Water | $ 116,820 | $ 0.2 |
| Raw Water | $ 395,305 | $ 0.7 |
| Neutralized Water | $ 86,820 | $ 0.2 |
| Acid Storage | $ 36,341 | $ 0.1 |
| Caustic Storage | $ 36,341 | $ 0.1 |
| Dedicated Fire Protection Water Storage | $ 212,316 | $ 0.4 |
| | | |

|  |  |  |
|---|---|---|
| **Cooling Tower** | **$ 15,094,192** | **$ 27** |
|  |  |  |
| **Auxiliary Cooling Water Heat Exchanger** | **$ 152,969** | **$ 0.3** |
|  |  |  |
| **Steam Turbine Crane** | **$ 1,403,592** | **$ 2.5** |
|  |  |  |
| **Station Instrument Air Compressors** | **$ 955,936** | **$ 1.7** |
|  |  |  |
| **General Plant Instrumentation** | **$ 446,686** | **$ 0.8** |
|  |  |  |
| **Medium Voltage Equipment** | **$ 8,499,153** | **$ 15** |
| Transformers | $ 1,225,828 | $ 2.2 |
| Circuit Breakers | $ 501,147 | $ 0.9 |
| Switchgear | $ 2,149,781 | $ 3.9 |
| Motor Control Centers | $ 4,217,678 | $ 7.6 |
| Miscellaneous | $ 404,719 | $ 0.7 |
|  |  |  |
| **Low Voltage Equipment** | **$ 2,328,973** | **$ 4.2** |
| Transformers | $ 822,781 | $ 1.5 |
| Circuit Breakers | $ 670,152 | $ 1.2 |
| Motor Control Centers | $ 725,143 | $ 1.3 |
| Miscellaneous | $ 110,898 | $ 0.2 |
|  |  |  |
| **Coal Handling Equipment** | **$ 77,179,135** | **$ 140** |
|  |  |  |
| **Ash Handling Equipment** | **$ 24,903,817** | **$ 45** |
|  |  |  |
| **Miscellaneous Equipment** | **$ 7,360,371** | **$ 13** |

|  |  |  |
|---|---|---|
| **Civil** | **$ 105,551,677** | **$ 191** |
| **Site Work** | $ 19,774,449 | $ 36 |
| **Excavation and Backfill** | $ 6,839,480 | $ 12 |
| **Concrete** | $ 77,768,896 | $ 141 |
| **Roads Parking and Walkways** | $ 1,168,852 | $ 2.1 |

| **Mechanical** | **$ 332,077,085** | **$ 602** |
|---|---|---|
| **On Site Transportation and Rigging** | $ 11,121,067 | $ 20 |
| **Equipment Erection and Assembly** | $ 239,556,407 | $ 434 |
| **Piping** | $ 78,972,668 | $ 143 |
| **Steel** | $ 2,426,944 | $ 4.4 |

| **Electrical Assembly and Wiring** | **$ 30,318,365** | **$ 55** |
|---|---|---|
| **Controls** | $ 18,598,808 | $ 34 |
| **Assembly and Wiring** | $ 11,719,557 | $ 21 |

| **Buildings and Structures** | **$ 22,448,094** | **$ 41** |
|---|---|---|
| **Boiler House and Turbine Hall** | $ 20,400,100 | $ 37 |
| **Administration Control Room, Machine Shop, Warehouse** | $ 2,021,483 | $ 3.7 |
| **Guard House** | $ 26,510 | $ 0.05 |

| **Engineering and Plant Startup** | **$ 56,170,844** | **$ 102** |
|---|---|---|
| **Engineering** | $ 45,503,738 | $ 82 |
| **Start Up** | $ 10,667,106 | $ 19 |

| **Totals** | | |
|---|---|---|
| **Subtotal Contractor's Internal Cost** | **$ 1,310,949,901** | **$ 2,375** |
| Contractors Soft & Misc Costs | $ 253,644,708 | $ 460 |
| **Subtotal Contractor's Price** | **$ 1,564,594,609** | **$ 2,834** |
| Owner's Soft and Misc Costs | $ 293,990,948 | $ 533 |
| **Total Owner's Cost** | **$ 1,858,585,556** | **$ 3,367** |

**Table 32** shows the calculated annual costs for the power block configured for $CO_2$ capture. The fixed operating costs and the maintenance and material costs in this case were assumed to be equal to the values in DOE case 12 of the cost updates to the Bituminous Baseline Study.

**Table 32.** Annual costs from power plant modeling of Case H (see details in Table 19)

| | Consumption / day | Unit Cost | Annual Cost | Annual Unit Cost |
|---|---|---|---|---|
| | | | $ | $/kWh-net |
| **Fixed Operating Costs** | | | **$ 61,032475** | **$ 0.01262** |
| **Maintenance Material Costs** | | | $ 18,136,161 | $ 0.00375 |
| Water (/1000 gallons) | 4,647 | 1.67 | $ 2,407,817 | $ 0.00050 |
| Chemicals | | | | |
| MU & WT Chem.(lbs) | 22,493 | 0.27 | $ 1,884,197 | $ 0.00039 |
| Limestone (ton) | 638 | 33.48 | $ 6,625,304 | $ 0.00137 |
| Ammonia (19% $NH_3$) ton | 97 | 330 | $ 9,961,176 | $ 0.00206 |
| **Subtotal Chemicals** | | | $ 18,470,677 | $ 0.00382 |
| Other | | | | |
| SCR Catalyst ($m^3$) | 0.41 | 5775.94 | $ 730,381 | $ 0.00015 |
| **Subtotal Other** | | | $ 730,381 | $ 0.00015 |
| Waste Disposal | | | | |
| Total Ash (ton) | 627 | 25.11 | $ 4,882,568 | $ 0.00101 |
| **Subtotal Waste Disposal** | | | $ 4,882,568 | $ 0.00101 |
| **Total Variable Operating Costs** | | | **$ 26,491,442** | **$ 0.00548** |
| Fuel (ton) | 6461 | 68.60 | **$ 137,516,215** | **$ 0.02844** |

Capital cost estimations for the aminosilicone cases were done using Aspen Cost Estimator with a cost basis of Q1, 2010. The costs were then adjusted using the CEPCI index to get a final cost basis of 2011. The total CAPEX for the DOE Case 12 as compared to Case H and Case J are shown in **Figure 45**. Case H is <75% and Case J is <77% of the CAPEX of a system using MEA solvent. The lower CAPEX for Case L (SSC) as compared to Case H is due to the lower overall CO2 capture plant due to an increased working capacity with steam stripper column desorption,. Furthermore, increased water content in the working solution let to an improved heat transfer coefficient in the cross HX, hence lower CAPEX.

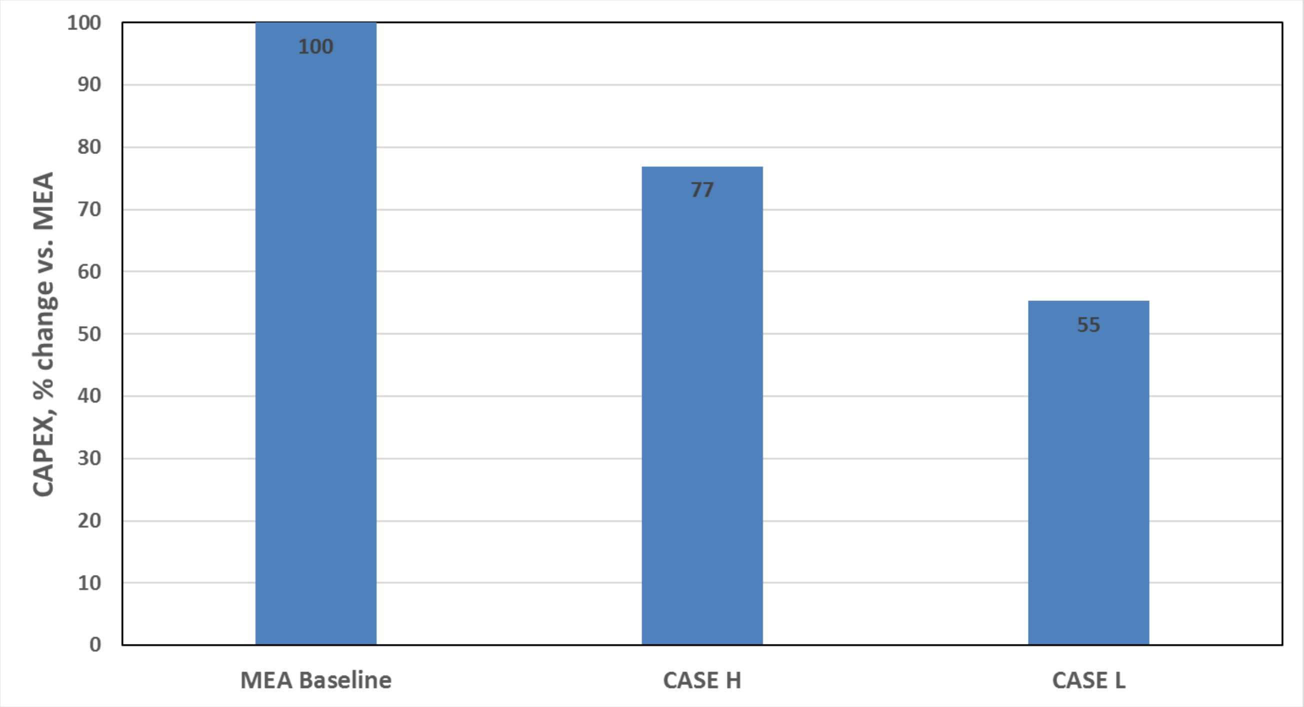


**Figure 45.** Total CAPEX comparison of two scaled-up cases using GAP-$1_m$/TEG vs. DOE Case 12 using MEA.

First year COE was calculated (with and without TS&M) as shown in **Figure 46** and **Figure 47**. Case L COE w/o TS&M is 11.9 as compared to 13.73 cents/kWh for the MEA based system. When TS&M is included in the analysis, then Case L COE is 12.8 vs. 14.73 cents/kWh for the MEA based system.

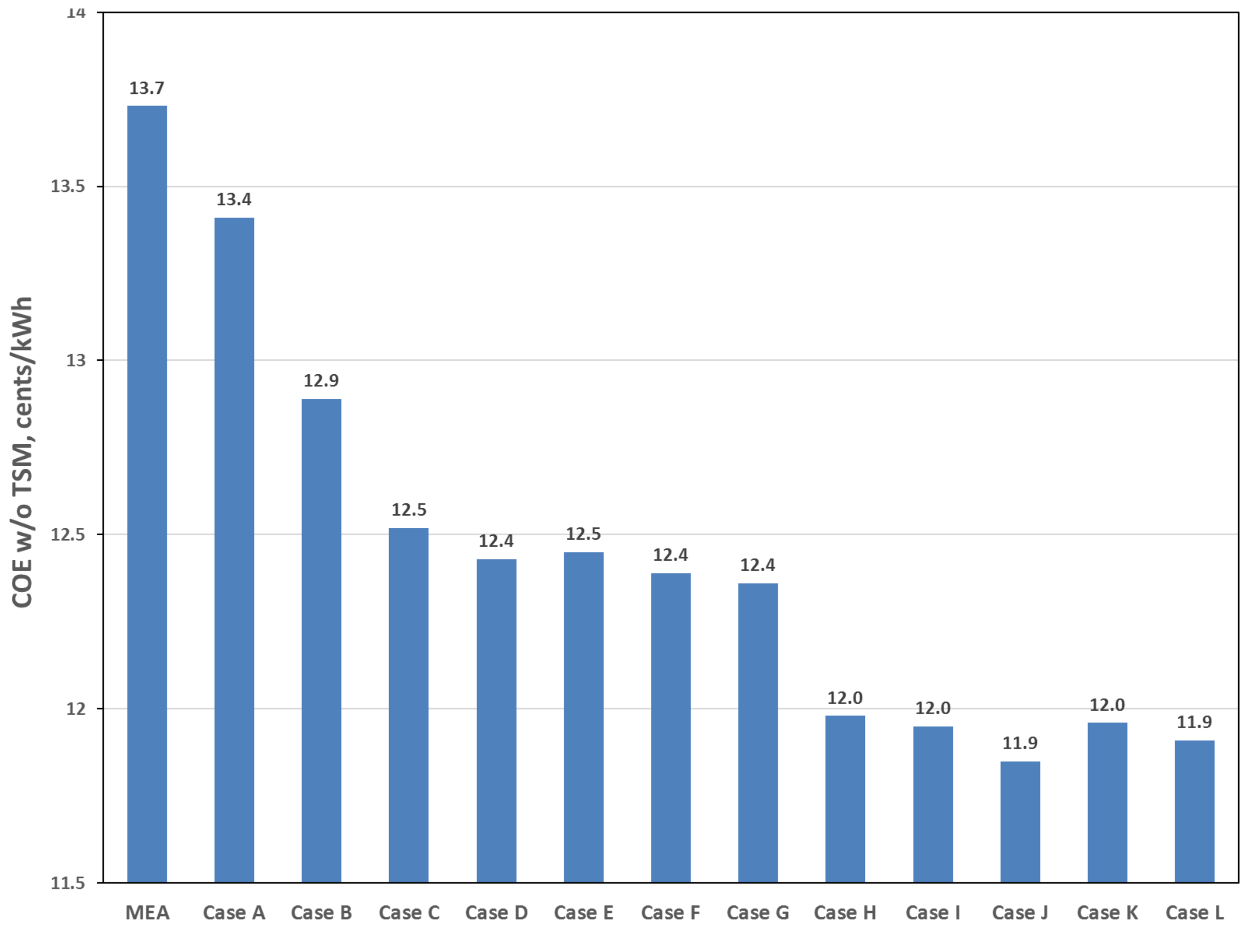


**Figure 46.** Cost of electricity without TS&M for various cases as compared to DOE Case 12

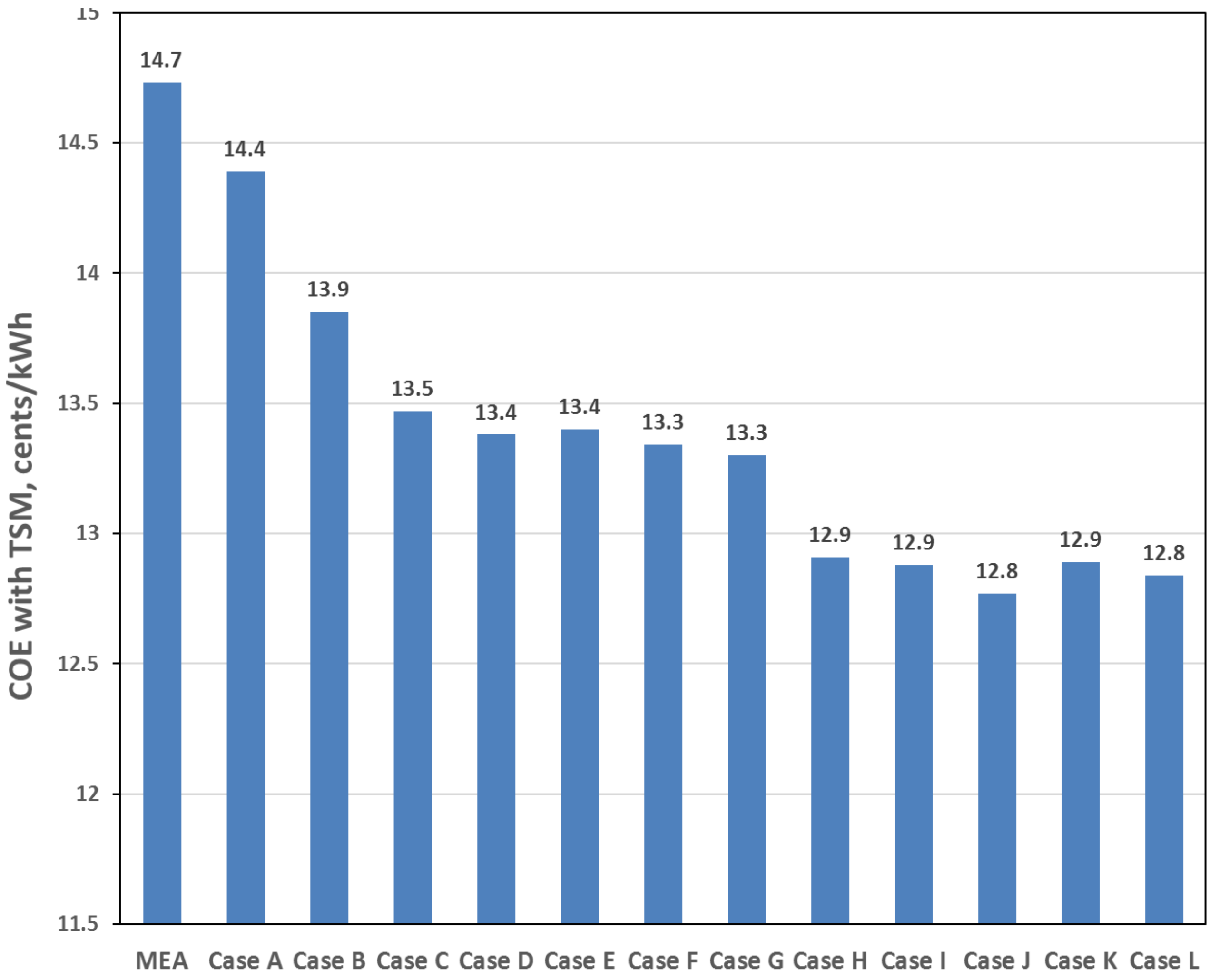


**Figure 47.** Cost of electricity with TS&M for various cases as compared to DOE Case 12

The first year removal cost of $CO_2$ for Case K (CSTR, low P) is \$52.6 \$/tonne of $CO_2$ as compared to \$66.3/tonne of $CO_2$ when MEA is used. For steam stripper desorber, the first year removal cost of $CO_2$ for case L (SSC, low P) is 46\$/tonne of $CO_2$. This shows a significant reduction in removal cost when aminosilicone solvent is used for carbon capture. (**Figure 48**)

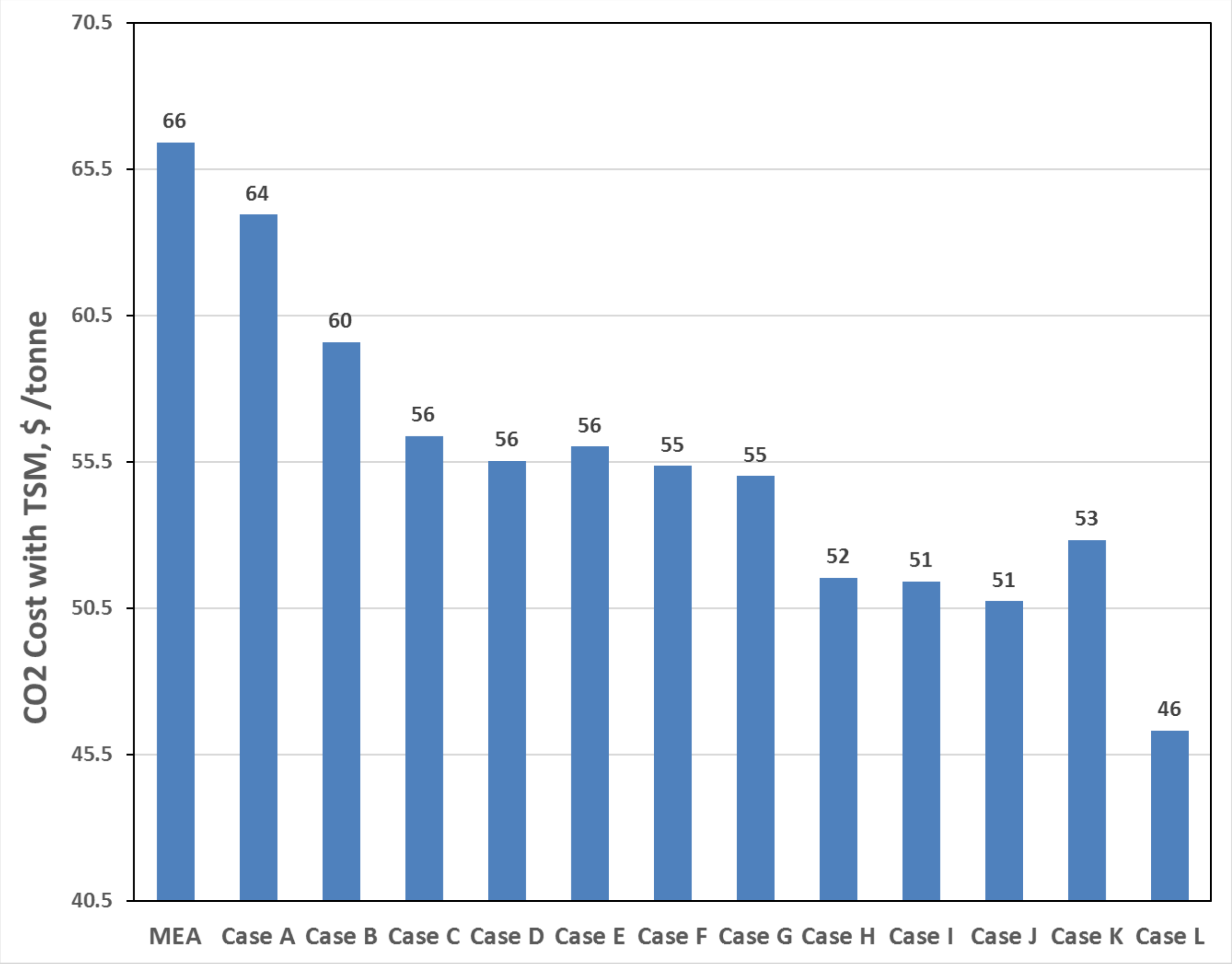


**Figure 48.** First year removal cost of $CO_2$ in \$/tonne for various cases as compared to DOE Case 12.

## 4.10 Sensitivity Analysis

In order to understand the effect of the main parameters on the cost of $CO_2$ removal and efficiency of the power plant, the sensitivity analysis was conducted with respect to the following parameters:

- Heat rate of the desorber
- Auxiliary load of the pumps and compressors for $CO_2$ capture island
- Required amount of cooling water
- Installed CAPEX of $CO_2$-capture island
- Power island capital cost
- Solvent cost
- Sulfur amount in incoming flue gas
- Solvent make-up yearly rate

The results of the sensitivity analysis are presented in below.

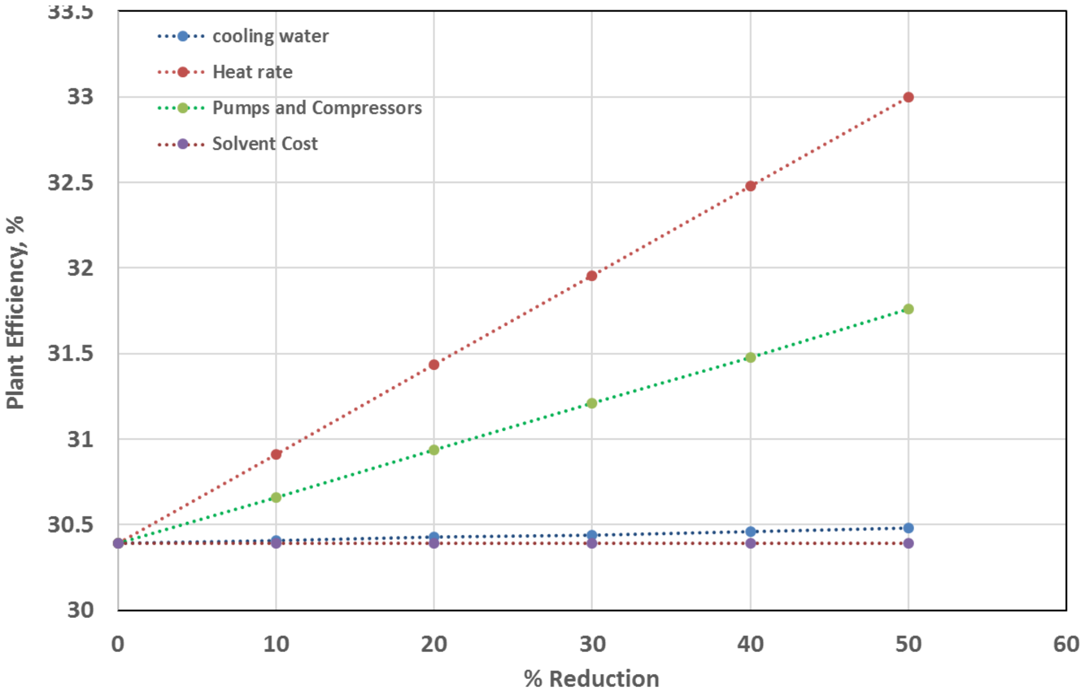


**Figure 49.** Sensitivity analysis of effect of different variables on plant efficiency for Case K (see details on **Table 19**)

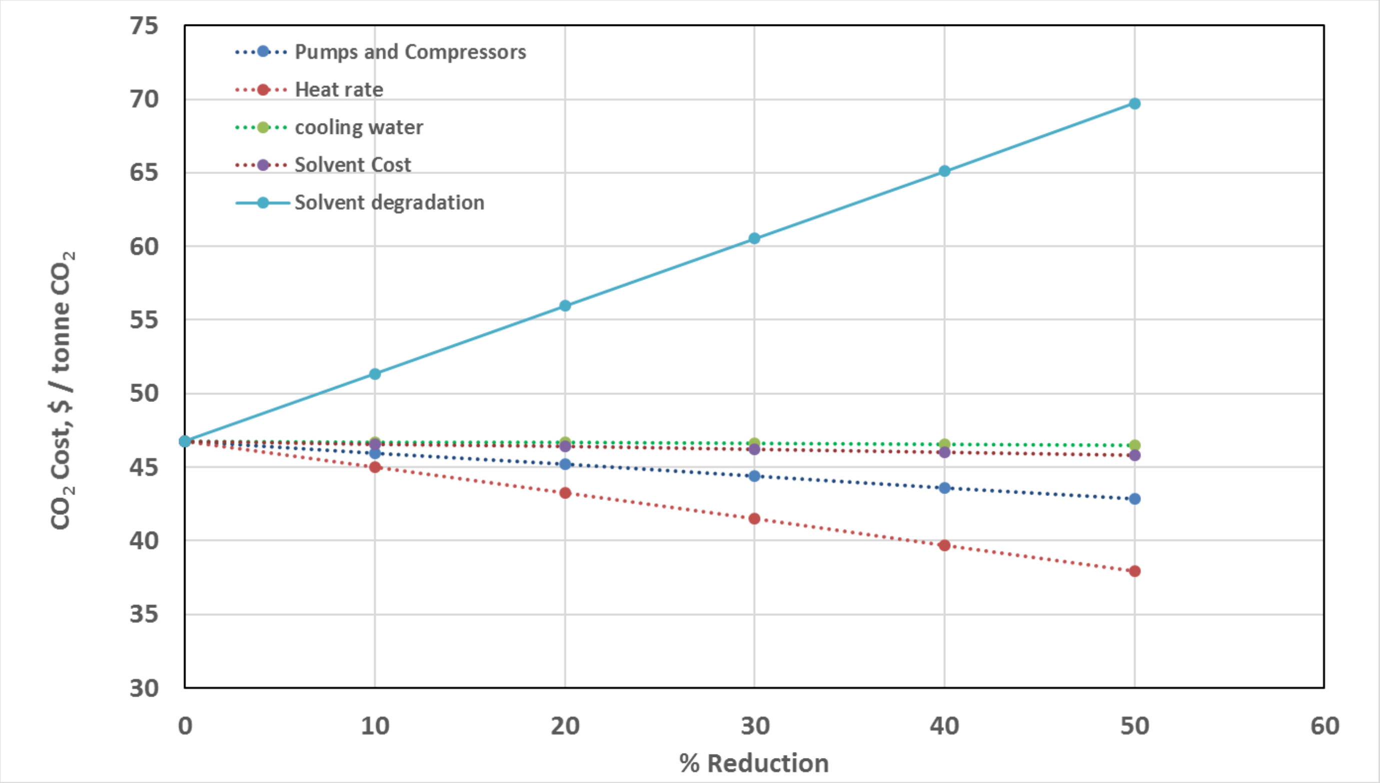


**Figure 50.** Sensitivity analysis of effect of different variables on removal cost of $CO_2$ for Case K (see details on **Table 19**)

It can be seen from the results presented in **Figure 49** and **Figure 50**, that Installed CAPEX of the $CO_2$-capture island and desorber heat rate have the most positive significant impact on $CO_2$ removal cost. Cooling water amount, auxiliary power, and solvent cost (at this low level of degradation) have a lesser effect. However, the $CO_2$ cost is negatively dominated by the solvent degradation rate, as the aminosilicone is a more expansive solvent than MEA. Based on the 0.5 $MW_e$ Demo performed at NCCC, the solvent make-up rate was 15% / yr. for SSC, and 120% / yr. for CSTR. **Figure 51** and **Figure 52** show the predicted values for $CO_2$ cost assuming the measured make-up solvent degradation rates. For CSTR absorber, the high solvent degradation rate renders a cost of $CO_2$ over $100/ tonne $CO_2$. On the other hand, lower solvent make-up rate and improved performance for the steam stripper column led to a cost of $CO_2$ of $52.9 / tonne of $CO_2$. This shows a significant reduction in removal cost vs MEA when aminosilicone solvent is used for carbon capture.

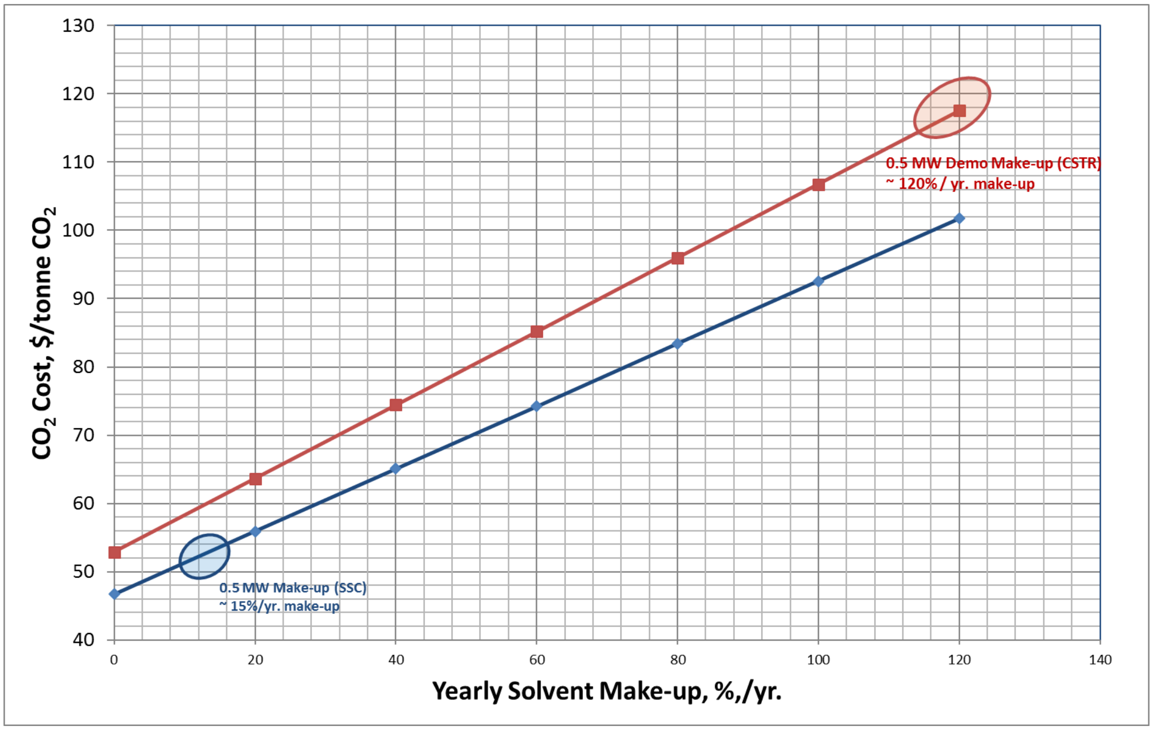


**Figure 51.** Sensitivity analysis of effect of yearly solvent make-up on removal cost of $CO_2$ for Case K (CSTR desorber, low P) and Case L (SSC, low P)

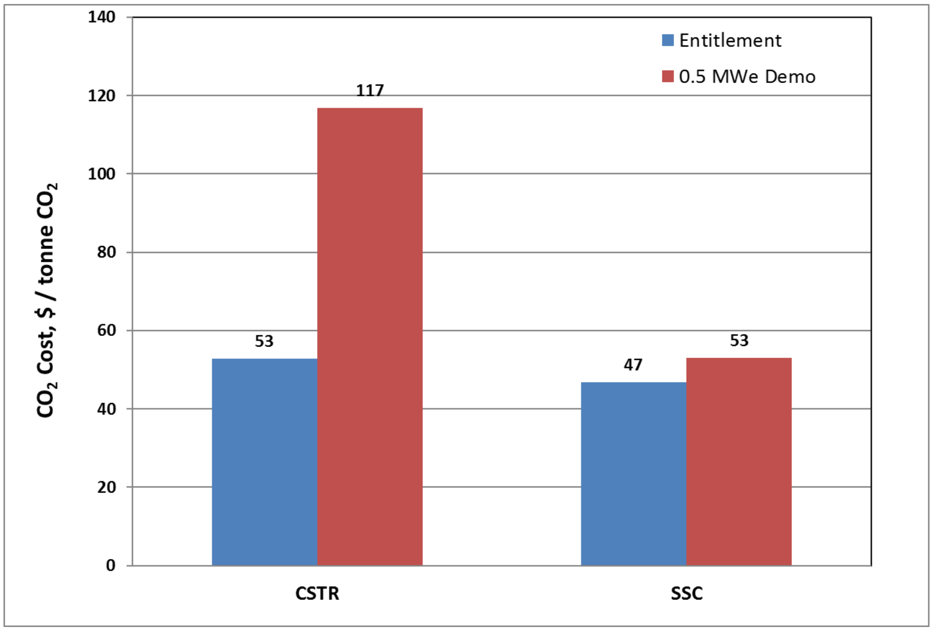


**Figure 52.** $CO_2$ cost for CSTR (continuous stirred tank reactor) and Steam Stripper Column (SSC) desorbers: Entitlement vs. Prediction based on measured yearly solvent make-up rates at 0.5 $MW_e$ Demo (NCCC)

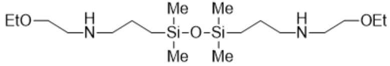
## 4.11 Advanced Aminosilicone – Preliminary Techno-Economic Analysis

While the current GAP-$1_m$/TEG technology has many positive attributes, there are areas for improvements to enable its widespread deployment. Based on the process and economic models discussed before and recent experiments performed in our laboratory, four attributes have been identified that will significantly reduce the cost of $CO_2$ captured for the aminosilicone solvents: a) $CO_2$ working capacity, b) solvent stability, c) solvent viscosity, and d) heat of reaction. Preliminary experiments that examined a related aminosilicone solvent (EEAP) showed promising results. The advanced amino silicone solvent exhibits lower heat of reaction, greater thermal stability, lower viscosity and the ability to remain as a flowable liquid when fully reacted without the need for a co-solvent. (**Table 33**)

**Table 33.** Advanced Aminosilicone Solvents: Physical Properties

| **Solvent Attribute** | **EEAP***<br>(Gen 2 Candidate) | |
|---|---|---|
| | | Note |
| **$CO_2$ Capacity** (wt.%) | 8 | Absorption at 35 °C; desorption at 100 °C |
| **Solvent Make-up** (%/yr.) | 20 | Thermally stable up to 140 °C |
| **Viscosity** (cP, $CO_2$ loaded) | 286 | No co-solvent required |
| **Heat of Reaction** (kJ/Kg) | 1863 | |

**EEAP*:**



A comparative techno-economic analysis was conducted to demonstrate the potential of the advanced aminosilicone technology over the current state-of-the-art systems. Design basis for this technology evaluation, approach, assumptions and results are discussed below.

### 4.11.1 Technology Evaluation—Design Basis

The design basis that we adopted to benchmark the advanced aminosilicone technology is described in Case 12 of the DOE Bituminous Baseline Study.[1] The proposed advanced aminosilicone process utilize four key processes, $CO_2$ absorption, $CO_2$ desorption, solvent handling, and $CO_2$ compression.

ASPEN Plus models developed for GAP-$1_m$ / TEG were used along with a new spreadsheet model with transfer functions for a supercritical commercial-scale process with advanced aminosilicone-based solvent. Solvent design targets of the advanced aminosilicone working solution evaluated are shown in **Table 33**. The base case chosen was similar to Case 11 in the DOE-NETL study.[1] Cases were further developed to carry out sensitivity related to varying solvent properties. In order to compare the different cases of the carbon-capture island, the flue gas flow rate was fixed to match the Case 11 (550 MW net power without capture). The best case was then scaled up to 550 $MW_e$ net power with $CO_2$ capture. Each property change and its effect were used to estimate the COE improvement. Cost of the advanced aminosilicone solvent was estimated based on previous studies conducted for the GAP-$1_m$/TEG technology. The assumptions and approach used are presented below.

Cost of the solvent

***Assumptions***

For the large scale manufacture of GAP-$1_m$ solvent, SiVance/Millikin had estimated that implementation of an improved synthetic process could result in a solvent cost of 40 $/kg.[12] The advanced aminosilicone solvent will be composed of the same silicone backbone, is anticipated to have the same number, or fewer, intermediate synthetic steps, and should result in a higher overall yield of final product. Given this information, we anticipate that the ultimate cost of the new advanced aminosilicone solvent will be less than or equal to that estimated for GAP-$1_m$.

***Outcome***

Cost of the advanced aminosilicone solvent utilized in the sensitivity analysis is 40 $/kg.

Heat of Reaction Optimization

***Assumptions***

The heat of reaction for the current GAP-$1_m$/TEG working solution is 2263 kJ/kg $CO_2$. Design target for the advanced aminosilicone working solution is 1900 kJ/kg of $CO_2$. It is assumed that the reduction in heat of reaction does not impact any other solvent properties and working capacity of the solvent.

***Outcome***

It is estimated that the reduced heat of reaction will lower the desorber reboiler duty by 12%, and correspondingly on the amount of steam which needs to be extracted from power plant steam turbines. COE cost (without TS&M) is estimated at 12.0 cents/kWh. (case 2, **Table 34)**

$CO_2$ Working capacity

***Assumption and Approach***

Design target for the advanced aminosilicone working solution is 0.1 kg $CO_2$/ kg working solution. A sensitivity analysis was conducted using the GAP-$1_m$/TEG process model with respect to solvent flow rate and the results were used to estimate the benefit for the advanced aminosilicone. It is assumed that the outcomes from the GAP-$1_m$/TEG solvent sensitivity cases would result in a proportional benefit for the advanced solvent with higher working capacity.

***Outcome***

Working solution flow rate is decreased by 40 % vs. GAP-$1_m$/TEG. This leads to a smaller size overall system with 25 % reduction in CAPEX and an additional 12 % reduction in reboiler duty). COE cost (without TS&M) is estimated at 11.6 cents/kWh. (Case 3, **Table 34**)

Viscosity

***Assumption and Approach***

Design target for the advanced aminosilicone working solution at the absorber outlet is 100 cP. To estimate the potential benefit of the reduced solvent viscosity on the size of the absorber, we made the assumption that the mass transfer resistance is dominated by the liquid side resistance. This assumption was consistent with the estimated Sherwood numbers (Sh) and diffusivities from Aspen Plus™ simulations of the absorber.

$$Sh = \frac{k_l d}{D}$$

where $k_l$ is the mass transfer coefficient, d is the nominal packing size, and D is the diffusivity.

Based on the engineering correlations for $k_L$ in a packed column described in the following equation,[13]

$$\frac{k_L d}{D_l} = 25.1 \left(\frac{d_s L}{\mu}\right)^{0.45} \left(\frac{\mu}{\rho D_l}\right)^{0.5}$$

and the Wilke-Chang correlation (equation (3)) for the dependence of diffusivity ($D_l$) on viscosity ($\mu$),

$$D^{\circ}_{AB} = \frac{7.4x10^{-8}(\emptyset_B M_B)^{1/2}T}{\mu_B V_A^{0.6}}$$

we estimate the liquid side mass transfer coefficient to vary with ($\frac{1}{\mu^{0.45}}$). Assuming a three-fold reduction in viscosity, we estimate up to a 40% reduction in the height of the absorber.

Similarly, it was assumed that, due to viscosity reduction, the heat transfer resistances on both sides of the rich lean heat exchanger can be reduced according to Dittus-Boelter correlation (equation (4)).**Error! Bookmark not defined.** Hot side resistance is reduced by $3.2^{0.5}$ and cold side resistance is reduced by $3.2^{0.4}$.

$$Nu = 0.023 \mathrm{Re}^{0.8} \mathrm{Pr}^{0.4}$$

where: Nu (Nusselt number) = $\frac{hD}{k}$, Re (Reynolds number) = $\frac{Dv\rho}{\mu}$, Pr (Prandlt number) = $\frac{C_p \mu}{k}$

h = heat transfer coefficient, D = pipe diameter, k = thermal conductivity, v = fluid bulk velocity, $\mu$ = density, $\rho$ = viscosity, $C_p$ = heat capacity.

***Outcome***

40% reduction in absorber height and 30% reduction in rich/lean heat exchanger size. We have used this reduction to estimate the reduction in the size and capital expense associated with the absorber column and rich/lean heat exchanger. COE cost (without TS&M) is estimated at 11.2 cents/kWh. (Cases 5-6, **Table 34)**

**Table 34.** Advanced aminosilicone solvent: sensitivity analysis and process impact

| Case | Technology | | Solvent Design Target | | | COE w/o TS&M* | Cumulative Process Impact vs. GAP-1$_m$/TEG |
|---|---|---|---|---|---|---|---|
| | | Scale | ΔH (KJ/kg $CO_2$) | $CO_2$ Working Capacity (kg $CO_2$/ kg solution) | μ solution† @ absorber outlet (cP) | cents/ kWh | |
| 1 | GAP-1$_m$/TEG | Power plant size same as Case 11** | 2263 | 0.05 | 325 | 12.4 | |
| 2 | Adv. Aminosilicone | | 1900 | 0.05 | 325 | 12.0 | 12% reduction reboiler duty |
| 3 | | | 1900 | 0.08 | 325 | 11.6 | 40% reduction in working solution flow<br>24% reduction reboiler duty<br>25% reduction in CAPEX |
| 4 | | | 1900 | 0.10 | 325 | 11.5 | 50% reduction in working solution flow<br>30% CAPEX reduction |
| 5 - 6 | | | 1900 | 0.10 | 100 | 11.2 | 30% reduction cross HX<br>40% reduction absorber height |
| 7 | | Scaled up power plant for 550 MWe net power | 1900 | 0.10 | 100 | 10.6 | 23% reduction in COE vs. Case 9 |
| 8 | GAP-1$_m$/ TEG | | 2263 | 0.05 | 325 | 11.6 | |
| 9 | MEA* (1) | | 1825 | 3 | 1 | 13.7 | |

* TS&M – transportation, storage, and monitoring; μ = viscosity

Effects of the improved properties for the advanced aminosilicone technology on COE and $CO_2$ cost are detailed of the analysis are listed in **Table 34.**

- Case 1 corresponds to the best simulation for GAP-1$_m$ / TEG as previously reported using SSC. Power plant size is the same as Case 11.
- Cases 2-6 represent the sensitivity analysis for the advanced aminosilicone solvent starting from Case 1 as the baseline, while implementing the improvements in solvent properties. For this sensitivity analysis, it was assumed that each individual property improvement does not affect other solvent properties.
- Case 7 represents Case 6 scaled-up to 550 MW plant including limited heat integration.

Best scaled-up case for the advanced aminosilicone (Case 7) is then compared to the corresponding cases for GAP-$1_m$/TEG (Case 8, 550 MWe net power) and MEA (Case 9, 550 MW net power). The results indicate that the improvements in heat of reaction, working capacity, and viscosity can potentially reduce the cost of $CO_2$ to 44.1 $/tonne and COE (w/o TS&M) to 10.6 cents/kWh. This represents 20% improvement in COE impact vs. MEA.

**Figure 53** compares performance of the proposed technology to the 2nd generation capture technologies showing the progress towards meeting the 40 $/tonne $CO_2$ cost target.[14] We anticipate that additional process optimization and material developments such as: (i) absorber, desorber and cross heat exchanger advanced designs, (ii) $CO_2$ capture plant flowsheet optimization, (iii) development of additives to further reduce thermal and chemical solvent degradation and its corrosivity, (iv) solvent cost-out and (v) advanced heat integration will further drive the reduction in COE.

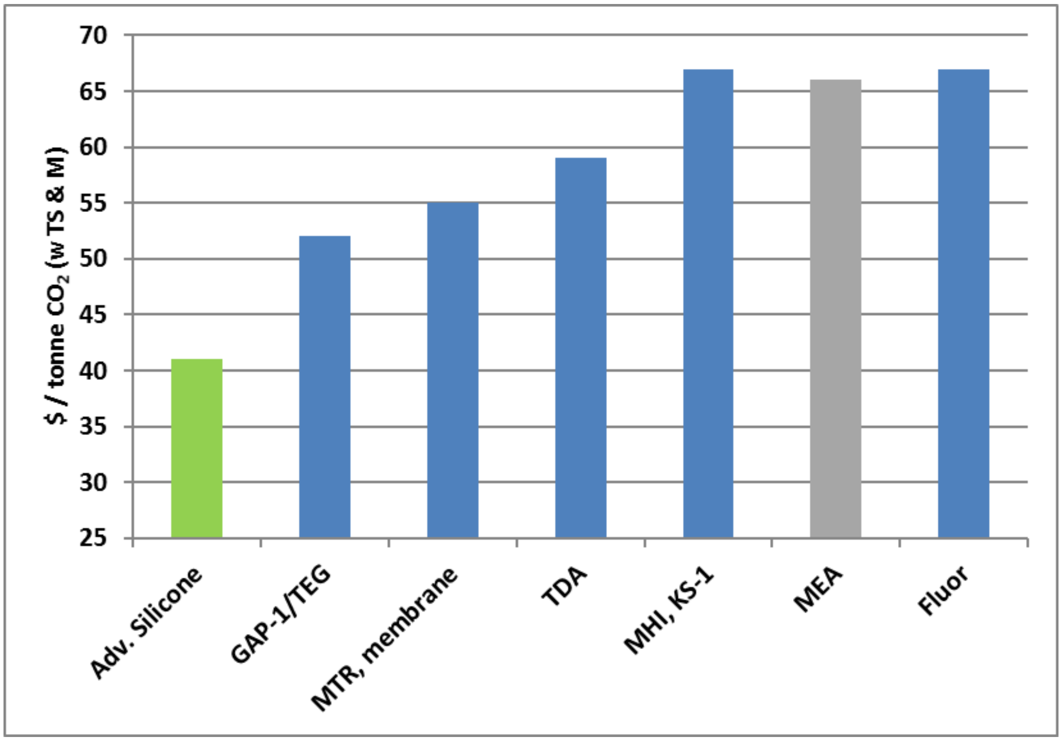


**Figure 53.** Advanced Aminosilicone (Gen 2) vs. Second Generation Capture Technologies. Data for Competitive Technologies from Reference 14. $CO_2$ cost for transportation, sensing & monitoring (TS&M) included.

## 4.12 Conclusions

System and economic analysis for a carbon capture unit which uses GAP-$1_m$ / TEG solvent for $CO_2$ capture in a pulverized coal (PC) boiler demonstrates that the amino-silicone solvent has significant advantages relative to an MEA-based system. An ASPEN process model was developed for the GAP-$1_m$/TEG solvent. Techno-economic analysis developed for a 550 MW supercritical coal plant[1] showed a 20 – 30 % improvements in both CAPEX and $CO_2$ removal cost vs. aqueous amine systems. The 1st year $CO_2$ removal cost for the aminosilicone-based carbon-capture process was evaluated at $52.9/tonne $CO_2$ using the steam stripper column. $CO_2$ cost using the CSTR desorber is dominated by the economics of the solvent make-up. The steam stripper desorber is the preferred unit operation due to a more efficient desorption, and reduced solvent make-up rate.

While the current GAP-$1_m$/TEG technology has many positive attributes, there are areas for improvements to enable its widespread deployment. The advanced amino silicone solvent recently identified in our laboratory is addressing these improvements. It exhibits lower heat of reaction, greater thermal stability, lower viscosity and the ability to remain as a flowable liquid when fully reacted without the need for a co-solvent. Preliminary techno-economic analysis conducted for the advanced aminosilicone solvents demonstrated significant improvements towards reaching the DOE goal of 90% capture rate, with 95% purity, at a cost of electricity of 30% less than MEA for a supercritical PC power plant.

# 5 Solvent Manufacturability and Scale-up Study

## 5.1 Introduction

Identifying a reliable, high quality, cost-acceptable manufacturer of the GAP-$1_m$ aminosilicone being used in GE's process for the post-combustion capture of $CO_2$ from coal-fired power plants is a critical component in the move towards commercialization of this technology. To this end, Wacker Chemie has been a willing participant in supplying GAP-$1_m$ for evaluation. Small scale samples have been shown to be of acceptable quality, but to maintain a high level of confidence in the effectiveness of their aminosilicone, testing at the bench-scale as well as thermal degradation and steam stripping experiments were performed to compare with results obtained after extensive testing of the previously qualified GAP-$1_m$ supplier (GAP-$1_m$ benchmark). 100 kg of GAP-$1_m$ (representative of a full scale manufacturing process) was purchased from Wacker and tested as described below.

## 5.2 Analyses

Evaluation of the large Wacker GAP-$1_m$ sample included NMR and GC analyses as well as titration to determine amine content. $CO_2$ uptake was measured as was thermal degradation and cyclic formation during steam stripping. Finally, the bench-scale skid unit was run under a limited set of conditions to mimic some of those used for the benchmark GAP-$1_m$.

GC analysis of the Wacker sample showed a composition similar to that of the benchmark GAP-$1_m$ material as seen in **Table 35**. While the Wacker solvent was slightly higher in GAP-0 and GAP-$1_m$, both materials were within an acceptable range to give an overall GAP value of approximately 1.0. The Wacker solvent showed only gamma isomers present; none of the beta isomers were detected. The GAP-$1_m$ benchmark values include all beta and gamma isomers.

**Table 35.** GC Analyses (Area %) of GAP-$1_m$ Materials

| **Component** | **Baseline supplier** | **Wacker** |
|---|---|---|
| GAP-0 | 44.5 | 49.1 |
| GAP-1 | 26.1 | 29.1 |
| GAP-2 | 13.8 | 13.0 |
| GAP-3 | 8.0 | 5.3 |
| GAP-4 | 4.6 | 2.3 |
| GAP-5 | 1.7 | 1.0 |
| GAP-6 |  | 0.3 |

Titration of the Wacker sample showed an average GAP-X value of 1.07. This compared favorably with that obtained for the GAP-$1_m$ benchmark material which was 1.05. Again, both were satisfactory values.

$^1$H NMR spectra of the 2 materials (**Figure 54** and **Figure 55**) showed a very large difference. The Wacker aminosilicone was free from the beta-isomer seen at 0.7, 0.9, 2.5 and 2.9 ppm in the benchmark material. Additionally, the amine smell of the Wacker material was greatly reduced from that experienced with benchmark GAP-$1_m$.

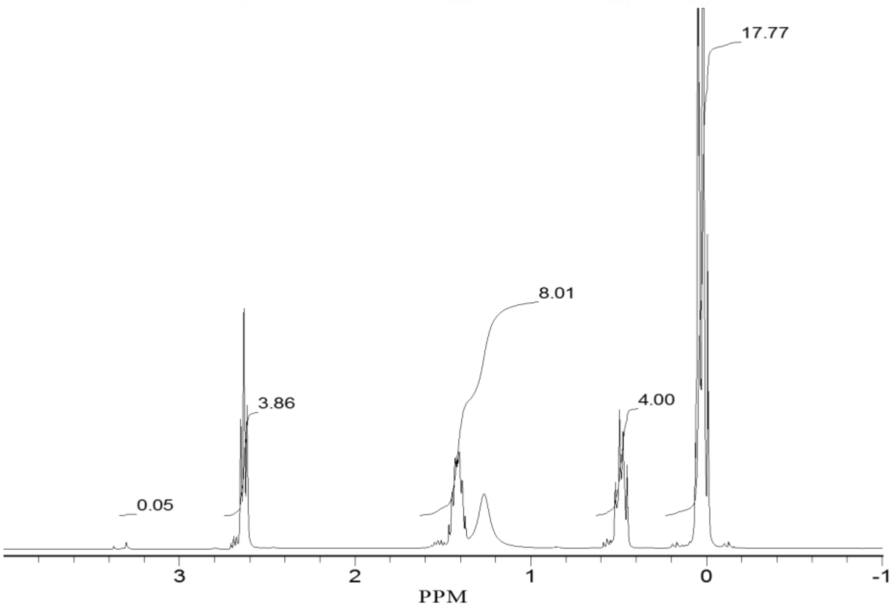


**Figure 54.** $^1$H NMR of Wacker batch SLM 92514 (234308)

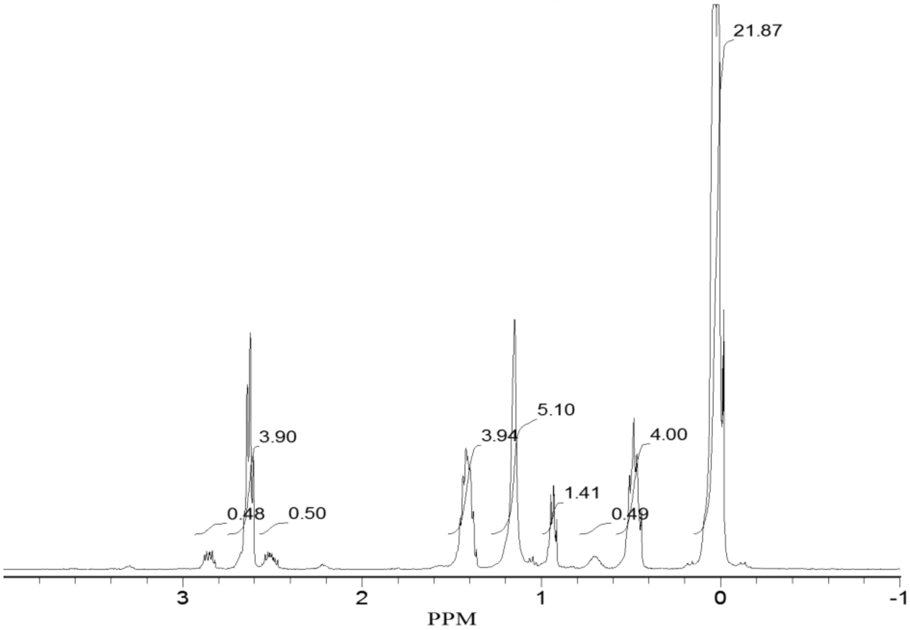


**Figure 55.** $^1$H NMR of Benchmark GAP-$1_m$

Likewise, the $^{13}$C NMR of the Wacker sample (**Figure 56**) was much cleaner than that from benchmark material (**Figure 57**). In addition, no imine, seen at ~64 ppm in the benchmark GAP-$1_m$, was detected.

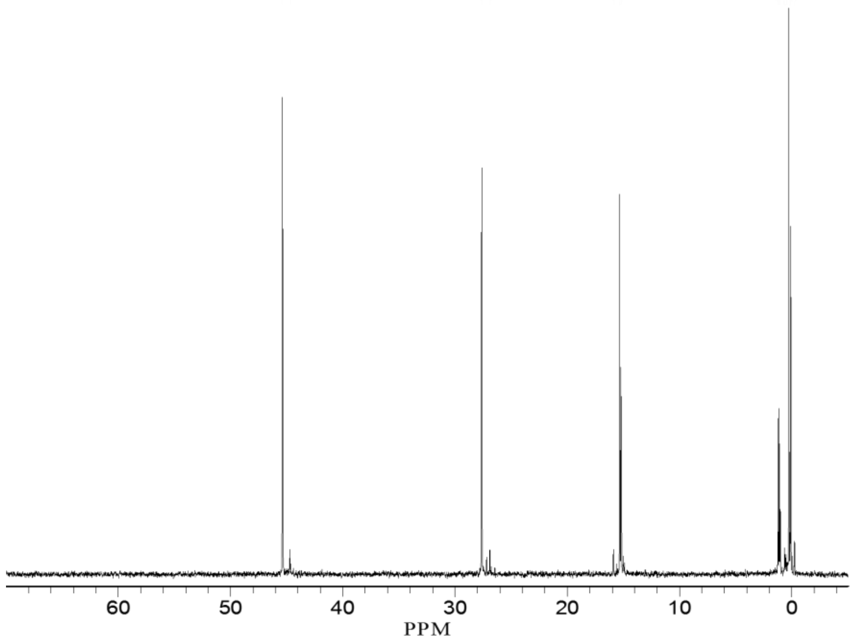


**Figure 56.** $^{13}C\{^1H\}$ NMR of Wacker GAP-$1_m$ (batch SLM 92514 (234308))

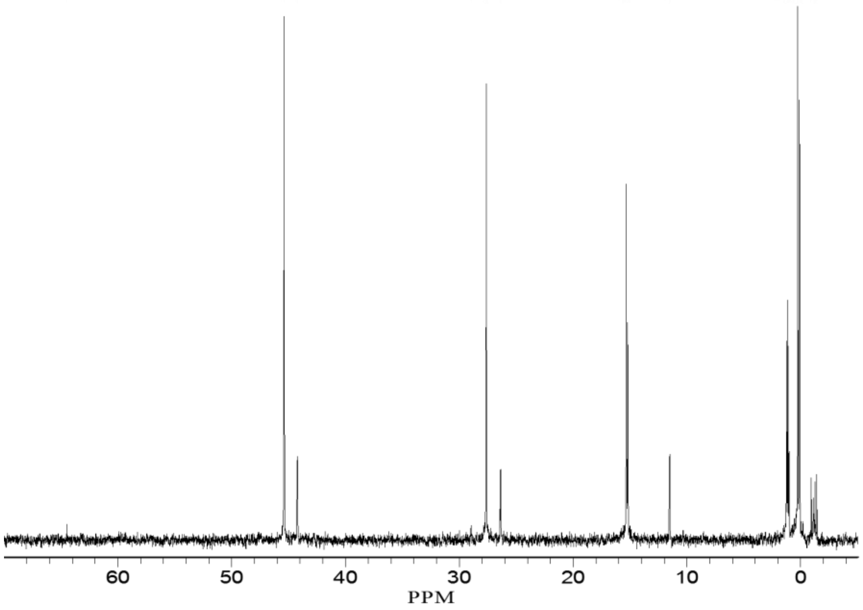


**Figure 57.** $^{13}C\{^1H\}$ NMR of Benchmark GAP-$1_m$.

Finally, the $^{29}Si$ NMR spectrum of Wacker (**Figure 58**) exhibited a few differences from those seen in the benchmark GAP-$1_m$ (**Figure 59**). Resonances at ~ -14 to -15 ppm and 12 ppm in

**Figure 59** are attributed to small amounts of silanol (Si-OH) or methoxysilane (Si-OMe) endcapped material arising from the manufacturing process.

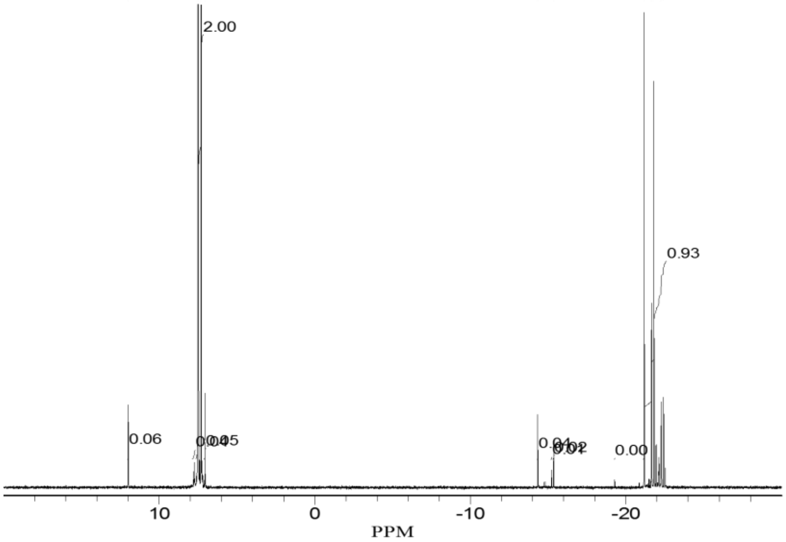


**Figure 58.** $^{29}$Si NMR of Wacker GAP-$1_m$ batch SLM 92514 (234308)

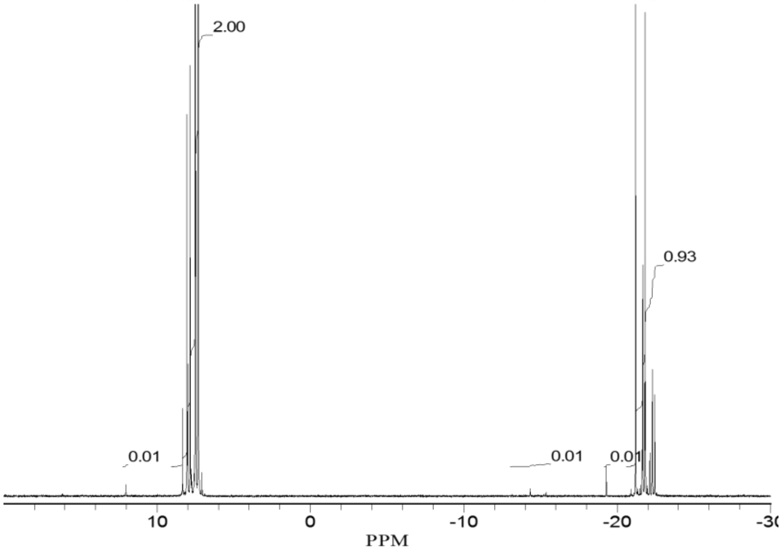


**Figure 59.** $^{29}$Si NMR of benchmark GAP-$1_m$

$CO_2$ uptake experiments (performed on a 60/40 GAP-$1_m$ /TEG mixture) showed a small difference between the two samples, but both were greater than 100% theoretical uptake as shown in **Table 36**.

**Table 36.** Summary of Analyses

| **Supplier** | **GAP-X by $^1H$ NMR** | **GAP-X by $^{29}Si$ NMR** | **GAP-X by titration** | **Beta content** | **$CO_2$ Uptake (wt %)** | **$CO_2$ Uptake (% of theory)*** |
|---|---|---|---|---|---|---|
| Benchmark | 0.95 | 0.93 | 1.05 | 19.0 | 9.1 | 111.1 |
| Wacker | 0.96 | 0.93 | 1.07 | 0 | 8.9 | 109.0 |

*Based on the average GAP-X value from $^1H$, $^{29}Si$ and titration results.

## 5.3 Thermal Degradation

Thermal degradation experiments were performed on 60/40 mixtures of GAP-$1_m$/TEG in small tubular reactors. Factors interrogated were temperature, water content and time. The carbamate concentration remained constant at 100% loading as this provided the worst case conditions for degradation of the carbamate.

Initial experiments were run with a total of 5 g of solvent mixture in the tubes, which were sealed and exposed to 100, 120 and 140 $^oC$ temperatures for up to 22 days. As expected lower temperatures resulted in decreased amine loss relative to the higher temperatures and less urea formation (determined by $^1H$ NMR) as shown in **Table 37, Table 38**, **Figure 60** and **Figure 61**, respectively. The addition of water also suppressed the degradation of the GAP-$1_m$ solvent. These same trends were seen with the GAP-$1_m$ benchmark material.

**Table 37.** **GAP-1$_m$ (Wacker) Thermal Degradation:** % Amine Retention over Time

| 100% Loading | Temp (°C) | Day | | | | | |
|---|---|---|---|---|---|---|---|
| | | 0 | 1 | 2 | 4 | 7 | 22 |
| **0% water** | 100 | 96.3 | | 96.3 | 95.5 | 95.5 | 91.25 |
| | 120 | 96.3 | | 95.8 | 92.8 | 89.5 | 76.75 |
| | 140 | 96.3 | 85 | 76.3 | 62.5 | 49 | 24 |
| **5% water** | 100 | 96.3 | | 95.8 | 95.3 | 95.3 | 92.5 |
| | 120 | 96.3 | | 94.5 | 93.5 | 91.3 | 81.75 |
| | 140 | 96.3 | 90 | 81.8 | 69.5 | 59 | 37.75 |

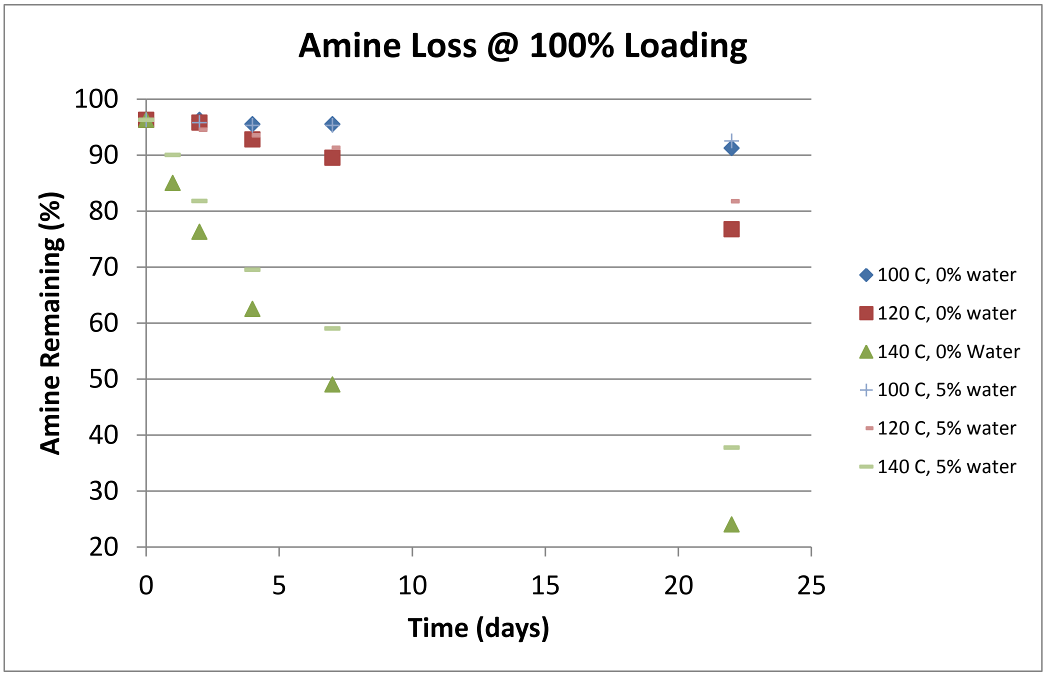


**Figure 60.** **GAP-1$_m$ (Wacker) Thermal Degradation:** Loss of GAP-1$_m$ over time

**Table 38.** **GAP-1$_m$ (Wacker) Thermal Degradation:** % Urea Formation over Time

| 100% Loading | Temp (°C) | Day | | | | | |
|---|---|---|---|---|---|---|---|
| | | 0 | 1 | 2 | 4 | 7 | 22 |
| **0% water** | 100 | 0 | | 0 | 1 | 1.3 | 4 |
| | 120 | 0 | | 2.5 | 4 | 6.8 | 18.5 |
| | 140 | 0 | 10.3 | 19.8 | 34 | 47.3 | 70.75 |
| **5% water** | 100 | 0 | | 0 | 0.5 | 0.8 | 2.5 |
| | 120 | 0 | | 1.8 | 3 | 4.5 | 12.75 |
| | 140 | 0 | 5.8 | 14.5 | 27.3 | 37 | 57.75 |

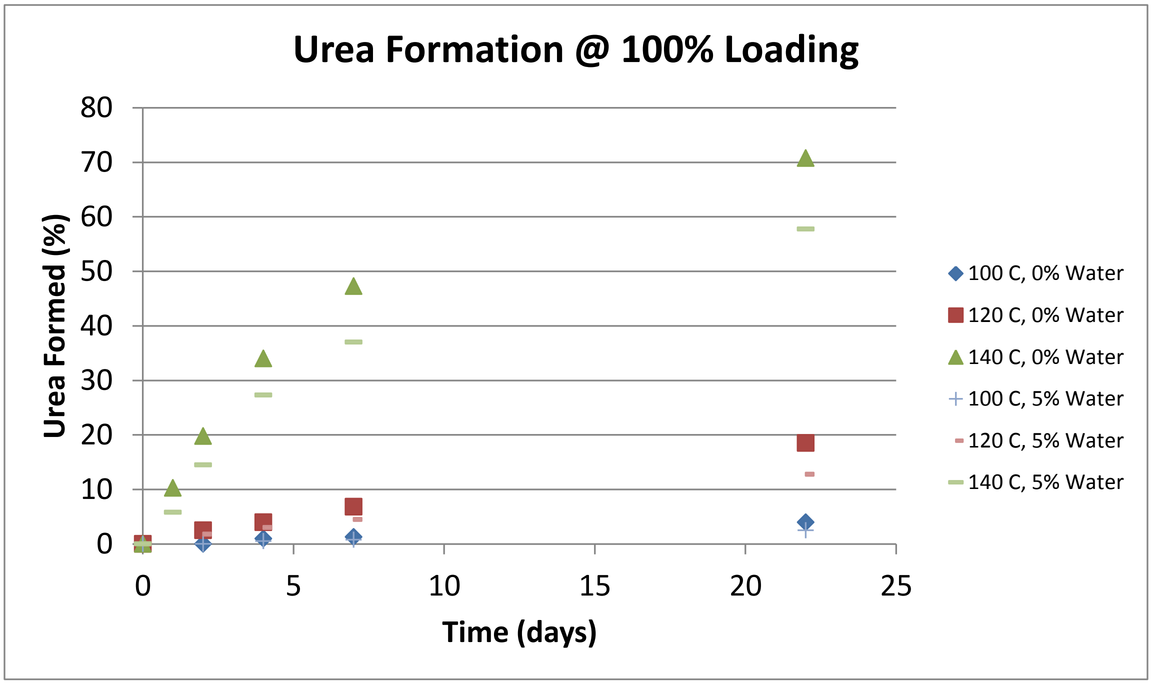


**Figure 61.** **GAP-1$_m$ (Wacker) Thermal Degradation:** % Urea Formation over time

Wacker GAP-$1_m$ was then compared to the benchmark solvent at 100% carbamate loading and 140 °C. **Table 39** and **Table 40** summarize these results indicating that the Wacker solvent is similar to the benchmark material with regards to thermal degradation to form urea.

**Table 39. Thermal Degradation (GAP-$1_m$ (Wacker) vs. Benchmark):** Amine Loss

| **Material** | **Water** | **Day** | | | | |
|---|---|---|---|---|---|---|
| | wt. % | **0** | **1** | **2** | **4** | **7** |
| Benchmark | 0 | 96 | 85.3 | 68 | 52.3 | 40.8 |
| Wacker | 0 | 96 | 85 | 76.3 | 62.5 | 49 |
| Benchmark | 5 | 96 | 89.8 | 79.3 | 67.8 | 57.3 |
| Wacker | 5 | 96 | 90 | 81.8 | 69.5 | 59 |

**Table 40. Thermal Degradation (GAP-$1_m$ (Wacker) vs. Benchmark):** Urea formation

| **Material** | **Water** | **Day** | | | | |
|---|---|---|---|---|---|---|
| | Wt.% | **0** | **1** | **2** | **4** | **7** |
| Benchmark | 0 | 0 | 12.8 | 30 | 45.5 | 57.3 |
| Wacker | 0 | 0 | 10.3 | 19.8 | 34 | 47.3 |
| Benchmark | 5 | 0 | 8.3 | 19.5 | 29.3 | 41 |
| Wacker | 5 | 0 | 5.8 | 14.5 | 27.3 | 37 |

## 5.4 Metals Analyses

To determine if trace metals remained in the samples, inductively coupled plasma-optical emission spectroscopy (ICP-OES) was used**. Table 41** shows that, to the limits of detection, the samples were metal free. This held for both the Wacker and benchmark materials. Additional analyses for Pd, Pt, Rh, Ir and Ru were also negative (<10 ppm).

**Table 41. Metal Analysis by ICP-OES:** Wacker vs. Benchmark

| *Material* | Sample | Ag | Al | As | B | Ba | Be | Ca* | Co | Cr | Cu | Fe* | K | Li | Mg | Mn |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Benchmark | 1 | x<1 | x<1 | x<5 | x<2 | x<1 | x<1 | x<5 | x<1 | x<2 | x<2 | x<2 | x<10 | x<1 | x<1 | x<1 |
|  | 2 | x<1 | x<1 | x<5 | x<2 | x<1 | x<1 | x<5 | x<1 | x<2 | x<2 | x<2 | x<10 | x<1 | x<1 | x<1 |
|  | 3 | x<1 | x<1 | x<5 | x<2 | x<1 | x<1 | x<5 | x<1 | x<2 | x<2 | x<2 | x<10 | x<1 | x<1 | x<1 |
| Wacker | 1 | x<1 | x<1 | x<5 | x<2 | x<1 | x<1 | x<5 | x<1 | x<2 | x<2 | x<2 | x<10 | x<1 | x<1 | x<1 |
|  | 2 | x<1 | x<1 | x<5 | x<2 | x<1 | x<1 | x<5 | x<1 | x<2 | x<2 | x<2 | x<10 | x<1 | x<1 | x<1 |
|  | 3 | x<1 | x<1 | x<5 | x<2 | x<1 | x<1 | x<5 | x<1 | x<2 | x<2 | x<2 | x<10 | x<1 | x<1 | x<1 |

| *Material* | Sample | Mo | Na | Ni | P | Pb | S | Se | Sr | Ti | V | W | Zn | Zr |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Benchmark | 1 | x<2 | x<5 | x<1 | x<5 | x<5 | x<5 | x<5 | x<1 | x<1 | x<1 | x<2 | x<1 | x<1 |
|  | 2 | x<2 | x<5 | x<1 | x<5 | x<5 | x<5 | x<5 | x<1 | x<1 | x<1 | x<2 | x<1 | x<1 |
|  | 3 | x<2 | x<5 | x<1 | x<5 | x<5 | x<5 | x<5 | x<1 | x<1 | x<1 | x<2 | x<1 | x<1 |
| Wacker | 1 | x<2 | x<5 | x<1 | x<5 | x<5 | x<5 | x<5 | x<1 | x<1 | x<1 | x<2 | x<1 | x<1 |
|  | 2 | x<2 | x<5 | x<1 | x<5 | x<5 | x<5 | x<5 | x<1 | x<1 | x<1 | x<2 | x<1 | x<1 |
|  | 3 | x<2 | x<5 | x<1 | x<5 | x<5 | x<5 | x<5 | x<1 | x<1 | x<1 | x<2 | x<1 | x<1 |

Results in ppm (ug/g). *Raised detection limits due to trace contamination of the microwave vessels.

## 5.5 Hydrothermal Stability

Hydrothermal stability experiments have been performed in a lab-scale stripping column (Autocol, Pope, 1") for both benchmark and Wacker GAP-$1_m$ materials (fresh, lean). **Figure 62** shows a picture of the experimental set-up. **Table 42** lists column specifications.

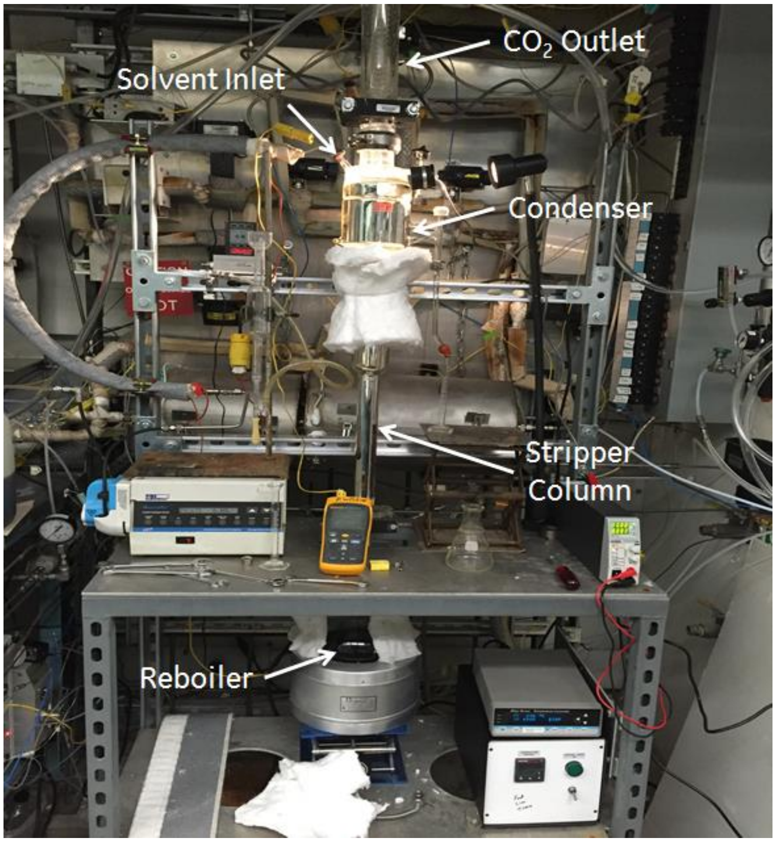


**Figure 62.** **Hydrothermal Stability:** Lab-scale stripping column

**Table 42.** **Hydrothermal Stability:** Column Specification (AUTOCPL, Pope)

| | |
|---|---|
| Column Diameter | 1" |
| Boiling Flask Size | 5 liters |
| No Theoretical Plates | 15 |
| Column Height | 24 inches |
| Packing Material | Perforated 316 SS |
| Cooling Water | 0.3 gal/min |
| Column Pressure | 2 Psig |

During the hydrothermal stability testing, it became apparent that the composition of the GAP-$1_m$ solvent was changing. As shown in **Figure 63** , re-equilibration can occur with the GAP-$1_m$ solvents with or without the presence of water and is accelerated by elevated temperatures. The primary amine functionality in the GAP-$1_m$ solvent is sufficient to catalyze this reaction. This re-equilibration reaction produces cyclic silicone compounds (known as $D_3$, $D_4$,$D_5$, etc.) and linear species with shorter average change lengths commensurate with the amount of cyclics formed. At equilibrium, this ratio is typically on the order of 15:85 molar ratio of cyclics: linears.

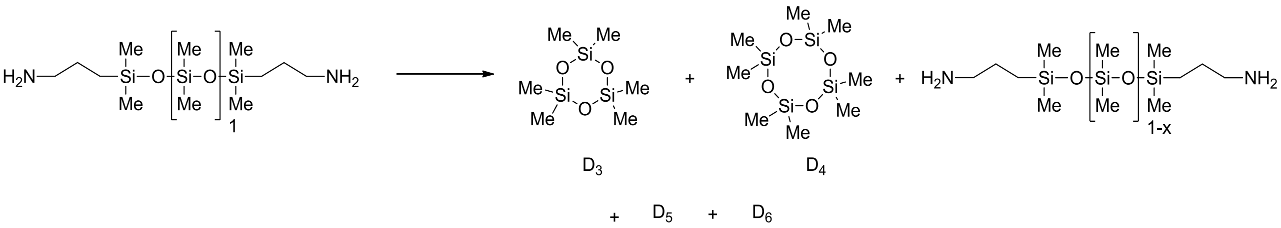


**Figure 63.** **GAP-$1_m$ Hydrothermal Stability:** Equilibration Reaction

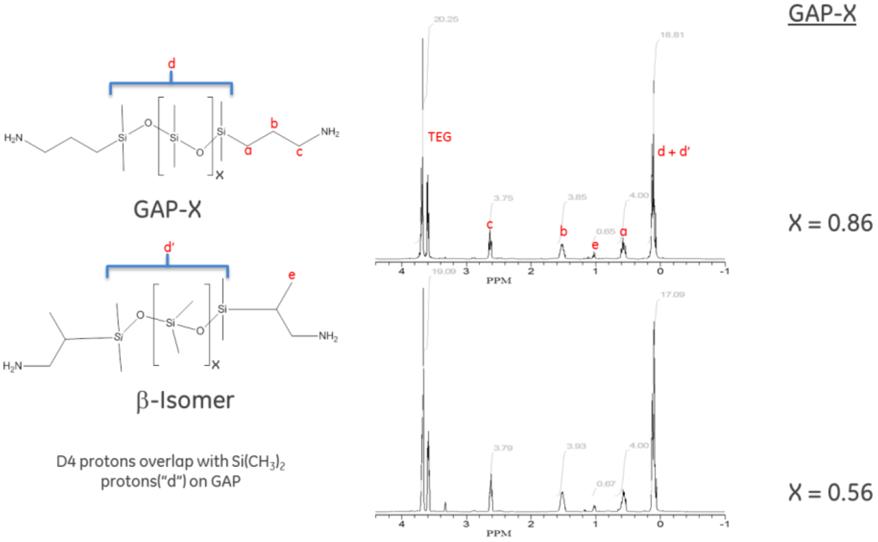
### 5.5.1 Experimental Conditions

600 mL of lean working solution (55 wt. % GAP-$1_m$, 45 wt. % TEG and 10 wt. % $H_2O$) was placed in a 1 L boiling flask and heated at the working temperature of 120 °C. Water (DI, 70 °C, 1 ml/min) was delivered using a MasterFlex pump into the top of the column. The condensate was removed from the column directly above the reboiler for analysis ($^1H$ NMR). During the run, the condensate generated is continuously collected on the top of the column, and the liquid samples were analyzed by $^1H$ NMR to evaluate GAP number.

### 5.5.2 GAP-X Number Calculations

Determination of the GAP-X number was a facile way to monitor this re-equilibration reaction. GAP-X numbers derived from both $^1H$ NMR and $^{29}Si$ NMR were used to evaluate hydrothermal stability of the aminosilicone solvent.

GAP-X numbers from $^1H$ NMR were calculated from the ratio of **d** to **a** protons after subtracting out the contribution of β-isomer by using **e** protons from the $^1H$ NMR analysis as shown in **Figure 64**.



D4 protons overlap with $Si(CH_3)_2$ protons("d") on GAP

**Figure 64. Hydrothermal Stability:** $^1H$ NMR Calculations for GAP-X number

Similarly, using $^{29}$Si NMR, the GAP-X numbers were calculated using the following expression:

$$\text{GAP-X} = (2/\text{Integral M'})*\text{Integral D}$$

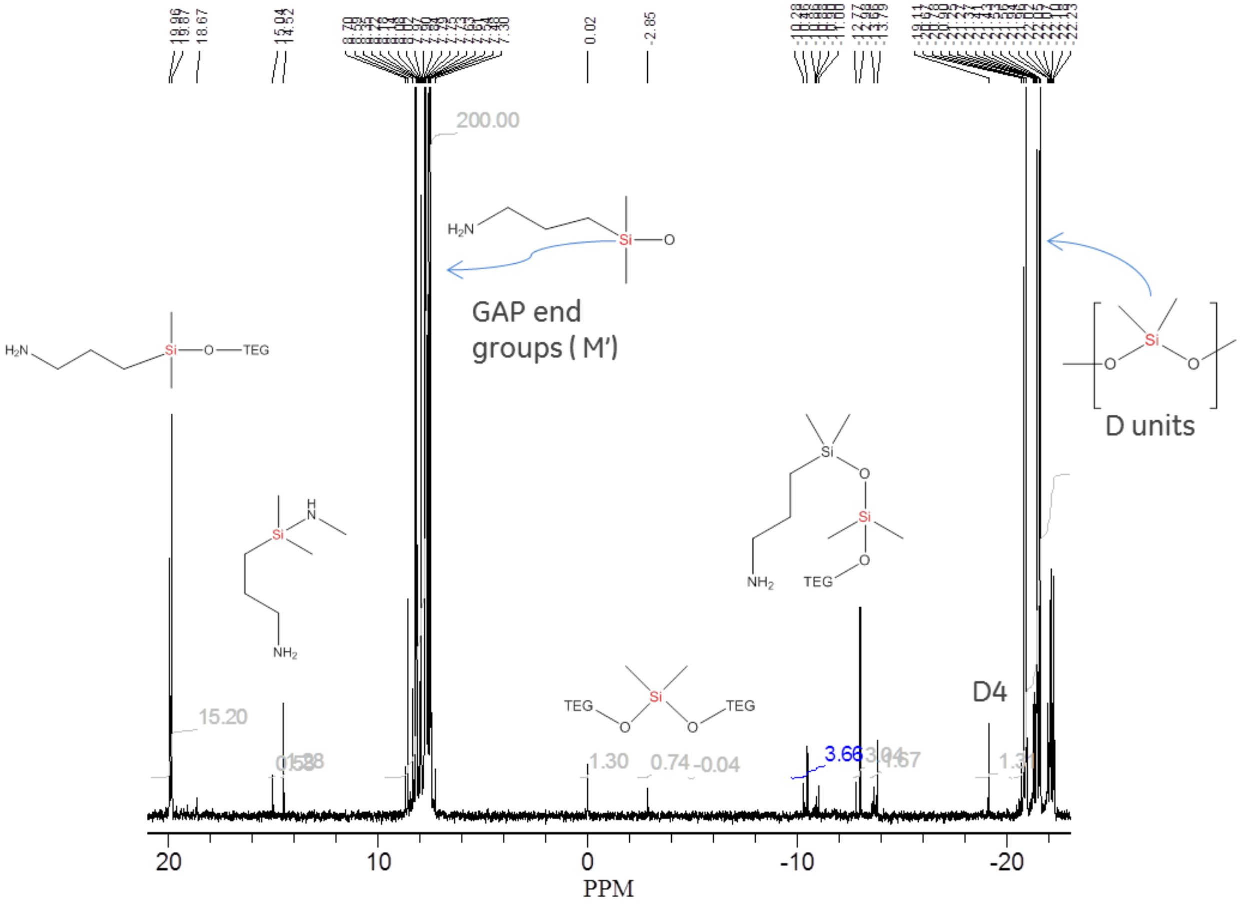


**Figure 65.** **Hydrothermal Stability:** $^{29}$Si NMR Calculations for GAP-X number

GAP-X can be distinguished from $D_4$ only by $^{29}$Si NMR as the protons in the D units in GAP-1 and $D_4$ are overlapping in $^1$H NMR. GAP numbers calculated from both $^1$H NMR and $^{29}$Si NMR measurements were compared for several $D_4$ containing GAP-X samples to evaluate the validity of the $^1$H NMR analysis. As shown in **Figure 66** and **Table 43**, good correlations were obtained between the two NMR methods. The concentration of $D_4$ in the mixtures was less than 0.3 wt %. It is expected that the $^1H$ NMR will not yield a reliable GAP # for GAP-X/$D_4$ mixtures with higher concentrations of $D_4$. As the current studies did not produce GAP-X/$D_4$ mixtures with $D_4$ concentrations higher than 0.5 wt. %, we used $^1H$ NMR as a means to calculate GAP-X number and quantify hydrothermal stability.

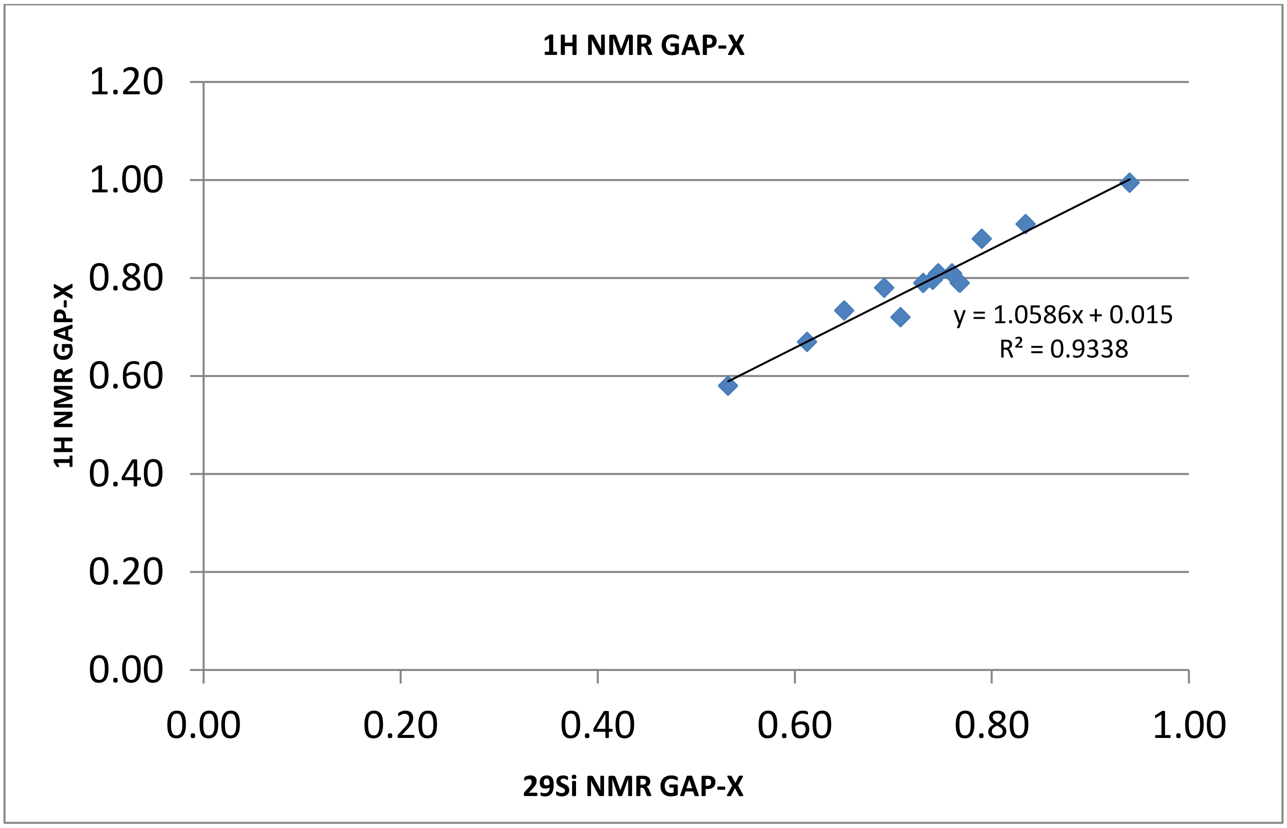
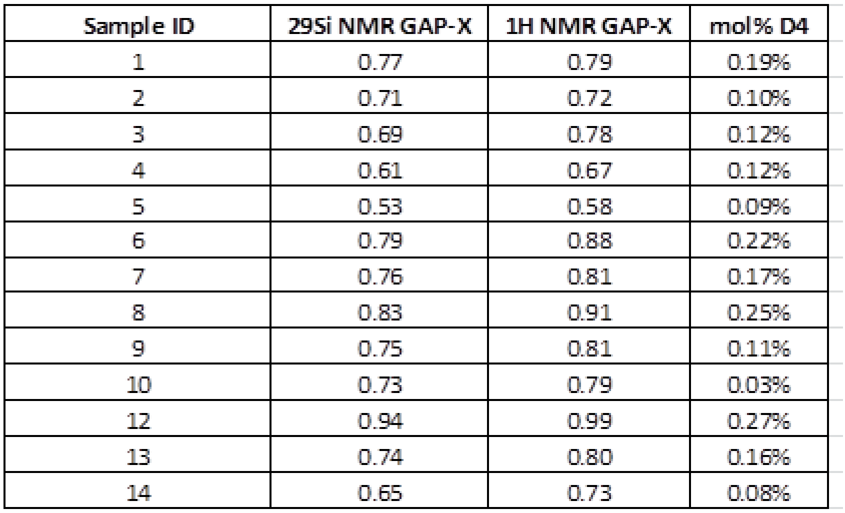


**Figure 66.** **GAP-X Number Calculations:** $^1H$ NMR vs. $^{29}Si$ NMR.

**Table 43. GAP-X Number Calculations for GAP-X /$D_4$ mixtures.**$^{29}$Si NMR vs. $^{1}$H NMR



| Sample ID | 29Si NMR GAP-X | 1H NMR GAP-X | mol% D4 |
|---|---|---|---|
| 1 | 0.77 | 0.79 | 0.19% |
| 2 | 0.71 | 0.72 | 0.10% |
| 3 | 0.69 | 0.78 | 0.12% |
| 4 | 0.61 | 0.67 | 0.12% |
| 5 | 0.53 | 0.58 | 0.09% |
| 6 | 0.79 | 0.88 | 0.22% |
| 7 | 0.76 | 0.81 | 0.17% |
| 8 | 0.83 | 0.91 | 0.25% |
| 9 | 0.75 | 0.81 | 0.11% |
| 10 | 0.73 | 0.79 | 0.03% |
| 12 | 0.94 | 0.99 | 0.27% |
| 13 | 0.74 | 0.80 | 0.16% |
| 14 | 0.65 | 0.73 | 0.08% |

### 5.5.3 Hydrothermal Stability: Wacker vs. Baseline GAP-$1_m$/TEG Materials

Hydrothermal stability tests were performed for both Wacker and baseline materials at 120 °C reboiler temperature. GAP-X numbers (determined based on $^{1}$H NMR) of the samples collected at the bottom of the stripper column were calculated based on $^{1}$H NMR following the methodology described above. The aminosilicone solvent was thermally equilibrated for 6 hours at 120 °C. This was done to mimic what happens in the real system in which the amine groups on the aminosilicone solvent catalyze the re-equilibration of the siloxane (Si-O-Si) linkages in the solvent to generate a mixture of cyclic and linear components in an approximate ratio of 15:85. The experimental apparatus used to test the hydrothermal stability is shown in **Figure 62.** The reboiler (pot) temperature was held at 120 °C with the top of the condenser column maintaining ~95 °C. Water was continuously added at ~ 1 mL/min to the lean solution. Temperature profiles of the reboiler and the top of the column are shown in **Figure 67**.

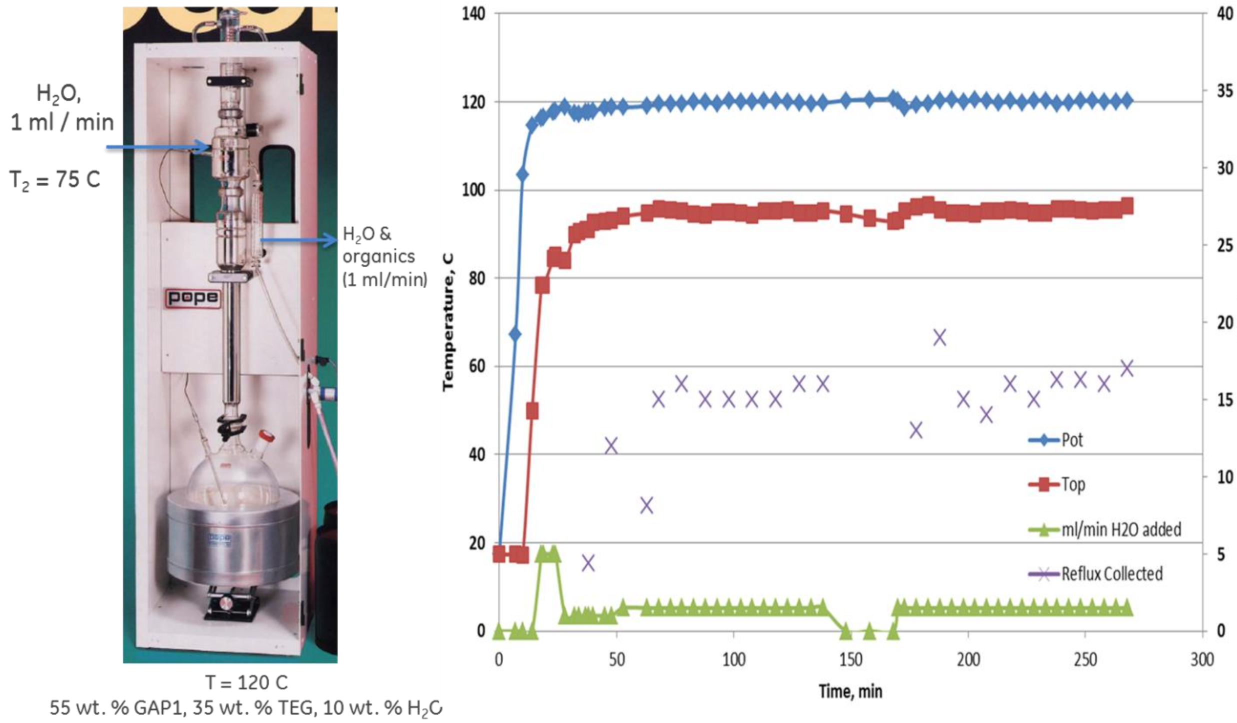


**Figure 67.** **Hydrothermal Stability:** Testing Apparatus and Data Profiles for GAP-1/TEG (Wacker)

If the volatile cyclic compounds are removed by distillation, this results in an overall shift in the GAP number from ~1.0 to a value approaching 0.5-0.6, if enough time is allowed. In these experiments, 6 hours resulted in a shift to ~GAP-0.8 as shown in **Figure 68**. Over the same period, the decrease in GAP-# is the same as that seen for the baseline solvent sample. As most of the hydrothermal degradation of the Wacker material occurs in the first 24 h of the water exposure, it is recommended to start with a material having GAP-X ~ 0.5.

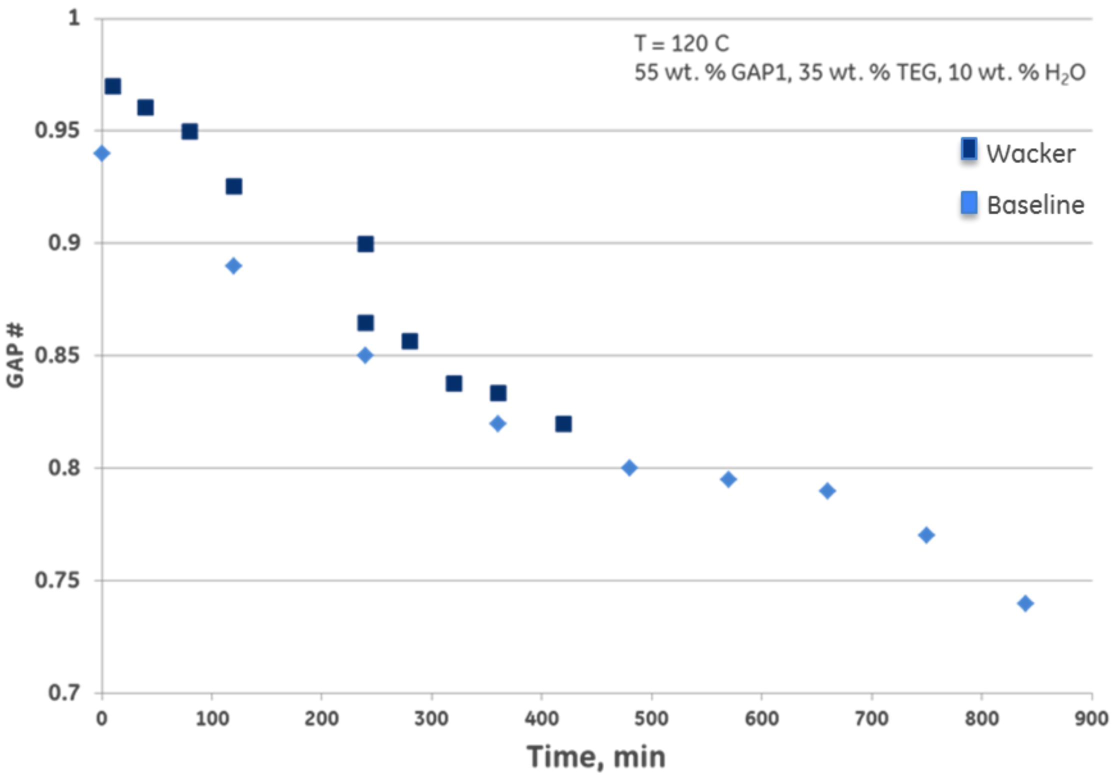


**Figure 68.** **GAP Numbers = f (time)** for Wacker and baseline solvent samples
55 wt. % GAP-1, 35 wt. % TEG, 10 wt. % $H_2O$; $T_{reboiler}$ = 120 °C; GAP Numbers calculated based on $^1H$ NMR of liquid samples collected at the bottom of stripping column.

### 5.5.4 Steam stripping performance of GAP-$1_m$ (Wacker)

The performance of the steam stripper column with Wacker GAP-$1_m$ / TEG solvent was determined by feeding a heated, rich solution of GAP-$1_m$ carbamate (55 wt. % carbamate, 35 wt. % TEG, 10 wt. % water) to the top of the steam stripper column. The reboiler was filled with lean working solution (600 mL, 55% wt. GAP-$1_m$, 35% wt. TEG, 10% wt. $H_2O$), and the temperature was set at 120 °C. **Table 44** lists the experimental conditions.

**Table 44.** **GAP-$1_m$ (Wacker)/TEG:** Steam Stripping Experimental Conditions

| | |
|---|---|
| Rich Solvent composition | 55 % wt. GAP-1m<br>10 % wt. $H_2O$<br>35 % TEG |
| Rich Solvent Slurry flowrate | 10 ml/min |
| Rich solvent , T | 75 $^{o}$C |
| Re-Boiler T | 120 $^{o}$C |
| Reboiler volume | 600 mL |
| Re-boiler composition | 55% wt. GAP-$1_m$<br>10% wt. $H_2O$<br>35% wt. TEG |
| Column Pressure | ~ 2 Psig |

Column performance was measured based on the $CO_2$ yield and $CO_2$ selectivity according to the equations below.

$$\text{CO}_2\ \text{Yield}_{\text{Column}} = \frac{\%\,\text{Rich}_{\text{column lean out (IR)}}}{\%\,\text{Rich}_{\text{rich in}\,(IR)}}$$

$$\text{Column Selectivity} = \frac{\text{CO}_2\ \text{Yield}_{\text{column}}}{\text{CO}_2\ \text{Yield}_{\text{total}}}$$

**Figure 69** illustrates where samples were taken.

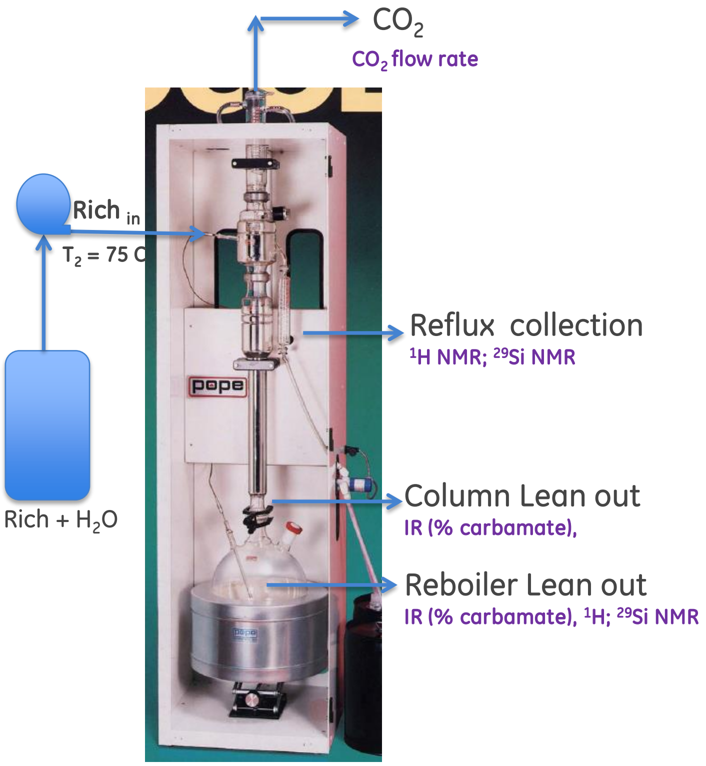


**Figure 69.** Sample points for column performance

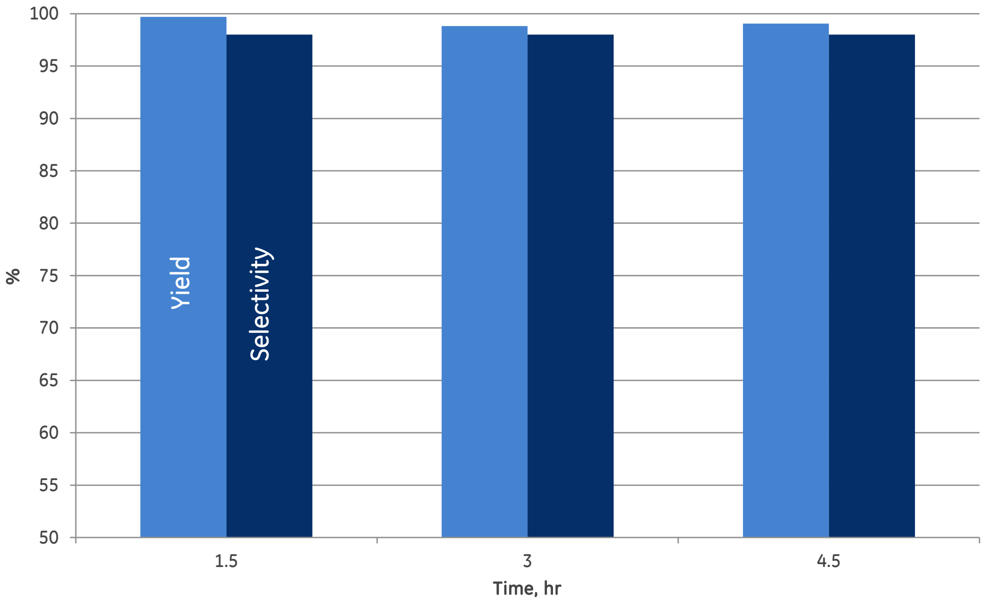


**Figure 70.** **Stripper Column Performance over time**
Reboiler: T = 120 °C, Lean solvent: 55 wt. % GAP-$1_m$, 35 wt. % TEG, 10 wt. % $H_2O$; Rich Solvent: 100 wt. % carbamate; 10 ml/min rich solvent.

**Figure 70** shows that, under these conditions, excellent yield and selectivity were achieved with the stripper column. Even though the column temperature is below 100 °C (column at atmospheric pressure), 90% of the $CO_2$ fed into the column with the rich solvent is desorbed. This is significantly higher than can be achieved at the same temperature with a CSTR. Because the solvent becomes progressive leaner as it flows down to the hotter regions of the column, the stripper column design ensures that only the leanest solvent contacts the highest temperatures. This decreases the rate of thermal degradation. Additionally, because the driving force for $CO_2$ desorption is increased by the presence of the steam, a lower maximum temperature is possible while achieving efficient removal of $CO_2$. Similar performance was observed in earlier experiments with the benchmark material.

## 5.6 Oxidative Stability

It is well established that ammonia production in aqueous amine solvents is indicative of oxidative degradation of these $CO_2$ capture solvents. Most research to-date has been focused on MEA, and **Figure 71** suggests one pathway, catalyzed by $Fe^{+3}$ or other radical sources, that leads to the formation of this volatile by-product.

Mass spectral analysis of head space samples in early experiments showed ammonia was also present in thermally treated GAP-$1_m$ samples. To provide quantitative data on ammonia generation, an FT-IR spectrometer was installed on the $CO_2$ capture skid at the top of the absorber unit. A heated line ensured that condensation of volatile products did not occur (**Figure 72**).

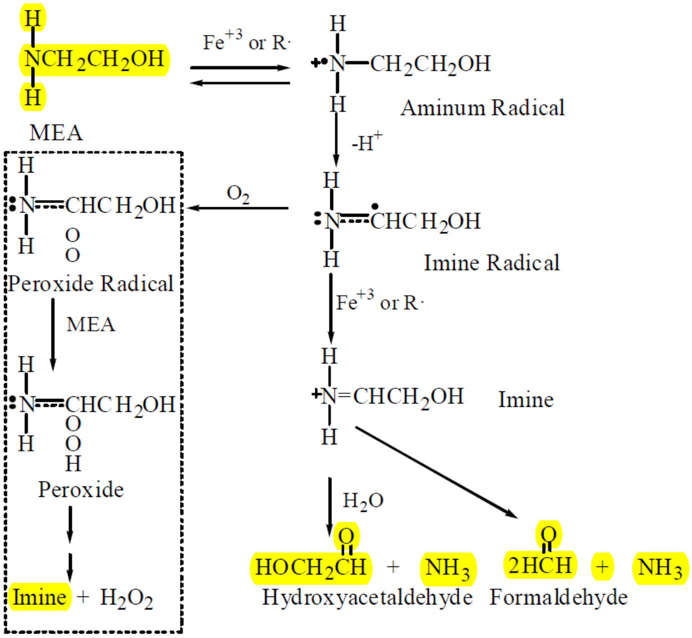
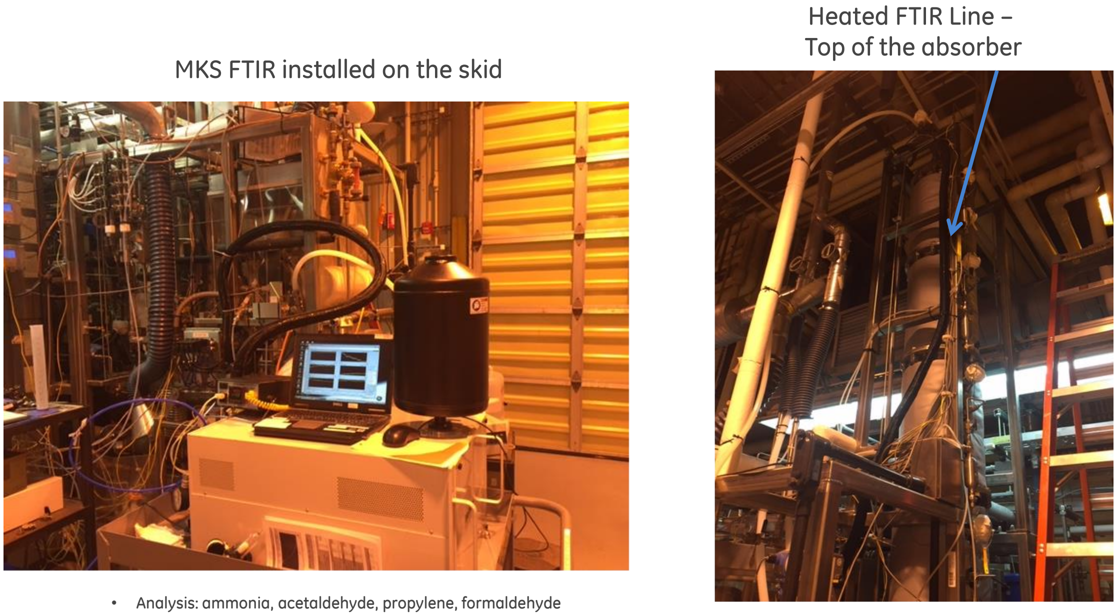


**Figure 71.** Proposed oxidative decomposition path to ammonia formation from aqueous MEA.[15]



- Analysis: ammonia, acetaldehyde, propylene, formaldehyde

- Heated transfer line at 190 C

**Figure 72.** **$CO_2$ Capture Bench Scale (0.2 kW skid):** FTIR Components Installation

Prior to collecting data from the skid, baseline experiments were performed in a 400 mL, windowed Parr reactor with mechanical agitation. The desired gas ($N_2$ or air) was introduced below the solvent surface of the 60/40 wt % mixture of GAP-$1_m$/TEG via a dip tube, and the temperature was controlled via an internal heating coil. Purging the virgin Wacker GAP-$1_m$ solvent at 50 °C with $N_2$ showed a large spike in ammonia concentration as seen in **Figure 73**. However, this rapidly dissipated and was likely due to ammonia already dissolved in the solvent from the manufacturing process or some degradation that occurred during shipping and storage. After 30 minutes, no ammonia was detected. Then the solvent was exposed to air for 100 minutes. No detectable ammonia, acetaldehyde or formaldehyde was seen. This procedure was followed by another $N_2$ purge that indicated no ammonia was present. This baseline experiment showed that, at absorber temperatures of 50 °C and 1 bar pressure, ammonia was not generated. This also showed that ammonia and GAP-$1_m$ signals did not overlap in the IR spectra.

The oxidative activity of GAP-$1_m$ / TEG (Wacker), baseline GAP-$1_m$/TEG and aqueous MEA (Aldrich) was evaluated by feeding air (1 SLM) into lean working solution (100 mL), under vigorous mixing, at 50 °C while dosing soluble Fe(2+) salts (0.5 to 2.5 mM). The ammonia concentration in the gas phase was measured by FTIR. Ammonia profiles (gas phase, FTIR) for $N_2$ baseline, air baseline and Fe (2+) doping are shown in **Figure 73** - **Figure 76**. Data are also summarized in **Table 45**. Wacker-produced material exhibits one order of magnitude lower ammonia generation than the corresponding baseline GAP-$1_m$ batch. Spiking of $Fe^{+2}$ salts was performed to simulate the conditions of an aged solvent containing corrosion impurities. Both GAP-$1_m$ batches showed no increase in ammonia generation upon $Fe(OAc)_2$ spiking (up to 2.5 mM). Contrary to the results obtained with GAP-$1_m$, ammonia generation for an aqueous MEA solution increased by more than 50 % upon addition of $Fe(OAc)_2$ (2.5 mM).

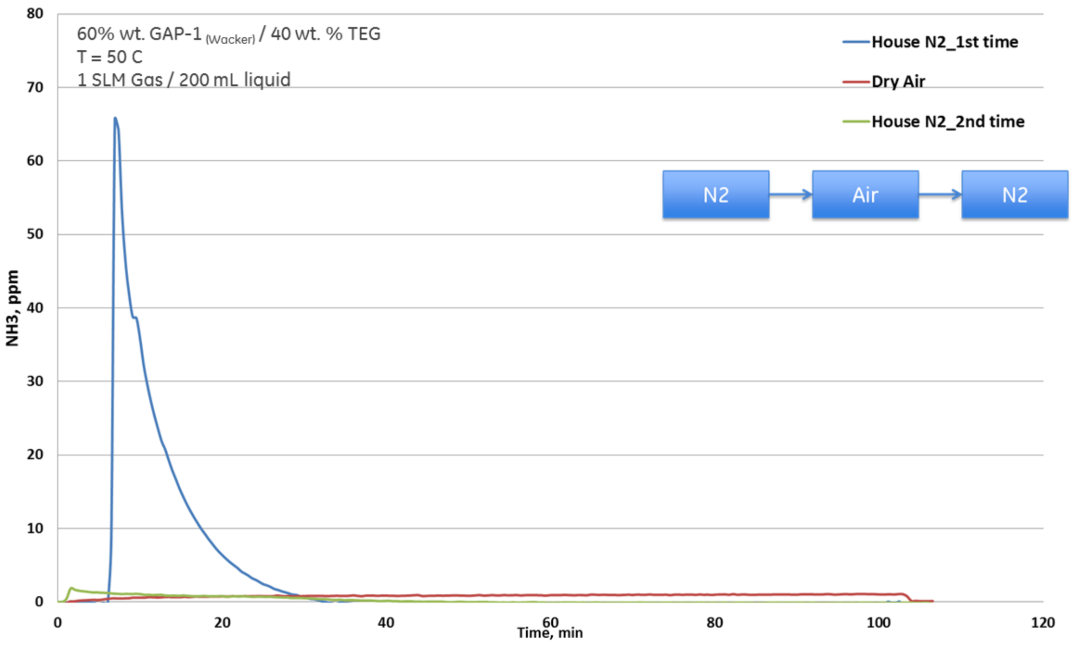


**Figure 73.** Calibration of FTIR (MKS) for measuring $NH_3$ evolution in oxidation of GAP-$1_m$ / TEG (Wacker)

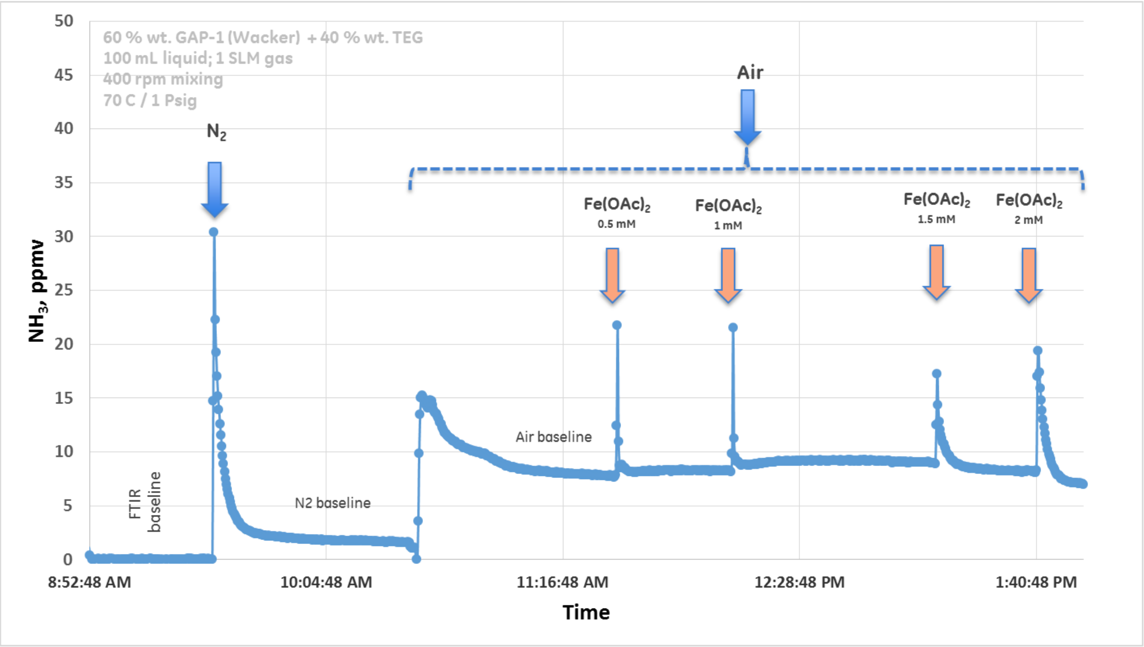


**Figure 74.** **Ammonia Generation for GAP-$1_m$ (Wacker) / TEG**: $N_2$ baseline, Air baseline, and Air + $Fe(OAc)_2$ doped. Fresh / lean solvent

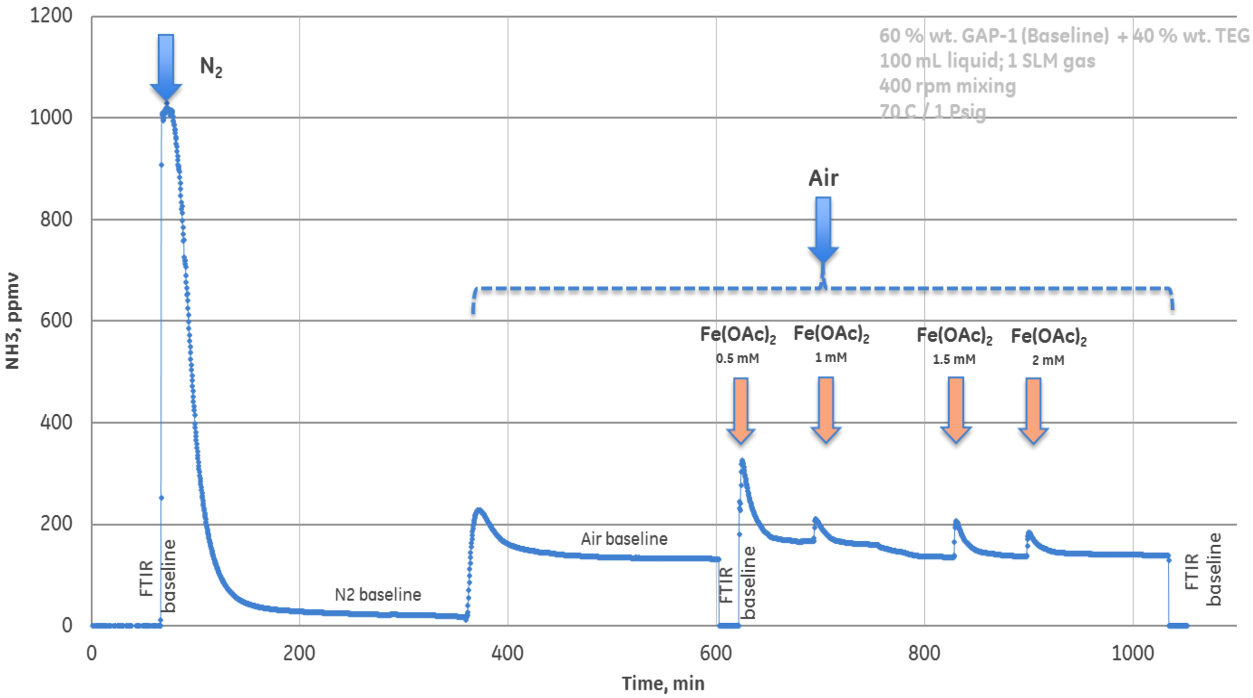


**Figure 75.** **Ammonia Generation for GAP-$1_m$ (Baseline) / TEG:** $N_2$ baseline, Air baseline, and Air + $Fe(OAc)_2$ doped. Fresh / lean solvent

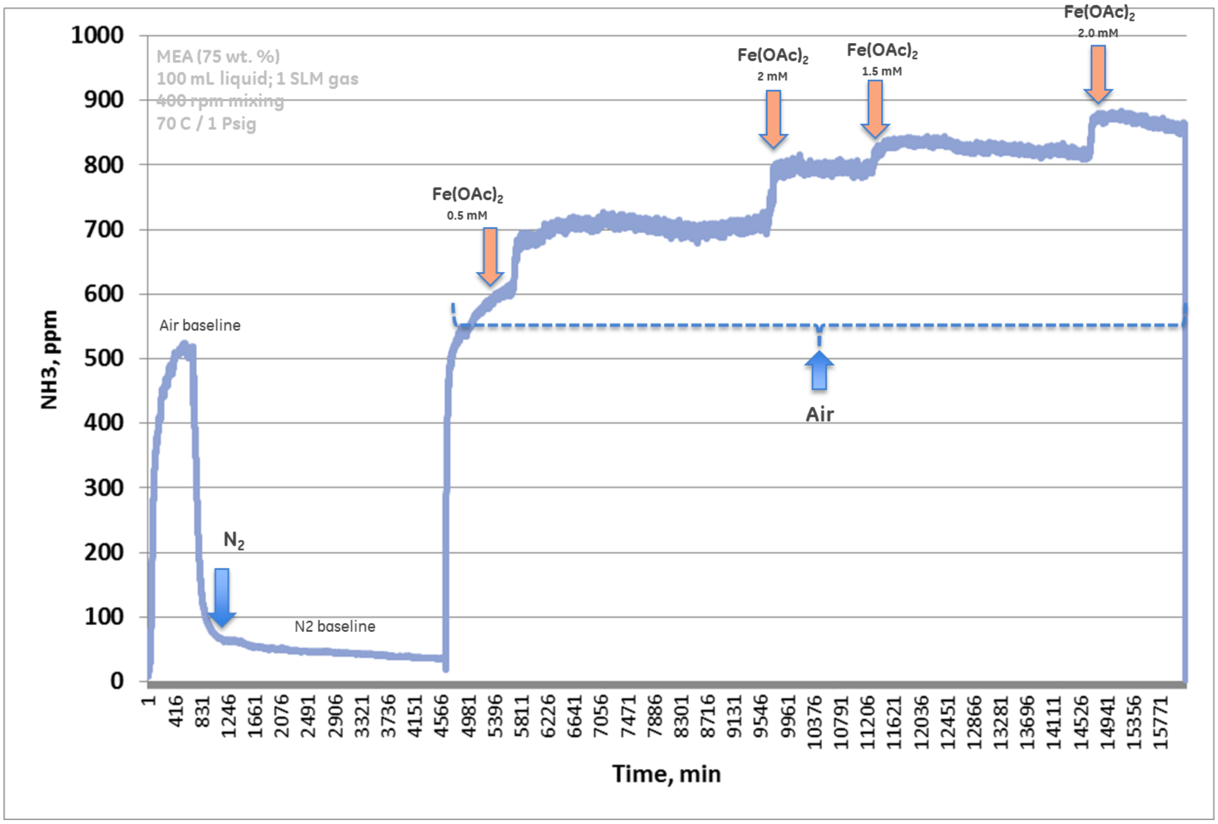


**Figure 76.** **Ammonia Generation for MEA:** $N_2$ baseline, Air baseline, and Air + $Fe(OAc)_2$ doped. Fresh / lean solvent

**Table 45.** **Ammonia Generation for 60 wt. % GAP-$1_m$/ 40 wt. % TEG:** Wacker vs. Baseline vs vs. MEA (75 wt. %)

| | Baseline GAP-$1_m$ | | | Wacker GAP-$1_m$ | | | MEA (75 wt.%) | | |
|---|---|---|---|---|---|---|---|---|---|
| | $NH_3$ ppmv | | $NH_3$, mol/min 10^4 | $NH_3$ ppmv | | $NH_3$ mol/min * 10^4 | $NH_3$ ppmv | | $NH_3$ mol/min 10^4 |
| | Av. | Max | Avg. | Av. | Max | Avg. | | | |
| Baseline, FTIR | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| N2, initial | 3 | 1005 | 0.1 | 1 | 30 | 0.04 | 31 | 1000 | |
| Air | 130 | 212 | 5.8 | 8 | 15 | 0.4 | 550 | 850 | 5.3 |
| Air & Fe2+ (2.5 mM) | 140 | 203 | 6.2 | 8 | 20 | 0.4 | 850 | 875 | 11* |

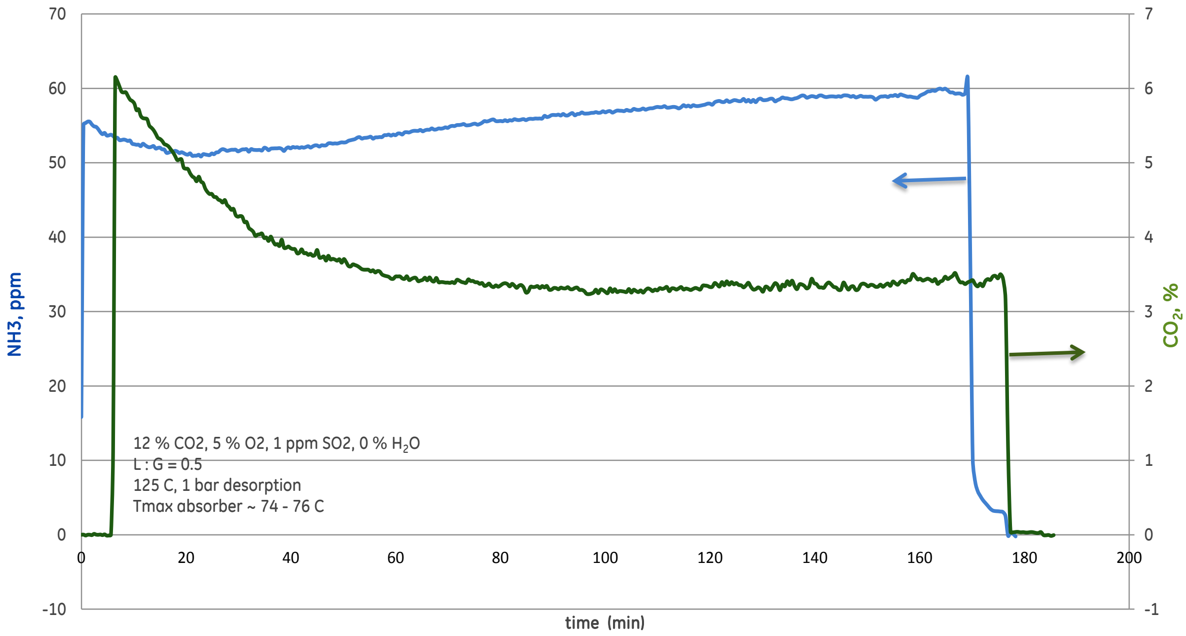
Parr reactor, P = 2.5 Psig, T = 70 C, 1 SLM gas / 100 mL liquid. (*) Normalized for amine content

**Figure 77** shows the data generated earlier from the baseline GAP-$1_m$ solvent that was run in the skid for a total of 280 hours. The plot shows an average ammonia content of ~55 ppm with no measurable amounts of acetaldehyde or propylene observed. No water was added to the system the day the data in **Figure 77** was collected, but most of the 280 hours of run time was completed under wet conditions.

Examining the results from running the following day with wet baseline GAP-$1_m$ solvent (**Figure 78**), about 55 ppm ammonia was again observed to be present along with 25-50 ppm of acetaldehyde. This represents a cumulative run time of over 280 hours. The presence of additional water did not appear to have an effect on the ammonia content but did increase the amount of acetaldehyde.

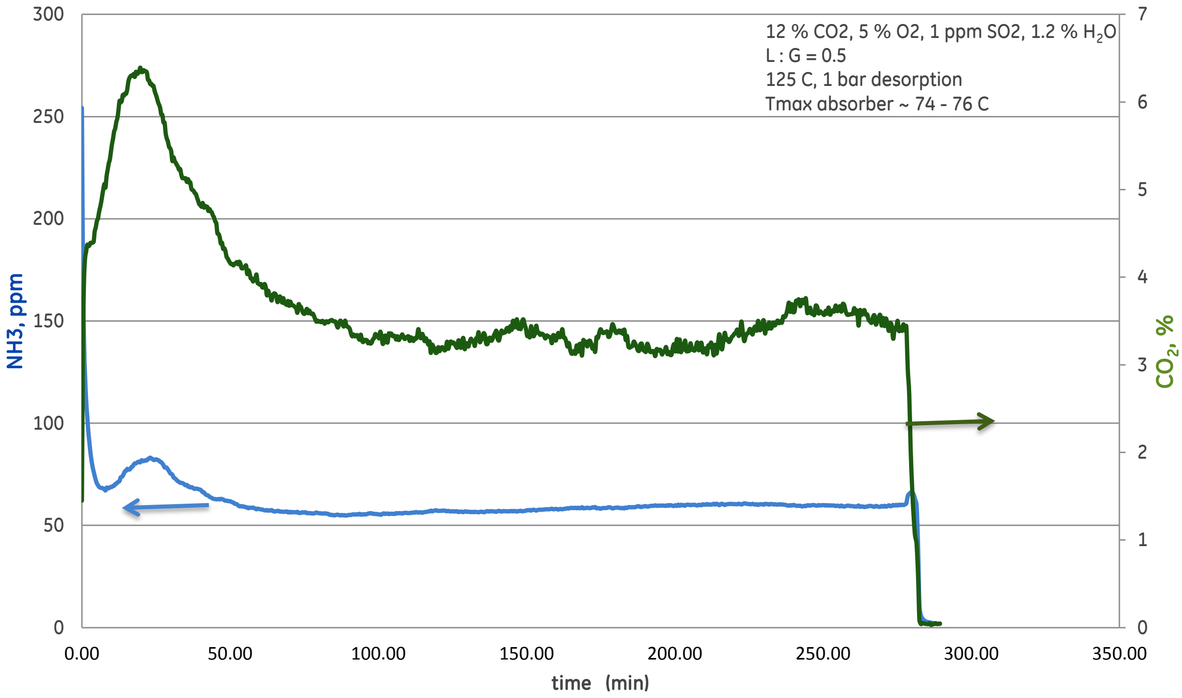
When fresh Wacker GAP-$1_m$/TEG solvent was run in the skid for 4 hours and analyzed by FT-IR, 6-7 ppm of ammonia was detected. No acetaldehyde was detected. Further analyses after running under wet conditions (**Figure 80**) showed ~ 5 ppm of both ammonia and acetaldehyde indicating that rate of oxidation of the Wacker material is 1/10 of the benchmark GAP-$1_m$ batch. The bench skid results are summarized in **Table 46** and are in agreement with the data obtained in the Parr reactor for the fresh materials (**Table 45**). They suggest that the increased ammonia generation for the benchmark material is intrinsic to the difference in composition rather than the aging time between the two batches. Furthermore, the limited data indicates that higher levels of water do contribute to increased levels of acetaldehyde. Long term experiments need to be conducted to confirm these observations.

To determine the effect of running under higher oxygen levels, one run with 20.3% $O_2$, instead of 5% $O_2$, was completed using the Wacker GAP-$1_m$/TEG solvent under wet conditions. The results from the FT-IR analysis are provided in **Figure 81** and showed approximately 3-4 ppm of ammonia and 20-25 ppm acetaldehyde. **Table 46** summarizes the differences between the two batches under low and high oxygen content.



12 % CO2, 5 % O2, 1 ppm SO2, 0 % $H_2O$
L : G = 0.5
125 C, 1 bar desorption
Tmax absorber ~ 74 - 76 C

**Figure 77.** **Ammonia Generation**: Baseline GAP-$1_m$/TEG (Dry Conditions, $2kW_e$ demo)



12 % CO2, 5 % O2, 1 ppm SO2, 1.2 % $H_2O$
L : G = 0.5
125 C, 1 bar desorption
Tmax absorber ~ 74 - 76 C

**Figure 78.** **Ammonia Generation**: Benchmark GAP-$1_m$/TEG (Wet Conditions, $2kW_e$ demo)

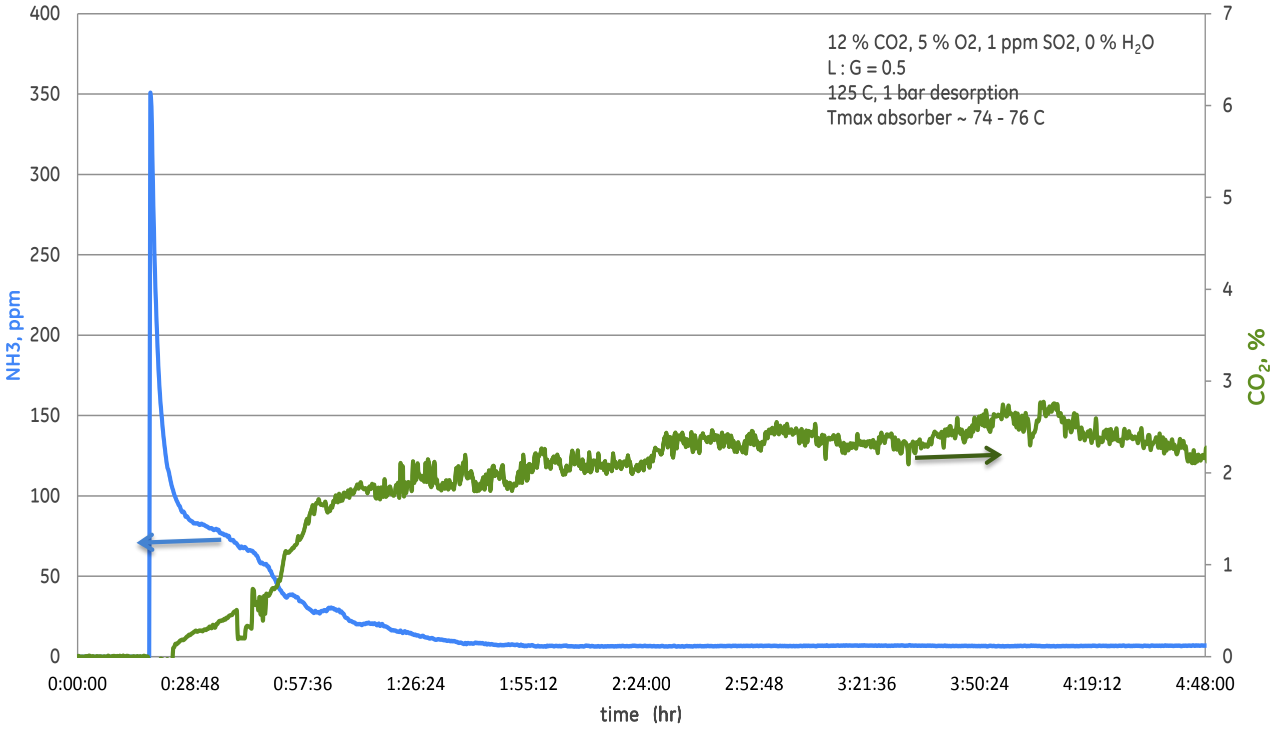


**Figure 79.** **Ammonia Generation:** Wacker GAP-$1_m$/TEG (Dry Conditions. $2kW_e$ demo)

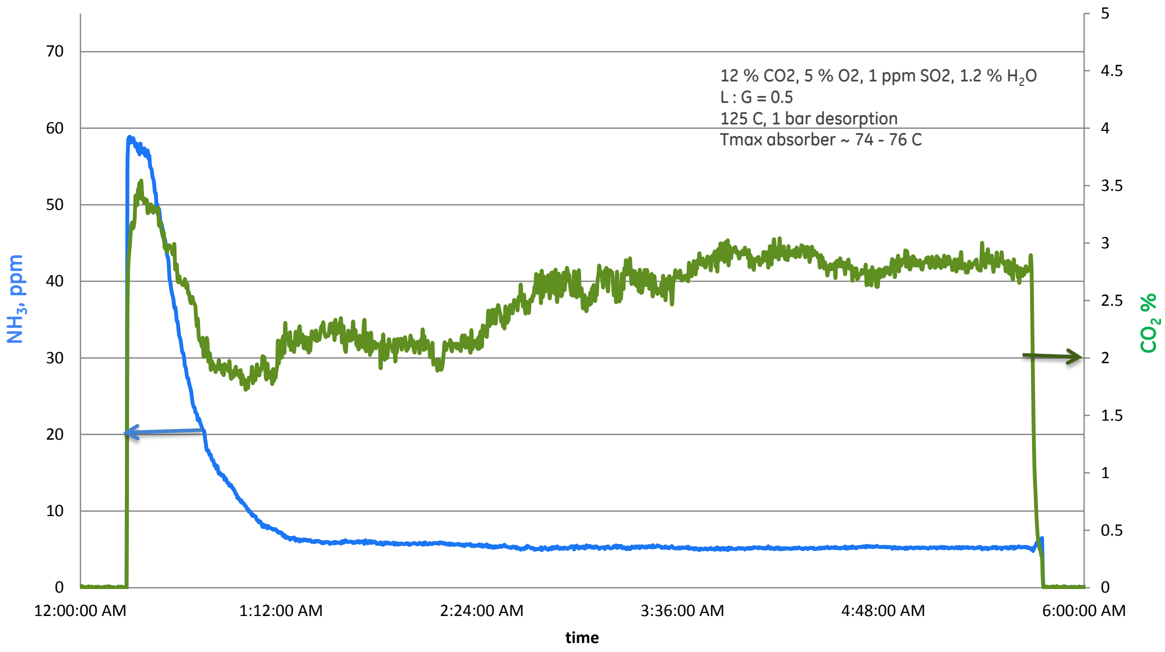


**Figure 80.** **Ammonia Generation:** Wacker GAP-$1_m$/TEG (Wet Conditions. $2kW_e$ demo)

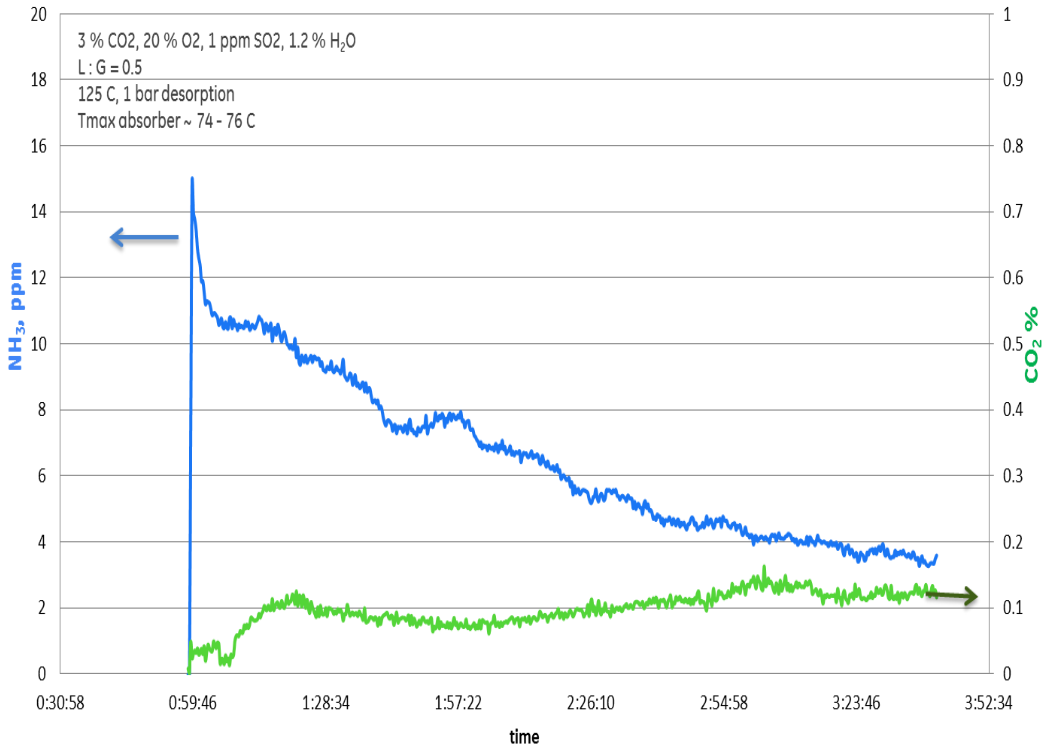


**Figure 81.** **Ammonia Generation:** Wacker GAP-$1_m$/TEG (Wet Conditions. 2kW$_e$ demo, 20 % $O_2$)

**Table 46.** **Ammonia Generation:** Baseline vs. Wacker GAP-$1_m$/TEG (2 kW$_e$ demo)

| | **Baseline GAP-$1_m$ ( 280 hrs.)** | | **Wacker GAP-$1_m$ (fresh)** | |
|---|---|---|---|---|
| | NH$_3$, ppmv | | NH$_3$ ppmv | |
| | Dry | Wet | Dry | Wet |
| Baseline, FTIR | 0 | 0 | 0 | 0 |
| 5 % O2, 12 % CO$_2$ | 60 | 59 | 7 | 6 |
| 20 % O2, 3 % CO$_2$ | NA | NA | NA | 4 |

Baseline GAP-$1_m$: 5 % $O_2$, 12 % $CO_2$; Wacker GAP-$1_m$: 5 % $O_2$, 12 % $CO_2$ and 20% $O_2$ 3 % $CO_2$

**Table 47** shows the list of runs that were completed so that the $CO_2$ capture efficacy could be compared between the baseline and Wacker GAP-$1_m$ solvents. Most of the runs were completed at 12% $CO_2$ with the exception of one run that was completed at 3% $CO_2$ and 20.3%

$O_2$. The % $CO_2$ capture and % GAP-$1_m$ reacted across the column are provided in **Figure 82** showing a similar performance of the system for the two solvents.

**Figure 83** shows the % GAP-$1_m$ reacted in the absorber and in the lean storage before it enters the absorber. The results show very similar performance for the two solvents. The % reacted in lean storage for the Wacker runs was a little lower than for the baseline material, which could indicate that more desorption occurred in the CSTR for the Wacker material. Additional experiments would also be needed to determine if that is a significant difference.

**Figure 84** compares the temperature profiles across the absorber for the two solvent samples showing little difference between the two materials. This is consistent with the similar values for % GAP-$1_m$ reacted across the column under the same run conditions.

**Table 47.** **GAP-$1_m$ / TEG: Baseline vs. Wacker:** Experimental Conditions (2kW bench)

| Solvent | Lm/Gm | Desorber Temp (°C) | Desorber Pressure (psig) | Liquid flowrate (LPM) | Total gas flowrate (SLPM) | $CO_2$ (%) | $SO_2$ (ppm) | Water flowrate (mL/min) | % $O_2$ |
|---|---|---|---|---|---|---|---|---|---|
| **Baseline** | 0.5 | 125 | 2.5 | 1 | 200 | 12 | 0 | 0 | 5.2 |
| | 0.5 | 125 | 2.5 | 1 | 200 | 12 | 1 | 10 | 5.2 |
| | 0.5 | 125 | 2.5 | 1 | 200 | 12 | 0 | 0 | 5.2 |
| | 0.5 | 125 | 2.5 | 1 | 200 | 12 | 1.25 | 0 | 5.2 |
| | 0.5 | 125 | 2.5 | 1 | 200 | 12 | 1.25 | 10 | 5.2 |
| **Wacker** | 0.5 | 125 | 2.5 | 1 | 200 | 12 | 1.25 | 0 | 5.2 |
| | 0.5 | 125 | 2.5 | 1 | 200 | 12 | 1.25 | 10 | 5.2 |
| | 0.19 | 125 | 2.5 | 0.5 | 270 | 3 | 1 | 10 | 20.3 |

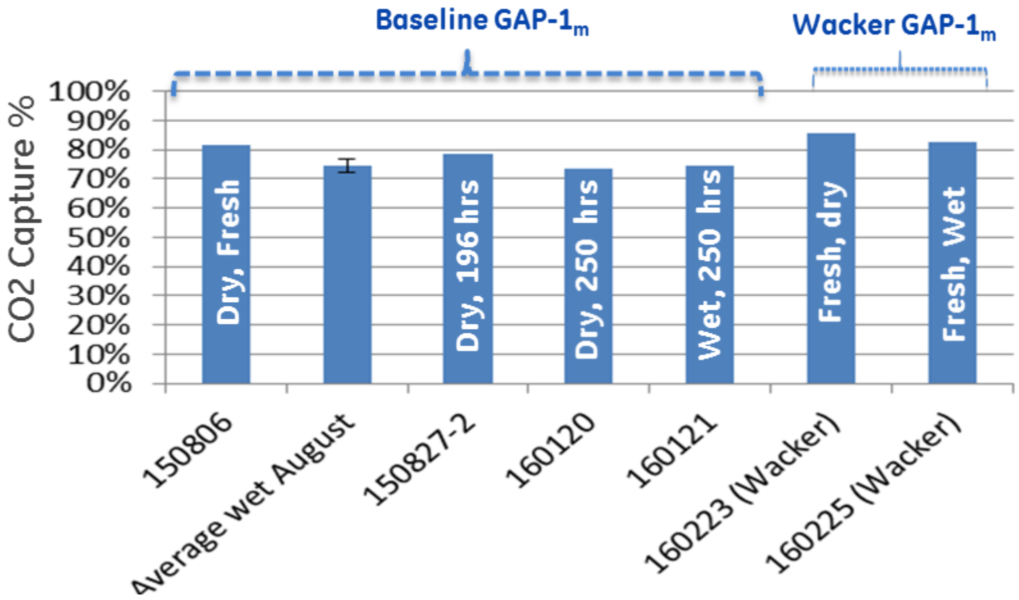


**Figure 82.** **GAP-1$_m$ / TEG: Baseline vs. Wacker:** $CO_2$ Capture Efficiency (2kW bench)
Experimental conditions in **Table 47**

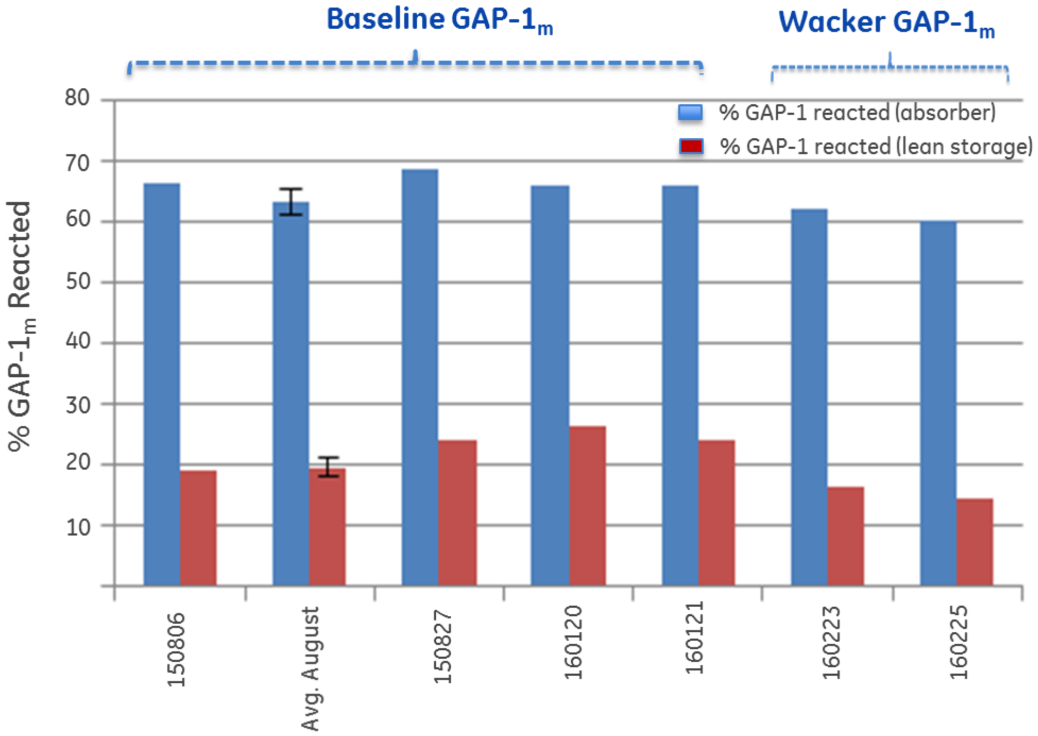


**Figure 83.** **GAP-1$_m$ / TEG: Baseline vs. Wacker:** GAP-1$_m$ reacted in absorber and lean storage.
Experimental conditions in **Table 47**

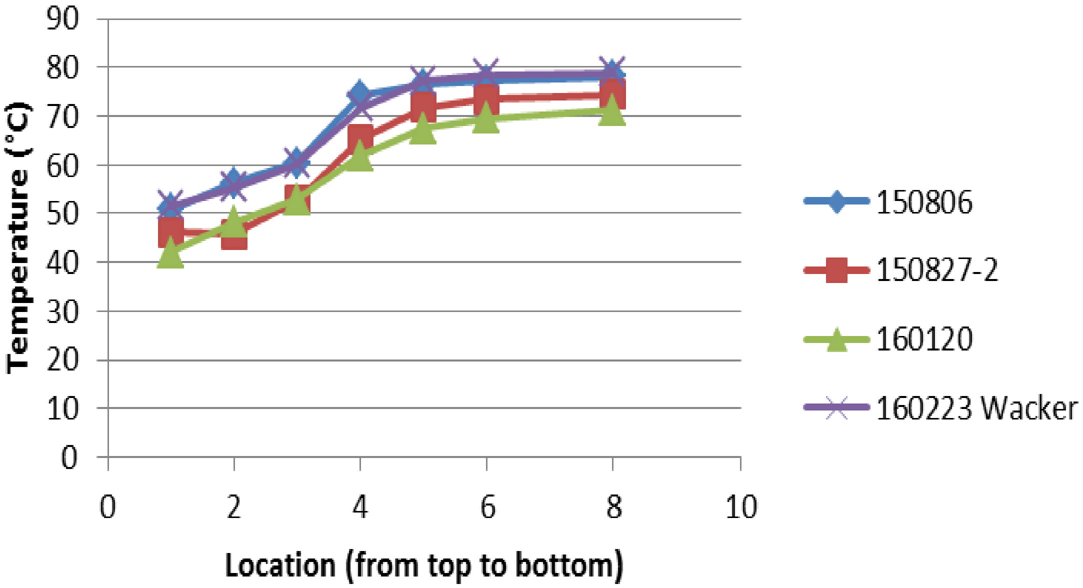


**Figure 84.** **GAP-$1_m$ / TEG: Baseline vs. Wacker:** Absorber temperature profile
Experimental conditions in **Table 47**

## 5.7 Conclusions

Analyses of the Wacker GAP-$1_m$ aminosilicone solvent showed that it was superior to the benchmark GAP-$1_m$ material from the standpoint of purity and thermal degradation but was comparable in $CO_2$ absorption, average composition and amine content. Metals analyses also showed no difference between the two samples.

The $CO_2$ capture rate for the Wacker material (fresh) was measured in the bench scale $CO_2$ capture system under both coal fired (12 % $CO_2$, 5 % $O_2$), and natural gas fired (3 % $CO_2$, 20 % $O_2$) simulated flue gas conditions. No statistical difference in initial performance was observed between the Wacker and the benchmark GAP-$1_m$ materials under similar conditions. Wacker material was also evaluated under hydrothermal degradation (steam stripping conditions, 120 $^oC$). In both cases, no statistical difference in degradation was measured between the Wacker and benchmark materials.

Finally, Wacker GAP-$1_m$/TEG showed better stability towards thermoxidation under absorber conditions (70 C, 2.5 Psig) both in the bench scale and lab scale testing. Overall, the aminosilicone solvents showed 2 times less oxidation activity vs. the baseline MEA solvent under the lab scale conditions. The Wacker GAP-$1_m$/TEG oxidation rate measured in the bench scale system corresponds to 40 % solvent make-up / year (0.13 kg amine/tonne $CO_2$). A similar degradation rate was observed in the Advanced Aqueous Amine pilot process (AAP). Considering the high cost of the aminosilicone solvent, it is recommended that the next activities should be concentrated in developing oxidation inhibitors to further reduce solvent make-up cost. Considering the similar or better performance, it is our opinion that Wacker has been qualified as a supplier of the GAP-$1_m$ aminosilicone solvent.

# 6 Technology Gap Analysis

The following sections discuss the technology gap analysis for a carbon-capture unit which uses an aminosilicone-based solvent for $CO_2$ capture for a pulverized coal (PC) power plant.

The GAP-$1_m$/TEG $CO_2$ separation units utilize four key processes, $CO_2$ absorption, $CO_2$ desorption, sorbent handling, and $CO_2$ compression. (**Figure 85**) The flue gas passes through a direct contact cooler to reduce the temperature to 40 $^oC$, and then enters the bottom of the $CO_2$ absorber. Here, the gas stream is contacted with the cooled lean solvent (40 $^oC$) entering the top of column. After reacting with $CO_2$, the rich aminosilicone solvent leaves the bottom of absorber. The $CO_2$ absorption reaction is exothermic, and increases the temperature of the sorbent. The absorber is operated between 40 - 65 $^oC$ and at atmospheric pressure. The rich solvent from the absorber is heated in the rich/lean heat exchanger before being fed to the solvent regenerator for separation of the absorbed $CO_2$. The lean solvent from the regenerator is cooled in the rich/lean heat exchanger and lean cooler, respectively before being fed back to the absorber column.

The regenerator is operated at 110 $^oC$ and 1.2 bar. Steam goes through a boiling heat exchanger to provide heat for $CO_2$ release from the rich solvent. The hot vapor from the top of the regenerator, consisting primarily of $CO_2$ and $H_2O$, is cooled in a partial overhead condenser and total condense, respectively. Water and entrained solvent are recovered in a mist separator, and then sent back to the lean storage tank to maintain water content in the working solution and to reduce solvent loss. The $CO_2$ product is then delivered to compression.

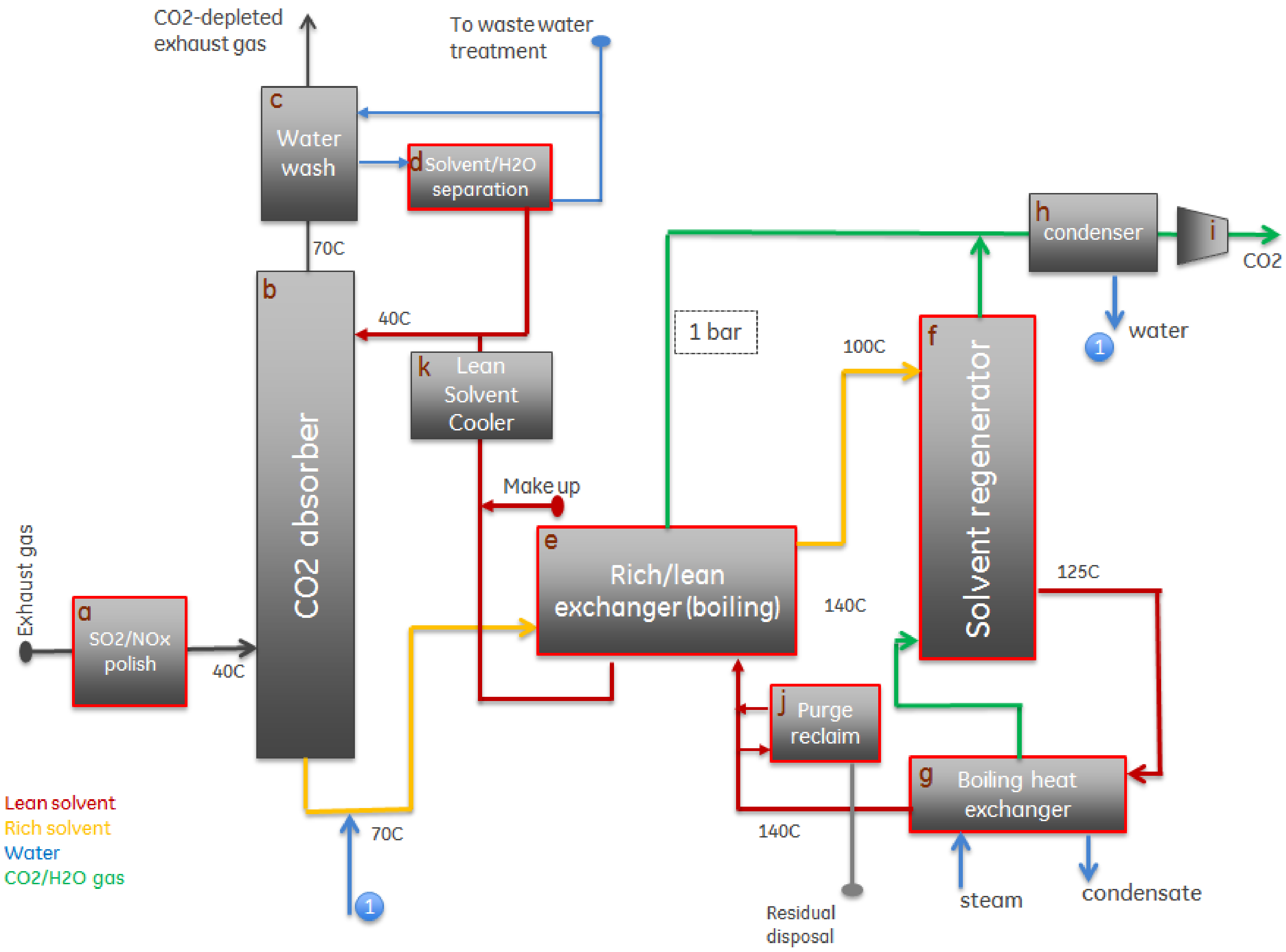


**Figure 85.** GAP-$1_m$ / TEG Process: Conceptual process flow diagram

## 6.1 Gaps and Technical Challenges

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The advantages of the GAP-$1_m$/TEG solvent technology are its higher $CO_2$ working capacity, low volatility, and low corrosivity. However, higher expected cost of the solvent vs. aqueous amines makes solvent management a top priority to maintain the low cost for the process. Our current techno-economic analysis indicates that a 20 % solvent make-up / yr. is required to meet the cost target of the DOE goals. Therefore, improving solvent management was identified as one of the main technical challenge for the development of the GAP-$1_m$ / TEG process at the commercial scale.

### 6.1.1 Solvent Management

Systematic analysis of the solvent loss in the GAP-$1_m$ / TEG process identified a number of areas for technology development (**Figure 86**). Thermal degradation of the rich solvent and oxidative degradation were found to be the main mechanisms for solvent loss, they were identified as the critical technology gap needed to be addressed.

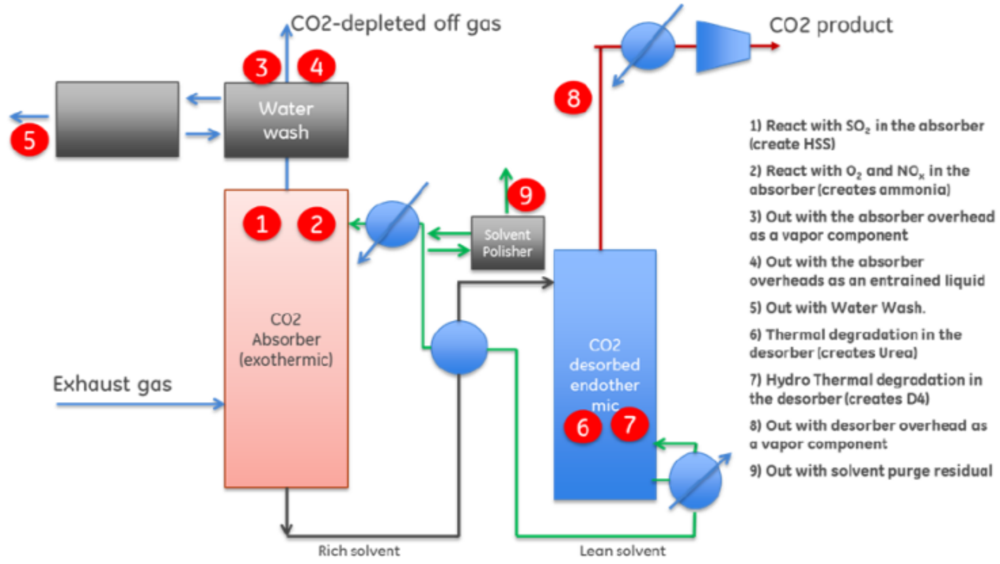


**Figure 86.** GAP-$1_m$/TEG process: Solvent management

#### 6.1.1.1 *Thermal degradation of rich solvent*

Small amounts of water in the working solution (up to 15 wt.%) were found to be an effective way to enable steam stripping, lower desorption temperature (110 °C), and hence reduce thermal degradation. The concept was first tested in a glass stripping column (TRL 3), optimized in a continuous bench scale system (TRL 4), and recently demonstrated in a 0.5 $MW_e$ pilot demo at NCCC (TRL 5). It was also demonstrated that steam stripping increased the $CO_2$ working capacity by 30 % due to a more efficient desorption. Controlled water addition had an additional benefit of reducing the viscosity of the working solution, making both the absorption and desorption steps more efficient. Low amine degradation (< 0.05 wt.%/day) was demonstrated for over 350 hours of operation (**Figure 87**). It is recommended that this concept be further optimized to reduce its effect on the specific steam duty, and increased corrosivity of the working solution.

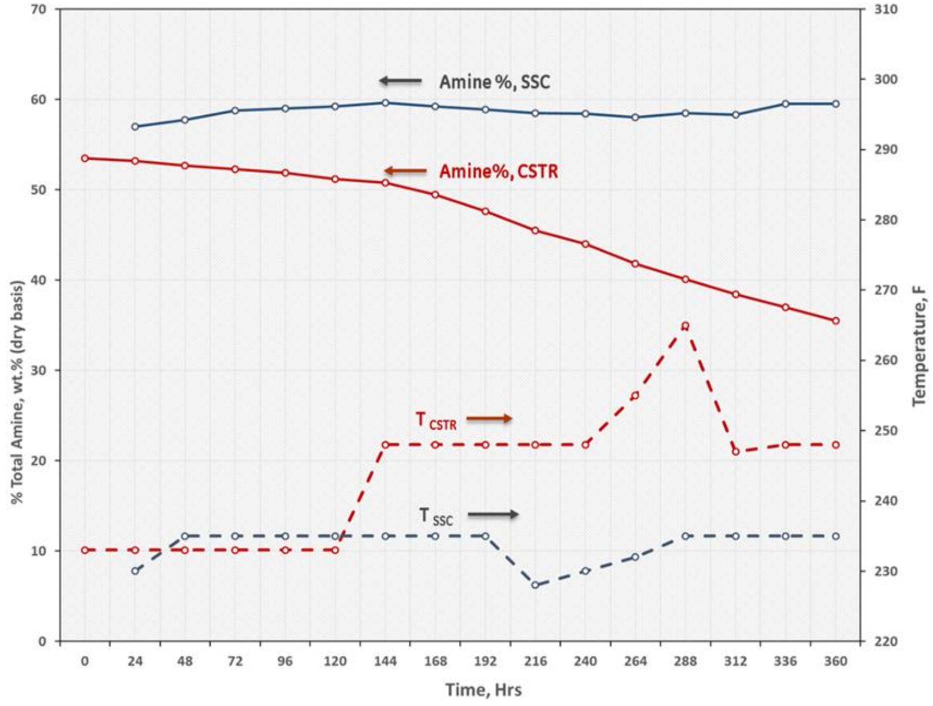


**Figure 87.** **Solvent Degradation at NCCC (0.5 $MW_e$ scale):** Steam stripping column (SSC) vs. Continuous Stirred Reactor (CSTR) Desorber

**SSC: $T_{desorber}$ = 230–235 °F; P = 2 Psig; 0.25–0.5 MWe, 14-35 wt.% $H_2O$**

**CSTR**: $T_{desorber}$ = 230 – 248 °F; P = 7 Psig; 0.25 – 0.5 MWe, 3-5 wt. % $H_2O$

### 6.1.1.2 *Thermal oxidation*

Aminosilicone solvents exhibited two times less oxidative activity vs. the baseline MEA solvent under the absorber conditions (70 $^{o}$C, 2.5 Psig) both in the lab and bench scale testing. As indicated by the ammonia formation, controlling the absorber temperature had a significant effect in reducing amine degradation by thermal oxidation as seen in **Figure 88**. Considering the high cost of the solvent, it is recommended that the next activities should be concentrated in developing oxidation inhibitors to further reduce solvent make-up cost while implementing rigorous temperature control through controlled water addition and optimized inter-stage cooling.

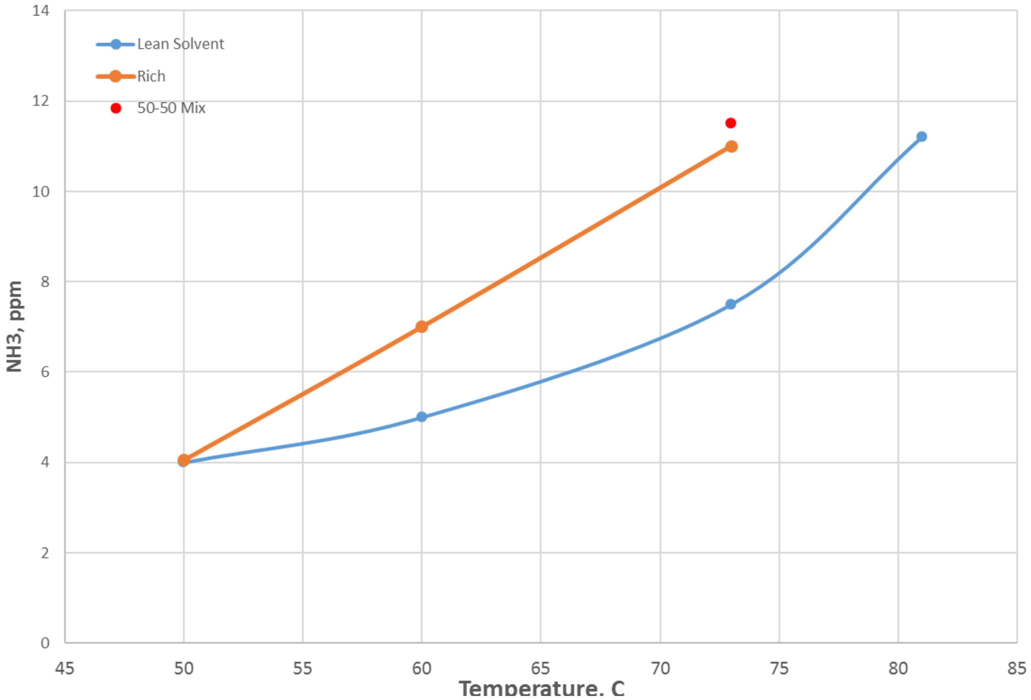


**Figure 88.** Thermal oxidation of GAP-1$_m$ / TEG as a function temperature
450 mL Parr reactor, P = 2.5 Psig, T = 70 C, 1 SLM gas (5 % $O_2/N_2$), 100 mL liquid.

#### 6.1.1.3 *Hydrothermal equilibration*

Evaluation of hydrothermal stability of GAP-$1_m$ / TEG working solution during the NCCC pilot test indicated that the solvent re-equilibrated and stabilized to lower GAP-1 numbers (0.3) after 300 hours of operation with the steam stripping desorber. This was expected as a re-equilibration reaction can occur under basic conditions and with heat and water present. Considering that the process of equilibration could form cyclic silicones such as $D_4$ and $D_5$, it is recommended that the GAP number of the starting material should be close to the equilibration value (i.e. GAP-0.3) noted above.

#### 6.1.1.4 *Heat stable salts formation: $SO_2$ polish unit*

Heat stable salts are formed from the reaction of $SO_x$ contained in the flue gas with the amine solvents. $SO_2$ levels in the flue gas from coal fired power plant can be controlled using a two-stage $SO_2$ polish unit. The first stage is a lime or limestone wet FGD (flue gas desulfurization) unit in which $SO_2$ removal is accomplished by recirculating an aqueous slurry of lime and limestone. Considering the high cost of the solvent, it is recommended that a second stage polishing unit should be considered to control the $SO_2$ content to less than 1 ppm to minimize solvent degradation. Some $SO_2$ scrubbers such as Mitsubishi double contact flow scrubber, Alstom open spray tower can reduce $SO_2$ concentration to single digit ppm level.

### 6.1.2 Specific equipment for non-aqueous solvents

In the following section, equipment related gaps and areas for technical development of commercial large-scale aminosilicone $CO_2$ capture are addressed. A summary of commercial availability of different equipment is presented in **Table 48**.

Summary of commercial availability of different equipment.

**Table 48.** **Technology Gap Analysis:** Equipment Availability

| Equipment | Commercial products can be applied | |
|---|---|---|
| a. SO2/NOx polish unit | 🟡 | Need 1 ppm or lower consistently |
| b. CO2 absorber | 🟡 | Need heat rejection to maintain liquid temp below 50C |
| c. Water wash | 🟢 | |
| d. Solvent/water separation | 🟢 | |
| e. Rich/lean heat exchanger | 🟡 | Plate and frame designs to maintain turbulent flow and a high heat transfer coefficient w viscous flow |
| f. Solvent regenerator | 🟢 | |
| g. Boiling heat exchanger | 🟢 | |
| h. Water condenser | 🟢 | |
| i. CO2 compressor | 🟢 | |
| j. Purge reclaim | 🔴 | Need separation not based on vapor pressure differential |
| k. Lean solvent cooler | 🟡 | Same as rich/lean heat exchanger |

🟢 Commercial products available
🟡 Technically feasible; Pilot scale
🔴 No obvious solution

#### 6.1.2.1 *$CO_2$ absorber*

$CO_2$ absorber is a gas-liquid contact tower with structured packing, where the flue gas contacts GAP-$1_m$ / TEG working solution. The exterior structure of the $CO_2$ absorber is made of lined concreate, and the internal support structure made of carbon steel. High temperatures in the absorber accelerate oxidative degradation of the lean solvent. The high $CO_2$ carrying capacity of the solvent combined with the high heat of reaction make heat rejection and temperature control in the absorber a challenge with the current multi-bed, intercooler design approaches. Based on the behavior observed in our 0.5 $MW_e$ pilot at NCCC, it is recommended that small amounts of water (up to 15 wt.%) are added to the working solution to reduce viscosity, improve mass and heat transfer in the column, and to lower temperature through evaporative cooling.

#### 6.1.2.2 *Water wash and Solvent/Water Separation*

The water wash is a packed bed tower. The flue gas from the top of the $CO_2$ absorber tower is contacted with water to remove entrained solvent droplets and lower the temperature of the vented gas. Packed beds and spray towers exist as commercial offerings but the effectiveness in capturing entrained droplets of the aminosilicone solvent has not been evaluated. Reducing the $SO_3$ content and particulates of the flue gas in the direct cooler is known to be effective in reducing the solvent loss in the overhead of the absorber.

Solvent/water separation is a gravity unit operation to recover the water and lean solvent from the water wash. There is a commercial gravity separation unit that is available for this application. It is recommended to recycle the condensate from the wash water tower back to the lean storage tank to maintain the water content in the working solution, and reduce solvent loss in the water wash tower.

#### 6.1.2.3 *Rich/lean heat exchanger*

The rich/lean heat exchanger is a liquid-liquid heat exchanger. The $CO_2$-loaded solvent needs to be heated in order to strip off $CO_2$ and regenerate the solvent. On the other hand, the regenerated lean solvent coming out of the regenerator has to be cooled down before it could be circulated back to the absorber column. Hence these two solvent streams are passed through a cross heat exchanger, where the rich ($CO_2$-loaded) solvent gets heated (from 65 $^{o}$C to 100 $^{o}$C) and the lean solvent gets cooled. Due to the high viscosity of the rich GAP-$1_m$ carbamate working solution, it is recommended that small amounts of water (up to 15 wt.%) are added to the working solution to reduce viscosity, improve mass and heat transfer. The concept has been proven in the 0.5 MW pilot scale demo (TRL 5).

#### 6.1.2.4 *Solvent regenerator*

The solvent regenerator is the gas-liquid contact packed column in which the main function is to remove $CO_2$ from the rich solvent by steam stripping. The absorption reactions are reversed with heat supplied by steam. The rich solvent flows down through the regenerator, and steam rising up through the column strips the $CO_2$ from the rich solvent. The exterior structure of solvent regenerator is made of concrete, and the internal support structure made of stainless steel. The regenerator is operated at 110 -115$^{o}$C at 1.2 bar. There is a commercial gas-liquid contact strip tower that is available for this application. It is recommended to maintain a low water content in the working solution (< 15 wt.%) to reduce the impact on the specific steam duty, and water carryover in the tower overhead.  Finally, implementation of the flash stripper could be considered as alternative to reduce the specific steam duty. This concept has been attempted at NCCC, however liquid level control was challenging due to foam formation. Specific design needs to be considered for the advanced flash stripper to limit foam formation during desorption.

#### 6.1.2.5 *Boiling heat exchanger*

The regenerator is connected to a boiling heat exchanger where low-pressure steam extracted from the power plant is used to heat the $CO_2$ loaded solvent. To save energy, steam and rich solvent stream are passed through a cross heat exchanger, where the steam gets cooled and the rich solvent gets heated. $CO_2$ released from the rich solvent is fed back to the solvent regenerator. There are commercial shell and tube heat exchanger available for this application.

#### 6.1.2.6 *Water condenser*

The total condenser is a heat exchanger that is used to condense water from the $CO_2$ rich stream. The inlet temperature of the condenser is ~90 $^{o}$C and the outlet temperature is 30$^{o}$C. There is commercial unit available for this application. It is recommended to recycle the condensate from the total condenser back to the lean storage tank to maintain water content in the working solution, and reduce solvent loss in the water condenser tower. The concept has been proven in the 0.5 MW pilot scale demo (TRL 5).

#### 6.1.2.7 *$CO_2$ compressor*

$CO_2$ compression is achieved by a centrifugal multi-stage compressor unit with inter-stage cooling to obtain liquid $CO_2$. There is centrifugal multi-stage compressor available for this application.

#### 6.1.2.8 *Purge reclaim*

The presence of acid gas impurities (such as $SO_x$, $NO_x$) in the flue gas leads to formation of heat stable salts (HSS) in the lean solvent stream. In order to avoid accumulation of these salts in the working solution, and to recover some of GAP-$1_m$ solvent, a part of the solvent stream is purged periodically. The recovered GAP-$1_m$ is sent to the lean solvent stream, and the HSS stream is disposed. Possible pathways to separate HSS and GAP-$1_m$ include selective solvents, selective chemical reactions, distillation and precipitation, and chemical reactions to convert the HSS back to GAP-$1_m$. None of these concepts have been proven at pilot scale.

#### 6.1.2.9 *Lean solvent cooler*

After the rich/lean heat exchanger, a lean solvent cooler has been used to cool the lean solvent before is fed to the absorber to increase the loading of $CO_2$ in the absorber. The lean solvent cooler lowers the lean solvent temperature from approximately 84$^{o}$C to 40 $^{o}$C using cooling water in a counter-current, shell and tube heat exchanger. The high viscosity of the lean solvent is a challenge for the lean solvent cooler. Controlled water addition in the working solution could improve performance of the lean solvent cooler through reduction of the viscosity of the working solution and decreased desorption temperature. The concept has been proven in the 0.5 $MW_e$ pilot scale demo (TRL 5).

## 6.2 Future R&D Directions

It is proposed that future R&D directions would focus on the design and demonstration of an advanced aminosilicone solvent (Gen 2) and process to meet the $CO_2$ cost target of 40 \$/t$CO_2$ at a 90% $CO_2$ capture efficiency with 95% $CO_2$ purity. **Table 49** shows the solvent design targets, the cost impact of those targets and their relevance to process changes and modifications based on our preliminary techno-economic analysis (TEA) performed for a 550 MW pulverized coal (PC) power plant.

**Table 49.** Solvent Design Targets and Impact

| **Solvent Attribute** | **Baseline** (MEA) | **GAP-1$_m$ / TEG** (Gen 1) | **Adv. Aminosilicone** (Gen 2) | **Process Impact**[(1)] (Gen 2 vs. Gen 1) |
|---|---|---|---|---|
| **$CO_2$ Working Capacity** (wt.%) | 4 | 5 | 10 | -30 % CAPEX; -11% OPEX |
| **Solvent Make-up** (% / yr) | 100 | 75 | 20 | -40% OPEX |
| **Viscosity** ($CO_2$ loaded, cP) | 1 | 576 | 100 | -40% absorber; -30% RLHX[(2)] |
| **Heat of Reaction** (KJ/Kg) | 1825 | 2263 | 1900 | -12 % reboiler duty |
| **$CO_2$ Cost** (\$/t$CO_2$)<br>**COE** (cents / kWh) | 67<br>(13.7) | 48<br>(11.6) | 40<br>(10.6) | |

(1) Individual process impact. (2) Rich/Lean heat exchanger

The following approach is proposed to achieve these targets.

(i) **Solvent Design:** Advanced aminosilicone solvents will be developed through molecular modeling, and rational design to improve the $CO_2$ capacity and solvent stability, to reduce viscosity of the working solution, minimize solvent make-up, and optimize heat of reaction.

(ii) **Process intensification:** Controlled water addition and steam stripping desorption will be evaluated for reduction in capital and operating costs and improved solvent management.

(iii) **System integration:** Heat integration between $CO_2$ capture and the reference plant will be performed to seek further reductions in $CO_2$ capture cost / cost of electricity.

Recent work in our laboratory identified promising advanced aminosilicone candidates that could meet the solvent attributes listed in **Table 49**. We determined that secondary amine functional disiloxanes with unhindered alkyl substituents exhibit improved total theoretical $CO_2$ uptake (up to 11 wt. % $CO_2$) and lower heat of reaction (1900 kJ/mol) than their primary amine containing counterparts. Improved performance was observed with advanced silicones having the general structure shown in **Figure 89**. If X is an electron donating group, we found that the carbamate salts were freely flowing liquids at room temperature, with excellent thermal and hydrothermal stability.

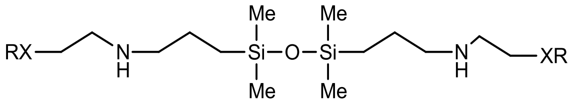


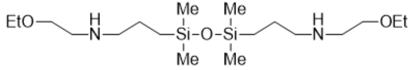
**Figure 89.** Advanced Aminosilicone Solvent

Preliminary experiments that examined one of the advanced aminosilicone solvents (EEAP, **Table 50**) showed promising results. These results included lower heat of reaction, greater thermal stability, lower viscosity and the ability to remain as a flowable liquid when fully reacted without the need for a co-solvent.[16] (**Table 50**) This enhanced class of aminosilicones could address the short-comings of the current solvent system, and will provide a material that is superior to the existing GAP-$1_m$/TEG.

**Table 50.** Advanced Aminosilicone Solvents (Gen 2) Candidate: Preliminary Data

| **Solvent Attribute** | **Adv. Aminosilicone** (Gen 2) - target | **EEAP*** (Gen 2 Candidate) | |
|---|---|---|---|
| | | | Note |
| **$CO_2$ Capacity** (wt.%) | 10 | 8 | Absorption at 35 °C; desorption at 100 °C |
| **Solvent Make-up** (%/yr.) | 20 | 20 | Thermally stable up to 140 °C |
| **Viscosity** (cP, $CO_2$ loaded) | 100 | 286 | No co-solvent required |
| **Heat of Reaction** (kJ/Kg) | 1900 | 1863 | |

**EEAP*:**



# 7 Environmental, Health, and Safety (EH&S) assessment

The following sections describe the Environmental, Health, and Safety (EH&S) assessment for a $CO_2$ capture system for a 550 MW coal-fired power plant and for the manufacturing process of GAP-$1_m$. Plant-wide engineering controls are described. Five components of the solvent, CAS#2469-55-8 (GAP-0), CAS#106214-84-0 (GAP-1-4), TEG, and methanol and xylene (minor contaminants from the aminosilicone) are included in this assessment. One by-product, GAP-1m/$SO_X$ salt, and DDBSA were also identified for analysis. The chemicals associated with the manufacturing process include methanol, xylene, allyl chloride, potassium cyanate, sodium hydroxide (NaOH), tetramethyldisiloxane (TMDSO), tetramethyl ammonium hydroxide (TMAH), Karstedt catalyst, octamethylcyclotetrasiloxane ($D_4$), Aliquat 336, methyl carbamate, potassium chloride, trimethylamine, and (3-aminopropyl) dimethyl silanol (referred to as silanol in this report).

Finally, the toxicological effects of the chemicals associated with the $CO_2$ capture system and the manufacturing process are reviewed. Details of the containment, handling, disposal processes, safety data sheets, shipping, storage equipment requirements, and relevant regulatory requirements are also summarized.

## 7.1 Aminosilicone-based $CO_2$ Capture System for a 550 MW Coal-Fired Power

### 7.1.1 Plant Air, Water, and Solid Waste Identification

This section describes the potential ancillary or incidental air, water, and solid wastes from the proposed technology and identifies and estimates their magnitude for a 550 MW coal-fired power plant. In addition to the absorption solvents, the possible by-products, waste products, and flue gas contaminants were considered. The $CO_2$ capture system was designed to minimize possible environmental degradation products and bioaccumulation thereof. The design also examined the full-scale conditions at the point of discharge to the environment.

The aminosilicone solvent used in the continuous $CO_2$ absorption/desorption process is a 60%wt GAP-$1_m$ / 40%wt TEG mixture. The GAP-$1_m$ (or DAP-0) is supplied by Milliken & Company (SiVance LLC). GAP-$1_m$ has some methanol and xylene contaminants that come from SiVance's manufacturing process. To estimate the concentration of the contaminants, SiVance measured the composition of 5 delivered lots of GAP-1m with an Agilent 6890 gas chromatogram (GC) and a model 5973 mass spectrometer (MS). The methanol was less than 100 ppm, and the xylene concentration was less than 50 ppm in the 5 lots. However due to statistical analysis of the capability of the current manufacturing process, SiVance specified the concentration limits to be 500 ppm for each, as shown in **Table 51**. Thus, 500 ppm will be used as the de-facto concentration in the mass balance discussed below. The molecular weight distribution of GAP-$1_m$ was also measured, showing a mixture of X = 0, 1, 2, 3, and 4 as included in **Table 52**. The GAP-0 and GAP-(1-4) components of GAP-1m have been registered separately as CAS#2469-55-8 and CAS#106214-84-0, respectively. The final solvent composition fed into the $CO_2$ absorption/desorption process is summarized in **Table 53.**

**Table 51.** Composition range and specifications of GAP-$1_m$ (SiVance)

| | **Methanol (ppm)** | **Xylene (ppm)** | **Molecular Weight (g/mol)** | **Total Amine Activity (%)** |
|---|---|---|---|---|
| Specification | <500 | <500 | <345 | >96% |
| Range of 5 lots | <100[17] | <50[18] | 301-317 | 96-100 |

**Table 52.** Representative distribution of GAP-$1_m$ components

| **GAP-0** | **GAP-1** | **GAP-2** | **GAP-3** | **GAP-4** |
|---|---|---|---|---|
| 44% | 30% | 15% | 8% | 3% |

**Table 53.** Composition of the aminosilicone solvent for the continuous $CO_2$ absorption/desorption system.

| **$CO_2$ Capture Solution** | **GAP-$1_m$ (60%wt)** | | | | **TEG (40%wt)** |
|---|---|---|---|---|---|
| **Components** | GAP-0 | GAP 1-4 | Methanol | Xylene | Triethylene glycol |
| **CAS #** | 2469-55-8 | 106214-84-0 | 67-65-1 | 1330-20-7 | 112-27-6 |
| **% wt Composition in $CO_2$ Capture System** | 26 wt % | 34 wt % | <300 ppm | <300 ppm | 40 wt % |

The flue gas composition for the 550 MW plant was specified in the cooperative agreement between GE Global Research and the DOE.[19] Before entering the $CO_2$ absorption/desorption system, flue gas is cleaned and prepared in Flue-Gas Desulfurization (FGD), pre-scrubber, cooler, and condenser units. The gas, labeled 1 in **Figure 90**, is fed into the $CO_2$ absorption unit (Absorber). The composition and flow rate of the gas is included in **Table 54**. It is primarily $CO_2$, nitrogen ($N_2$), water ($H_2O$), and oxygen ($O_2$), with low levels of sulfur oxides ($SO_x$) and nitrogen oxides ($NO_x$).

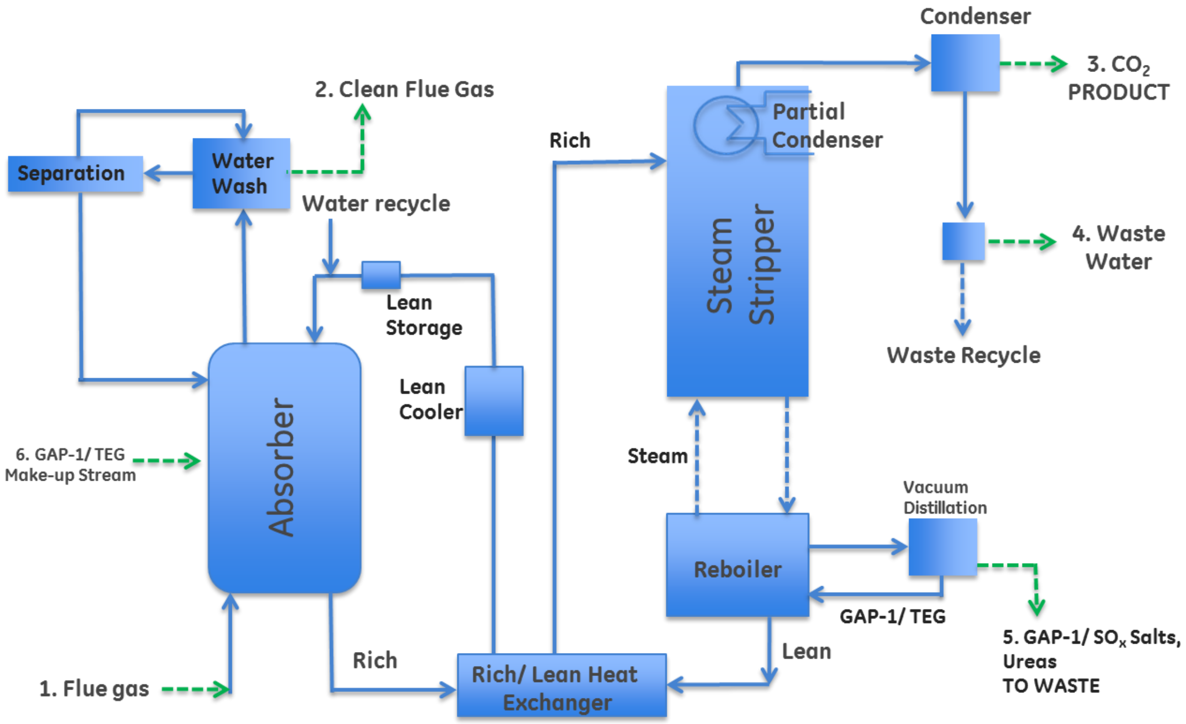


**Figure 90.** Continuous $CO_2$ absorption/desorption system for a 550 MW coal-fired power plant

**Table 54.** Composition and flow rate of stream 1, inlet flue gas

| | mass fractions | lb/hr |
|---|---|---|
| CO2 | 2.19E-01 | 9.64E+00 |
| H2O | 4.40E-02 | 7.93E-01 |
| N2 | 7.09E-01 | 1.99E+01 |
| O2 | 2.62E-02 | 8.39E-01 |
| SOx | 6.46E-06 | 4.14E-04 |
| NOx | 8.08E-05 | 3.72E-03 |

Flow Rate= 5.78E+06 lb/hr

As the gas enters the absorber (**Table 54**), it mixes with the 65%wt GAP-$1_m$/20%wt TEG and 15 wt $H_2O$ absorption solvent. The gas passes upward through the column while the liquid flows down. As it mixes, the GAP-$1_m$ reacts with $CO_2$ to make a carbamate salt. The column is designed to capture 90% of the inlet $CO_2$. The salt is soluble in the liquid and is carried down to the bottom of the column with the solvent. The GAP-$1_m$ also reacts with the $SO_x$ gases to form heat stable salts. This reaction is very efficient, and all of the incoming $SO_x$ is removed from the gas stream. This amino-sulfate salt is dispersed into the solvent and carried to the bottom of the column with the solvent. Since water and triethylene glycol are miscible, some water vapor dissolves into the solvent and is carried with the liquid to the bottom of the column. Meanwhile, none of the $N_2$, $O_2$, or $NO_x$ dissolves or reacts with the solvent, as confirmed by GE Global Research's bench-scale studies.[20] As the cleaned flue gas exits the top of the column, a small amount of GAP-$1_m$, TEG, xylene, and methanol may exit with the gases. To prevent release to the environment, these are captured with a water wash tower. The GAP-$1_m$ is separated from the water with a distillation column and returned to the top of the absorption column. The water is returned to the water wash tower. The cleaned flue gas, shown as stream 2 in **Figure 90**, is released to the atmosphere via a stack. Its composition and flow rate is shown in **Table 55**.

**Table 55.** Composition and flow rate of stream 2, cleaned flue gas

| | mass fractions | lb/hr |
|---|---|---|
| $CO_2$ | 4.70E-02 | 2.21E+05 |
| H2O | 4.80E-02 | 2.26E+05 |
| N2 | 8.70E-01 | 4.10E+06 |
| O2 | 3.50E-02 | 1.65E+05 |
| SOx | 1.50E-05 | 7.06E+01 |
| NOx | 1.00E-04 | 4.71E+02 |
| GAP-1m | 1.22E-05 | 5.75E+01 |
| NH3 | 2.00E-05 | 10.00E+01 |

Flow Rate= 4.71E+06 lb/hr

Meanwhile, the liquid at the bottom of the absorption column is pumped through a heat exchanger into a desorption vessel (Desorber). Here, the liquid is heated until the carbamate salt decomposes, releasing $CO_2$ gas. Some GAP-$1_m$, TEG, and water, may also vaporize with the $CO_2$ product. The gas stream goes through a series of condensers and compressors to remove the contaminants from the gas stream. The clean gas stream, shown as stream 3 in **Figure 90**, is collected as the $CO_2$ product. See **Table 56** for composition and flow rate. A second stream rich in GAP-$1_m$, TEG, xylene, and a fraction of water, is recycled to the Desorber. A third condensed stream, stream 4 in **Figure 90**, is mostly water and with a small amount of GAP-$1_m$, TEG, and D4 (see **Table 57**) and it would also be disposed of as non-hazardous waste, which could include sending it to a wastewater treatment facility, depending on site-specific considerations. This would not be an option if GAP-$1_m$ were still present in this waste stream. The classifications of solid waste in regards to RCRA are discussed in detail in Section E of this report.

**Table 56.** Composition and flow rate of stream 3, $CO_2$ product

| | mass fractions | lb/hr |
|---|---|---|
| **CO2** | 9.98E-01 | 9.61E+05 |
| **H2O** | 4.10E-05 | 3.95E+01 |
| **N2** | 2.00E-03 | 1.93E+03 |
| **O2** | 1.30E-04 | 1.25E+02 |
| **SOx** | 7.00E-07 | 6.74E-01 |
| **NOx** | 1.78E-08 | 1.71E-02 |
| **GAP-1m** | 0.00E+00 | 0.00E+00 |
| **TEG or D4** | 0.00E+00 | 0.00E+00 |

Flow Rate= 4.71E+06 lb/hr

**Table 57.** Composition and flow rate of stream 4, waste water

| | mass fraction | lb/hr |
|---|---|---|
| **H2O** | 9.99E-01 | 1.12E+05 |
| **CO2** | 1.00E-03 | 1.12E+02 |
| **GAP-1m** | 9.30E-08 | 1.04E-02 |
| **GAP1CARB** | 2.18E-07 | 2.44E-02 |
| **D4** | 4.00E-06 | 4.48E-01 |
| **TEG** | 1.00E-06 | 1.12E-01 |

Flow Rate= 1.12E+05 lb/hr

A second exit stream (stream 5, **Table 58**) from the Desorber prevents buildup of GAP-1m/SOx waste products in the system. This stream has the same composition as the material in the Desorber. It is rich in GAP-$1_m$ and TEG but contaminated with GAP-1m/$SO_x$ compounds. To remove the contaminants, it is proposed that the material is vacuum-distilled. The bottoms will consist of GAP-$1_m$/$SO_x$ compounds (stream 5, **Table 58**). Stream 5 would be disposed of as industrial, non-hazardous waste under Subpart C of RCRA as hazardous waste. The requirements for this disposal and the details of the waste classification are discussed in Section E of this report. The remaining GAP-$1_m$ and TEG is returned to the Desorber. A third, cleaned exit stream is recycled back to the Absorber as part of the continuous $CO_2$ removal system. GAP-$1_m$ and TEG are added to the Absorption tower (stream 6) to replenish that lost in waste streams 2, 4 and 5. Water is recovered from the water wash tower and the total condenser on the $CO_2$ streams are recycled back to the wash tower to replenish that lost in the flue gas.

**Table 58**. Composition and flow rate of stream 5, Desorber purge stream

| | mass fraction | lb/hr |
|---|---|---|
| **GAP-1m** | 6.59E-01 | 1.55E+02 |
| **TEG** | 2.00E-01 | 4.69E+01 |
| **H2O** | 1.41E-01 | 3.31E+01 |
| **GAP-1m/SO2** | 1.00E-06 | 2.35E-04 |

Flow Rate= 2.35E+02 lb/hr

## 7.1.2 Toxicological Effects of Components in the Continuous $CO_2$ Capture Process

### 7.1.2.1 *Absorption/Desorption Process*

The following section details a description of the various toxicological effects of the substances identified above in Section 1.1. A thorough literature search was conducted to examine potential human health effects and eco-toxicity. Where information was lacking for a particular material, the material was either compared to similar substances or Quantitative Structure Activity Relationships (QSARs) models[21] were used to predict toxicity levels of the particular chemical. The EPA has worked with various computer programming companies to develop numerous QSARs programs to predict the hazard and toxicological effects of many chemicals.

The substances of interest for the GAP-$1_m$ / TEG process are: GAP-$1_m$, xylene, methanol, TEG, GAP-$1_m$/$SO_x$, and DDBSA. As shown in **Table 52**, GAP-$1_m$ can be considered as a mixture of two compounds: CAS #2469-55-8 (GAP-0) and CAS #106214-84-0 (GAP-(1-4)). The GAP-$1_m$/$SO_x$ salt is not a registered compound, and toxicity information is not readily available. Typically, acid/primary amine salts are less toxic than the free amine itself. For example, 1, 4 diaminobutane is a linear alkyl amine similar in structure to the GAP materials, except it is a carbon chain. Its National Fire Protection Association (NFPA) rating is Health hazard: 4, Fire: 2, Reactivity Hazard: 0, on a scale of 0-4 where 4 is severe. In contrast, its acid salt, 1, 3-Diaminopropane dihydrochloride, has a NFPA rating of Health hazard: 2, Fire: 0, Reactivity Hazard: 0. The acid salt is much less severe. Thus, for analysis here the toxicity of GAP-$1_m$/$SO_x$ is assumed to be less than or equal to its components, GAP-$1_m$ and $SO_x$. Thus, the substances considered here are: the components of GAP-$1_m$ (CAS #2469-55-8 (GAP-0) and CAS #106214-84-0 (GAP-(1-4)), xylene, methanol, TEG, and DDBSA.

Several literature resources were searched including: MSDS, ATMI[22], REACH compliance registration[23], and SAP EHS Regulatory Content Substance Reports[24]. As discussed in footnote #8, much of the requested toxicology data has not been measured or published for CAS #2469-55-8 (GAP-0) and CAS #106214-84-0 (GAP-(1-4)). Instead, the QSAR models ECOSAR, EPIWIN, Toxtree, PBT Profiler, and T.E.S.T were used to predict potential human health effects and eco-toxicity for these materials. These models use the physical characteristics of the various parts of the chemical structure to predict the characteristics of the whole molecule. For example, molecules that contain the primary amine group, $-NH_2$, are known to have toxicity to fish. The siloxane group is known to be hydrophobic and decompose slowly in the environment. These and other "molecular descriptors" are combined through a series of mathematical equations to predict the hazard and toxicity properties of the entire molecule.

Through the years, the EPA has learned that the accuracy of the aquatic toxicity models (ECOSAR) is limited for very hydrophobic molecules. As the molecule becomes more hydrophobic, less disperses into water, preventing the chemical from contacting aquatic life. A common method of measuring hydrophobicity is the octanol/water partition coefficient (Kow). It is defined as the ratio of a chemical's concentration in n-octanol to its concentration in water at equilibrium. The log Kow is more commonly reported. When the log Kow is less than or equal to 5.0 for fish and daphnid, or 6.4 for green algae, ECOSAR provides reliable toxicity estimates for acute effects. If the log $K_{ow}$ exceeds those general limits, the decreased water solubility of these oleophilic chemicals limits the acute toxicity effects during a 48-hour to 96-hour test. For chronic exposures, the applicable log Kow range is extended up to log

Kow = 8.0. If the log Kow of the chemical exceeds 8.0, no chronic toxic effects are expected even with long-term exposures.[25]

The following sections summarize the results of various tests used to estimate the toxicity to humans and the environment of the chemicals used in the aminosilicone-based $CO_2$-capture process. When available, experimental data were included. If not available, modeling data were included and are indicated as predicted in the tables below. Resource information was also provided for clarification of how the data were obtained.

GAP-$1_m$: CAS# 2469-55-8 (GAP-0) and CAS# 106214-84-0 (GAP-1-4)

Some of the ingestion, eye, and skin effects for GAP-$1_m$ have been experimentally tested previously as shown in **Table 59** and **Table 60**. Generally, GAP-$1_m$ is a severe skin and eye irritant but has low ingestion toxicity. Toxtree and TEST models were used to predict the carcinogenic and mutagenic toxicity of the GAP-$1_m$ compounds. The models suggest low probability of genotoxic, carcinogenic, and mutagenic toxicity.

Since much of the aquatic toxicity data for the GAP-$1_m$ materials needed to be derived from modeling, the log Kow values were calculated to determine if the models are valid for this material. Specifically, the log Kow was calculated for the GAP-x series of x = 0, 1, 2, 3, and 4, the components of GAP-$1_m$. These are plotted in **Figure 91**. It shows that the log Kow values are directly proportional to the molecular weight of the GAP species. The log Kow validity limits are also plotted for fish, daphnia, and algae. ECOSAR model predictions are valid for the CAS# 2469-55-8 (GAP-0) component of GAP-$1_m$ for acute and chronic toxicity to fish, daphnia, and algae. The CAS# 106214-84-0 (GAP-1-4) component is more complex. The molecules become less water soluble as x increases. Thus for x = 1, only acute algae and chronic toxicity predictions are valid. For x = 2, only chronic toxicity predictions are valid. For x = 3 & 4, none of the predictions are valid. Knowing this information, the toxicity predictions were calculated and the results included in **Table 59** for CAS# 2469-55-8 (GAP-0) and **Table 60** for CAS# 106214-84-0 (GAP-1-4). Since GAP-(1-4) (CAS# 106214-84-0) is a mixture of x = 1-4, the most unfavorable, valid toxicity result was used to represent the mixture. The results suggest that the GAP-$1_m$ material can be quite toxic to aquatic ecosystems. This concurs with the results found with analogous organic amines that are known to be harmful to aquatic wildlife.

A second model, EPIWIN, predicted the effect of GAP-$1_m$ on soil-based environments. It suggests that it does not biodegrade easily, tending to persist in the environment. Compounds with siloxane segments are known to degrade slowly.[26] The lipophilic structure of the siloxane chain also tends to adsorb well to soil. A Koc > 500 L/kg suggests that it blends and adheres well to most soils. The results show that both CAS# 2469-55-8 (GAP-0) and CAS# 106214-84-0 (GAP-1-4) adhere well to soil, making it difficult to remove.

The modeling results for Bio-Concentration Factor, are graphed in **Figure 91**. Bio-Concentration Factor (BCF) is the measure of how readily a chemical moves in and out of the lipid layer of the fish. This is important because humans eat fish, possibly consuming concentrated amounts of the chemical. In the model, the BCF values are most affected by the molecular weight, structure, and solubility partition of the compound between non-polar, fatty substances and water. BCF values greater than 5000 are considered to be a concern for potential bioaccumulation in the environment. The BCF values for GAP-1m (x = 0-4) are plotted in **Figure 92**, showing a bell shaped curve. The GAP-0 and GAP-4 have the lowest BCF values while GAP-2 has the highest. It is possible that the model suggests that the molecular weight of GAP-0 is low enough that the fish can excrete the compound without it concentrating in the fat layers. GAP-4 is likely too big to be absorbed. GAP 1, 2, and 3 (especially 2) are small and lipophilic enough to be absorbed and difficult to excrete. As a result, they concentrate in the lipid layer of the fish.

**Table 59.** GAP-0 toxicity

| CAS# 2469-55-8, GAP-0 | Toxicity Test Result | Species | Time (hrs) | Resource/Model Software |
|---|---|---|---|---|
| **Ingestion $LD_{50}$ (mg/kg)** | 500 | Rat | N/A | SiVance MSDS[27] |
| **Eye Irritation/Damage** | Severe Irritant | Rabbit | 24 hours (100 μL) | SiVance MSDS |
| **Dermal $LD_{50}$ (mg/kg)** | >2 g/kg | N/A | N/A | SiVance MSDS**Error! Bookmark not defined.** |
| **Skin Corrosion/Irritation** | Severe Irritant | Rabbit | 24 hours (100 μL) | SiVance MSDS |
| **Predicted Octanol Water Partition Coefficient, log $K_{ow}$** | 4.27 | N/A | N/A | ECOSAR |
| **Predicted Genotoxicity** | Negative | N/A | N/A | Toxtree |
| **Predicted Non-Cancer Toxicity** | Negative | N/A | N/A | Toxtree |
| **Predicted Mutagenicity** | Negative | N/A | N/A | TEST |
| **Predicted Fish Toxicity $LC_{50}$ (ppm)** | 1.54 | N/A | 96 | ECOSAR |
| **Predicted Fish Toxicity $LC_{50}$ (ppm), Chronic** | 0.74 | N/A | N/A | ECOSAR |
| **Predicted Daphnia $LC_{50}$ (ppm)** | 0.24 | Daphnia | 48 | ECOSAR |
| **Predicted Daphnia Toxicity $LC_{50}$ (ppm), Chronic** | 0.020 | Daphnia | N/A | ECOSAR |
| **Predicted Algae $EC_{50}$ (ppm)** | 0.12 | N/A | N/A | ECOSAR |
| **Predicted Algae Toxicity $EC_{50}$ (ppm), Chronic** | 1.02 | N/A | N/A | ECOSAR |
| **Predicted Biodegradability** | Not readily biodegradable | N/A | N/A | EPIWIN |
| **Predicted Soil Adsorption Coefficient, $K_{oc}$ (L/kg)** | 1751 | N/A | N/A | EPIWIN |
| **Predicted Bioconcentration Factor (BCF)** | 305 | N/A | N/A | EPIWIN |

**Table 60.** GAP-1-4 Predicted toxicity based on molecular modeling

| CAS# 106214-84-0, GAP-1-4 | Toxicity Test Result | Species | Time (hrs) | Resource/Model Software |
|---|---|---|---|---|
| **Predicted Ingestion $LD_{50}$ (mg/kg)** | >2444 | Rat | N/A | T.E.S.T. |
| **Intraperitoneal $LD_{50}$ (mg/kg)** | 80 | Mouse | N/A | SiVance MSDS**Error! Bookmark not defined.** |
| **Eye Irritation/Damage** | Severe Irritant | Rabbit | 24 hours (100 µL) | SiVance MSDS |
| **Skin Corrosion/Irritation** | Severe irritant | Rabbit | 24 hours (100 µL) | SiVance MSDS |
| **Predicted Octanol Water Partition Coefficient $K_{ow}$** | See **Figure 90** | N/A | N/A | ECOSAR |
| **Predicted Developmental Toxicity** | Positive | N/A | N/A | Toxtree - GAP1-3 |
| **Predicted Genotoxicity** | Negative | N/A | N/A | Toxtree - GAP1-4 |
| **Predicted Non-Cancer Toxicity** | Negative | N/A | N/A | Toxtree - GAP1-4 |
| **Predicted Mutagenicity** | Negative | N/A | N/A | TEST - GAP1-4 |
| **Predicted Fish Toxicity $LC_{50}$ (ppm), Chronic** | 0.000279 | N/A | N/A | ECOSAR - GAP-2 |
| **Predicted Daphnia $LC_{50}$ (ppm), Chronic** | 0.000967 | N/A | N/A | ECOSAR - GAP-2 |
| **Predicted Algae $EC_{50}$ (ppm), Acute** | 0.014 | N/A | 96 | ECOSAR – GAP-1 |
| **Predicted Algae $EC_{50}$ (ppm), Chronic** | 0.000841 | N/A | N/A | ECOSAR - GAP-2 |
| **Predicted Biodegradability** | Not readily biodegradable | N/A | N/A | EPIWIN |
| **Predicted Soil Adsorption Coefficient, $K_{oc}$ (L/kg)** | >11,250 | N/A | N/A | EPIWIN |
| **Predicted Bioconcentration Factor (BCF)** | See **Figure 91** | N/A | N/A | EPIWIN |

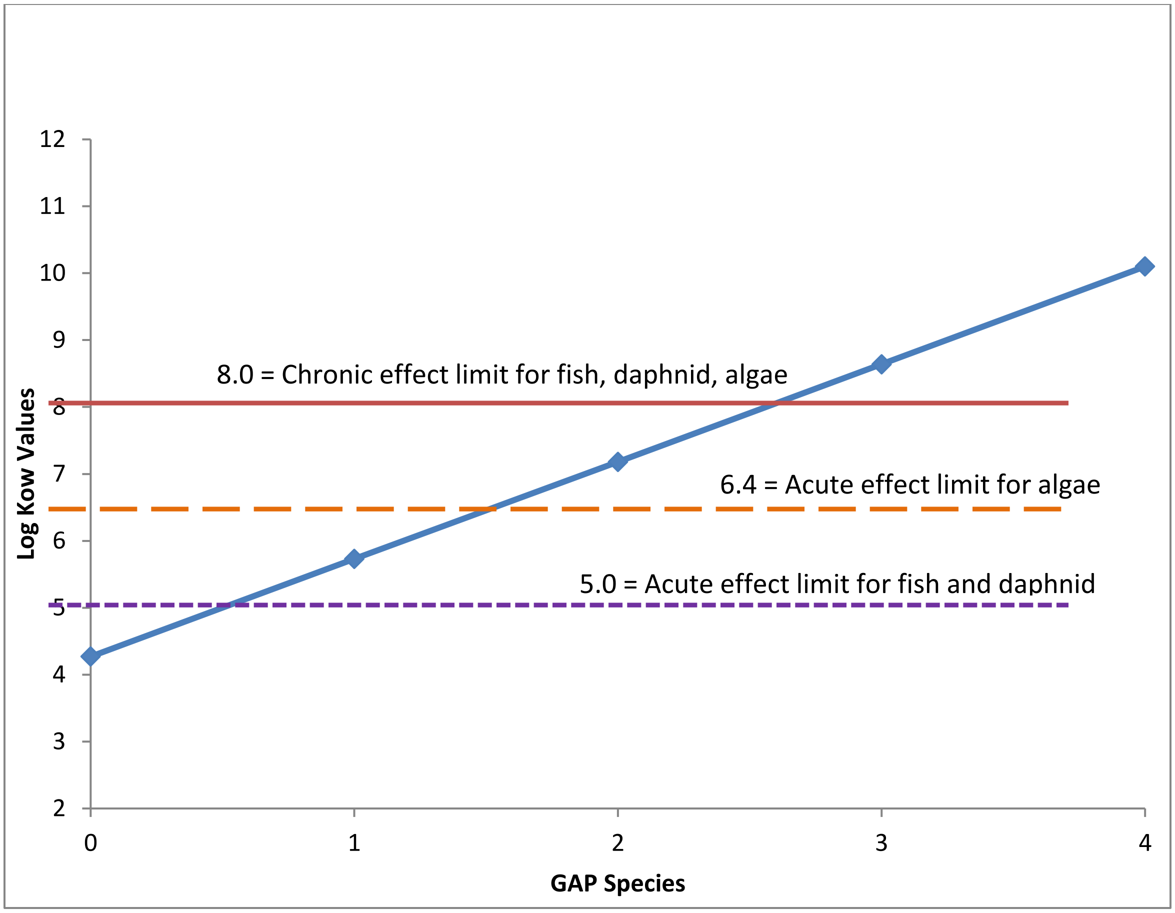


**Figure 91.** Log $K_{ow}$ values of GAP-0-4 with ECOSAR validity limits

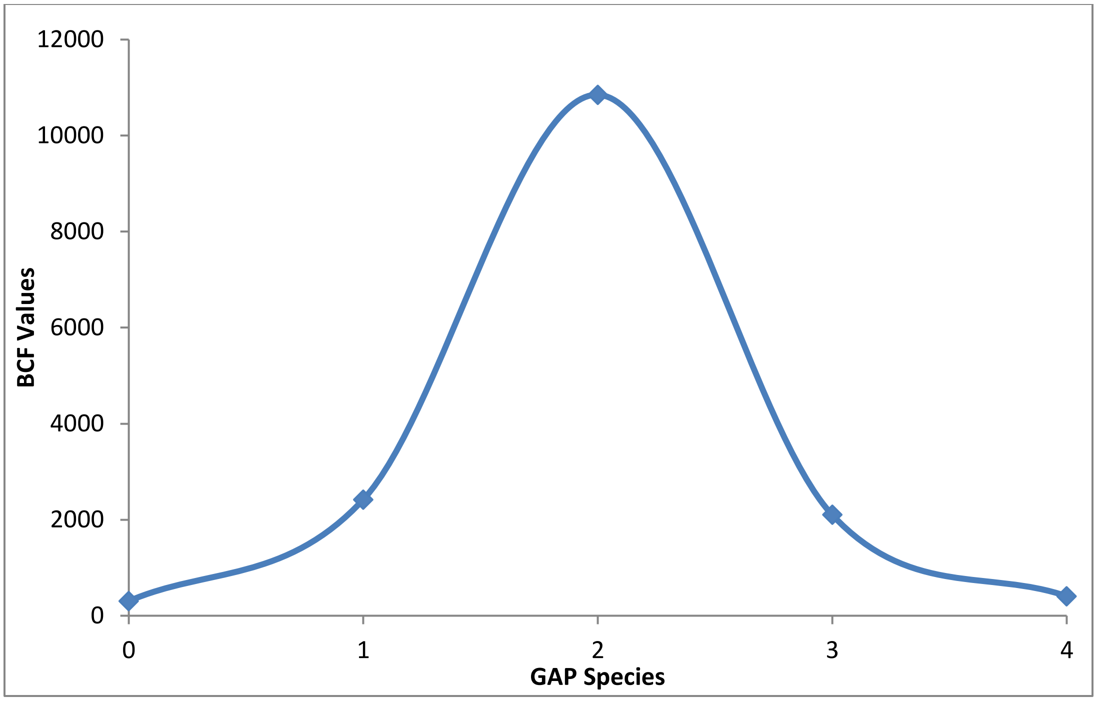


**Figure 92.** Predicted BCF values of GAP-0-4

### Xylene (CAS # 1330-20-7) Toxicological Data

Toxicological data for xylene is more widely available and is included in **Table 61**. Based on the ingestion, dermal and inhalation data, proper ventilation and protective equipment is recommended when using large volumes of xylene. Also, xylene is a severe eye irritant. Proper splash goggles should be worn around xylene. In the Integrated Risk Information System (IRIS), the EPA has documented the oral reference doses (RfD) and the inhalation reference concentration (RfC), defining the daily oral exposure (mg/kg/day) and continuous inhalation exposure (mg/m$^3$), respectively, that are likely to be without appreciable risk of health effects during a lifetime. RfD and RfC values only address the risk of non-cancer effects. For xylene, IRIS has stated “data are inadequate for an assessment of human carcinogenic potential.” [28] The octanol/water partition coefficient of 3.16 suggests that xylene is not very water soluble, but approximately 25 mg/L (LC$_{50}$) is toxic to fish. The BCF value for xylene is a range from 2.14-2.20 to include the three isomeric forms of xylene, suggesting that it is not bio- accumulative in fish (since BCF is less than 5,000). The data also suggest that it is readily biodegradable and does not adsorb well to soil.

**Table 61**. Xylenes toxicological data

| | Toxicity Test Result | Species | Time (hrs) | Resource |
|---|---|---|---|---|
| **Ingestion $LD_{50}$ (mg/kg)** | 4,300 | Rat | N/A | Ashland MSDS[29] |
| **Inhalation $LC_{50}$ (ppm)** | 6,700 | Rat | 4 | Ashland MSDS |
| **Dermal $LD_{50}$ (mg/kg)** | >2,000 | Rabbit | N/A | Ashland MSDS |
| **Developmental Toxicity** | Data Inadequate | N/A | N/A | Acros MSDS[31] |
| **Carcinogenicity** | Data Inadequate | N/A | N/A | Acros MSDS**Error! Bookmark not defined.** |
| **Mutagenicity** | Data Inadequate | N/A | N/A | Acros MSDS**Error! Bookmark not defined.** |
| **Skin Irritation** | Moderate | Rabbit | 24 | Acros MSDS**Error! Bookmark not defined.** |
| **Eye Irritation** | Severe | Rabbit | 24 | Acros MSDS**Error! Bookmark not defined.** |
| **Reference Concentration (RfC) ($mg/m^3$)** | 0.1 | N/A | 24 | IRIS |
| **Reference Dose (RfD) (mg/kg/day)** | 0.2 | N/A | 24 | IRIS |
| **Biodegradability** | readily biodegradable | N/A | N/A | EPA[32] |
| **Soil Adsorption Coefficient, $K_{oc}$ (L/kg)** | 196-311 | N/A | N/A | EPA[32] |
| **Bio-concentration Factor (BCF)** | 2.14-2.20 | N/A | N/A | EPA |
| **Octanol Water Partition Coefficient $K_{ow}$** | 3.16 | N/A | N/A | Ashland MSDS |
| **Fish Toxicity $LC_{50}$ (mg/L)** | 23.53 – 29.97 | Pimephales promelas | 96 | Ashland MSDS |
| **Daphnia $LC_{50}$ (mg/L)** | >100-<1,000 | Daphnia magna | 24 | Ashland MSDS |

## Methanol (CAS # 67-65-1) Toxicological Data

Like xylene, toxicological data for methanol are more readily available and are shown in **Table 62**. The inhalation value of 83.2 mg/L suggests that proper ventilation or respiration protection equipment is needed when working with large volumes of methanol.

The octanol/water partition coefficient is very low because methanol is miscible with water. It readily interacts with aquatic life when mixed with water. The low aquatic toxicity as shown by the >10000 mg/L $LC_{50}$ for fish and Daphnia suggest that use of proper wastewater treatment techniques can be an effective method to eliminate this waste.

**Table 62.** Methanol toxicological data

| | Toxicity Test Result | Species | Time (hrs) | Resource |
|---|---|---|---|---|
| **Ingestion $LD_{50}$ (mg/kg)** | 5,628 | Rat | N/A | Thermo Fisher Scientific MSDS[34] |
| **Inhalation $LC_{50}$ (mg/L)** | >83.2 | Rat | 4 | Thermo Fisher Scientific MSD |
| **Dermal $LD_{50}$ (mg/kg)** | 15,800 | Rabbit | N/A | Thermo Fisher Scientific MSDS |
| **Oral $LD_{50}$ (mg/kg)** | 5,600 | Rat | N/A | Airgas MSDS[35] |
| **Intravenous $LD_{50}$ (mg/kg)** | 2,131 | Rat | 4 | Airgas MSDS |
| **Intraperitoneal $LD_{50}$** | 7,529 | Rat | N/A | Airgas MSDS |
| **Developmental Toxicity** | Negative | N/A | N/A | Methanol Toxicology Review[36] |
| **Carcinogenicity** | Negative | N/A | N/A | Methanol Toxicology Review |
| **Mutagenicity** | Negative | N/A | N/A | Methanol Toxicology Review |
| **Reference Concentration (RfC) ($mg/m^3$)** | 20 | N/A | 24 | IRIS[37] |
| **Reference Dose (RfD) (mg/kg/day)** | 2.0 | N/A | 24 | IRIS |
| **Octanol Water Partition Coefficient $K_{ow}$** | -0.74 | N/A | N/A | Thermo Fisher Scientific MSDS[34] |
| **Biodegradability** | readily biodegradable | N/A | N/A | EPA[38] |
| **Soil Adsorption Coefficient, $K_{oc}$ (L/kg)** | 9 | N/A | N/A | EPA |
| **Estimated Bio-concentration Factor (BCF)** | 0.2 | N/A | N/A | EPA |
| **Fish Toxicity $LC_{50}$ (mg/L)** | 29,400 | Pimephales promelas | 96 | Airgas MSDS |
| **Daphnia $LC_{50}$ (mg/L)** | 23,400 | Daphnia magna | 48 | Thermo Fisher Scientific MSDS**Error! Bookmark not defined.** |

### TEG (CAS# 112-27-6) Toxicological Data

Toxicological data shown in **Table 63** suggest that TEG is not very harmful. An inhalation value of >5.2 mg/kg suggests that proper ventilation or respiration protection equipment is needed when exposed to mists or vapors of TEG. The fish toxicity of 10-100 mg/L suggests that use of proper wastewater treatment techniques is needed before it can be released to the environment.

**Table 63.** TEG toxicological data

| | **Toxicity Test Result** | **Species** | **Time (hrs)** | **Resource** |
|---|---|---|---|---|
| **Ingestion $LD_{50}$ (mg/kg)** | 17,000 | Rat | N/A | Sigma Aldrich MSDS[38] |
| **Inhalation $LC_{50}$ (mg/kg)** | >5.2 | Rat | N/A | Raw Material Supplier Form |
| **Dermal $LD_{50}$ (mg/kg)** | >22,500 | Rabbit | N/A | Sigma Aldrich MSDS |
| **Skin Irritation** | Mild Skin Irritation | Human | 24 | Sigma Aldrich MSDS |
| **Eye Irritation** | Mild Eye Irritation | Rabbit | 24 | Sigma Aldrich MSDS |
| **Fish Toxicity $LC_{50}$ (mg/L)** | 10-100 | Fish | 96 | Raw Material Supplier Form |
| **Daphnia $LC_{50}$ (mg/L)** | 48,900 | Daphnia magna | 48 | Dow MSDS[39] |
| **Algae $EC_{50}$ (mg/L)** | >100 | Pseudokirchneriella subcapitata | 168 | Dow MSDS[39] |
| **Biodegradability** | readily biodegradable | N/A | N/A | Dow MSDS[39] |
| **Estimated Soil Adsorption Coefficient, $K_{oc}$ (L/kg)** | 10 | N/A | N/A | Dow MSDS[39] |
| **Estimated Bio-concentration Factor (BCF)** | <100 | N/A | N/A | Dow MSDS[39] |
| **Estimated Octanol Water Partition Coefficient $K_{ow}$** | -1.75 | N/A | N/A | Dow MSDS[39] |
| **Carcinogenicity** | Negative | Lab Animals | N/A | Dow MSDS[39] |
| **Developmental Toxicity** | Negative | Lab Animals | N/A | Dow MSDS[39] |
| **Reproductive Toxicity** | Negative | Lab Animals | N/A | Dow MSDS |
| **Genotoxicity** | Negative | Lab Animals | N/A | Dow MSDS |

## DDBSA (CAS # 27176-87-0) Toxicological Data

The toxicological data for DDBSA are provided in **Table 64**. The predicted fish toxicity $LC_{50}$ and predicted Algae $EC_{50}$ values are listed as no effects at saturation (NES). According to ECOSAR, no effects are expected if these values are greater than 10 times the solubility in water, which is predicted to be 0.7032 mg/L. Since these values were predicted to be above that limit, they are not included in the table. It should be noted that the other aquatic toxicity values listed in the table are also above the solubility of DDBSA in water, though below the 10X solubility limit required for NES classification.

**Table 64.** DDBSA toxicological data

| | **Toxicity Test Result** | **Species** | **Time (hrs)** | **Resource/Model Software** |
|---|---|---|---|---|
| **Ingestion $LD_{50}$ (mg/kg)** | 650 | Rat | N/A | MSDS[40] |
| **Eye Irritation/Damage** | Severe irritant | N/A | N/A | MSDS[40] |
| **Skin Corrosion/Irritation** | Severe irritant | N/A | N/A | MSDS[40] |
| **Predicted Octanol Water Partition Coefficient, log $K_{ow}$** | 4.784 | N/A | N/A | ECOSAR |
| **Predicted Genotoxicity** | Negative | N/A | N/A | Toxtree |
| **Predicted Non-Cancer Toxicity** | Negative | N/A | N/A | Toxtree |
| **Predicted Mutagenicity** | Negative | N/A | N/A | TEST |
| **Predicted Fish Toxicity $LC_{50}$ (ppm)** | NES | N/A | 96 | ECOSAR |
| **Predicted Fish Toxicity $LC_{50}$ (ppm), Chronic** | 1.121 | N/A | N/A | ECOSAR |
| **Predicted Daphnia $LC_{50}$ (ppm)** | 6.218 | Daphnia | 48 | ECOSAR |
| **Predicted Daphnia Toxicity $LC_{50}$ (ppm), Chronic** | 1.24 | Daphnia | N/A | ECOSAR |
| **Predicted Algae $EC_{50}$ (ppm)** | NES | N/A | 96 | ECOSAR |
| **Predicted Algae Toxicity (ppm), Chronic** | 6.225 | N/A | N/A | ECOSAR |
| **Predicted Biodegradability** | Not readily biodegradable | N/A | N/A | EPIWIN |
| **Predicted Soil Adsorption Coefficient, $K_{oc}$ (L/kg)** | 3707 | N/A | N/A | EPIWIN |
| **Predicted Bioconcentration Factor (BCF)** | 71 | N/A | N/A | EPIWIN |

The BCF is significantly below 5000, so very little bioaccumulation in fish is expected. DDBSA is a severe irritant and is known to cause burns to skin, eyes, the digestive tract, and respiratory system.

### 7.1.3 Physical Properties of the Materials in the $CO_2$ Capture Process

The volatility, flammability, chemical reactivity, corrosivity, and other physical property data were collected from various databases and included in **Table 65** below. Data were collected for GAP-$1_m$, TEG, xylenes, methanol, and DDBSA. The information aids in the design and engineering of the $CO_2$ absorption/desorption system. It also helps in understanding how to handle and work with each chemical compound. The volatility and flash point data suggest that GAP-$1_m$ and TEG are not very volatile or flammable, but xylene and methanol are. All of the compounds react with oxidizing agents. GAP-$1_m$ and DDBSA are corrosive materials, but TEG, xylenes, and methanol are not. The storage and handling of these materials is discussed more fully in Section H.

**Table 65.** Physical properties of the $CO_2$ capture solution components

| | **GAP-1$_m$**Error! Bookmark not defined. **Stream 6** | **TEG[41] Stream 6** | **Xylenes Stream 7** | **Methanol Stream 4** | **DDBSA, Stream 4** |
|---|---|---|---|---|---|
| **Volatility (Evap. Rate)** | <1<br>(butyl acetate = 1) | <0.001 (butyl acetate = 1) | 0.86<br>(butyl acetate = 1) | 4.6 (butyl acetate =1) )[42] | Not available |
| **Flash Point** | >100 °C | 177 °C | 26.66 °C | 12 °C | > 200°C |
| **Lower Explosion Limit/Upper Explosion Limit** | Not available[43] | 0.9 % (V)/ 9.2 % (V) | 1.0 % (V)/ 7.0 % (V) | 6.0 % (V)/ 31.00 % (V) | Not available |
| **Auto-Ignition Temperature** | No data available | 349 °C | 527 °C | 455 °C | Not available |
| **Chemical Reactivity** | May react with oxidizing agents | May react with oxidizing agents | May react with oxidizing agents | May react with oxidizing agents | May react with metals, strong oxidizing agents, strong bases |
| **Corrosivity** | Corrosive | Not Corrosive | Not Corrosive | Not Corrosive | Corrosive |
| **State, STP** | Liquid | Liquid | Liquid | Liquid | Liquid |
| **Color** | Brownish | Colorless | Colorless | Colorless | Brown |
| **Odor** | Amine-like | Odorless | Mild, aromatic | Alcohol-like | Sulfur dioxide odor |
| **Melting Point** | ~ -90 °C | -7 °C | -47.00 °C | -98 °C | 10°C |
| **Boiling Point** | >155 °C | 288.0 °C | 137-140 °C | 64.7 °C | 315°C |
| **Vapor Pressure** | <0.13 kPa @ 20 °C | <0.001kPa @ 20 °C | 0.93 kPa @ 20 °C[44] | 12.8 kPa @ 20 °C | Not available |
| **Vapor Density** | >1<br>(Air = 1.0) | 5.2<br>(Air = 1.0) | 3.66<br>(Air = 1.0) | 1.11<br>(Air = 1.0) | Not available |
| **Density** | 0.93 g/cm$^3$@ 20 °C | 1.124 g/ cm$^3$ @ 20 °C | 0.86 g/cm$^3$ @20 °C | 0.791 g/ cm$^3$ @ 20 °C | 1.2 g/cm$^3$ |
| **Water Solubility** | Very slightly soluble in cold water | Soluble in water | Negligible (practically insoluble) | Soluble in water | Soluble in water |
| **Solubility Properties** | Soluble in chloroform, toluene, hexanes | Soluble in ethanol, benzene, ether | Ether; soluble in many organic liquids, alcohol | Ethanol, ether and many other organic solvents[45] | Not available |

### 7.1.4 U.S. EH&S Law Compliance and Regulation Implications for the $CO_2$ Capture Process

The compliance of the chemicals used in and potential emissions from the proposed continuous $CO_2$ absorption/desorption system to United States Environmental, Health, and Safety regulations is summarized below. The resulting implications on the proposed technology are also addressed. The applicable U.S. EH&S laws addressed include: Toxic Substances Control Act (TSCA), Comprehensive Environmental Response and Liability Act of 1980 (CERCLA), Clean Water Act (CWA), Clean Air Act (CAA), Superfund Amendments and Reauthorization Act (SARA) Title III, the Occupational Safety and Health Act (OSHA), and the Resource Conservation and Recovery Act (RCRA). **Table 66** summarizes the initial list of streams from the process (**Figure 90**) that were considered in preparing the regulatory review.

**Table 66.** Streams considered for regulatory review

| Stream # | Components | Comments |
|---|---|---|
| 1 | Flue gas | This stream would come directly from the plant and is not included in the regulatory review of this specific process. |
| 2 | Clean flue gas | This process does not add any components to this stream. It is not discussed further in the regulatory review. |
| 3 | $CO_2$ product | This stream is not a concern for the regulatory review and is not discussed further in this section. |
| 5 | GAP-$1_m$/SOx salts | -- |
| 6 | GAP-1/TEG make-up stream, includes xylene and methanol | -- |
| 7 | Xylene | -- |
| 12 | GAP-$1_m$, DDBSA | -- |
| 13 | Water, TEG, methanol, xylene | -- |

The following individual components are the primary focus of this review, based on the summary in **Table 66**:

- GAP-0
- GAP-1-4
- TEG
- Xylene

- DDBSA
- Methanol
- GAP-$1_m$/$SO_x$ salts

A summary of the applicable regulations for each of these components is provided in **Table 67**. Each regulation is discussed separately in the following sections. All substances are marked as being regulated by RCRA. This indicates that all of these materials are potential waste products of this process and would, therefore, be regulated under RCRA Subpart C or D. This table does not indicate hazardous or non-hazardous waste classification. For a detailed discussion of those classifications for each waste stream, see the RCRA section of this report.

**Table 67.** Regulatory overview for components of $CO_2$ capture system

| | TSCA | CERCLA RQ (lbs) | CWA | CAA HAP | CAA VOC | SARA 302 EHS | SARA 311/312 | SARA 313 | OSHA Regulated | RCRA |
|---|---|---|---|---|---|---|---|---|---|---|
| CAS#2469-55-8, GAP-0 | Y | N | N | N | Y | N | Acute<br>Fire | N | Y | Y |
| CAS#106214-84-0, GAP-1-4 | Y | N | N | N | Y | N | Acute | N | Y | Y |
| CAS#1330-20-7, Xylene | Y | 100 | Y | Y | Y | N | Acute<br>Chronic<br>Fire | Y | Y | Y |
| CAS#67-65-1, Methanol | Y | 5000 | N | Y | Y | N | Acute<br>Chronic<br>Fire | Y | Y | Y |
| CAS#112-27-6, TEG | Y | N | N | N | Y | N | Acute | N | Y | Y |
| CAS#27176-87-0, DDBSA | Y | 1000 | Y | N | Y | N | Acute | N | Y | Y |
| GAP-1/SOx salts | N | N | N | N | N | N | N | N | Y | Y |

## TSCA

GAP-0, GAP-1-4, xylene, methanol, TEG, and DDBSA are all on EPA's TSCA Inventory allowing companies to manufacture and use the chemical commercially.

## Clean Water Act

Xylene and DDBSA are designated as hazardous substances to the water supply in accordance with Section 311(b)(2)(A) of 40 CFR 116, the Clean Water Act (CWA).[46] As with CERCLA, the minimum reportable quantities for xylene and DDBSA are 100 lbs/day and 1000 lbs/day (40 CFR § 117.3), respectively.

## Clean Air Act

Xylene and methanol are also both regulated Hazardous Air Pollutants (HAPs) and Volatile Organic Compounds (VOCs) under the Clean Air Act (CAA).[47] GAP-$1_m$, TEG, and DDBSA are also VOCs. VOCs are defined in this case as any compound of carbon that participates in atmospheric photochemical reactions. Certain exclusions are listed in the regulatory definition (40 CFR §51.100(s)). The potential release rate for these chemicals for a 550 MW power plant is lower than required for reporting.

## SARA

None of these chemicals pose an immediate hazard to a community upon release as described by EPA's SARA 302 list. For Safety Data Sheet reporting (SARA 311/312), GAP-0, GAP-1-4, xylene, methanol, TEG, and DDBSA are considered as acute, immediate health hazards. Xylene and methanol are considered to be chronic, delayed health hazards, and GAP-0, xylene, and methanol are considered as fire hazards. SARA 313 rules require reporting chemical releases of xylene and methanol to public and government officials.[48]

## OSHA

All of the chemicals are regulated by OSHA, requiring proper safety data sheet, handling, shipping, and storage equipment. Safe handling and storage are discussed in further detail in Section G of this report.

## RCRA Subpart C requirements

### Generator requirements

Specific requirements for hazardous waste handling depend on the generator classification based on the quantity of hazardous waste generated per month. The only stream from this process for which the Subpart C requirements are relevant is stream 7.

The quantity of xylene generated based on the mass balance for stream 7 is estimated to be 28.4 lbs per month (calculated assuming 310.25 working days per year), or 12.9 kg per month. This would classify this process as a Conditionally Exempt Small Quantity Generator (CESQG) based on the RCRA definition and it would be exempt from RCRA requirements for this waste stream. CESQG facilities are required to identify their hazardous waste, comply with storage limit requirements, and ensure waste treatment or disposal. Locations for disposal or waste treatment for CEQSG facilities include:[48]

- Permitted or interim status hazardous waste transport, storage, and disposal facilities (TSDFs)
- State hazardous waste facilities
- State permitted, licensed, or registered solid waste disposal facilities
- State municipal solid waste landfills
- Recycling facilities
- Universal waste facilities

Depending on the classification of the overall power plant, small quantity generator (SQG) requirements may be applicable since it would add to existing hazardous waste streams at the power plant. In general, SQGs need to do the following:

- Identify and count waste
- Obtain an EPA ID number
- Comply with accumulation and storage requirements
- Prepare the waste for transportation
- Track the shipment and receipt of such waste
- Meet recordkeeping and reporting requirements

Since the exact requirements for hazardous waste disposal would vary based on plant classification and plant location, they are not discussed in detail in this assessment but would need to be evaluated on a site-specific basis.

<u>TSDF</u>

RCRA excludes generators from the permit requirements for TSDFs as long as the generators accumulate waste on-site in accordance with the generator regulations. It is assumed that this process would comply with the necessary generator requirements and would, therefore, not be subject to TSDF regulations.

### 7.1.5 Engineering Analysis and Controls for the $CO_2$ Capture Process

The entire system requires some plant-wide engineering controls. Many of these are common in the chemical industry but might be new for a power plant facility. For example:

1) To protect groundwater, a double containment drain system is necessary. These keep rainwater separated from any chemical drainage system, not allowing them to mix. The containment system should be built with chemical resistant, high strength concrete.
2) A volatile vapor detection sampling and monitoring system is necessary to identify when leaks occur. This is especially important for VOCs like xylene and methanol.
3) A pressure/relief, vapor condensation/recovery system should be considered for all vessels. This prevents undesired backflow from one vessel to another, and it is required to minimize leaks and meet VOC release standards.
4) The equipment and piping arrangement chosen for the system should be designed to minimize leaks. For example, a shell & tube heat exchanger is much better than a plate & frame heat exchanger for minimizing leaks. The large number of gaskets in the plate & frame are all potential VOC emission points.
5) The gas streams, #2 and #3 in **Figure 90**, require a final gas polishing process like an activated carbon absorption bed. This removes any remaining VOCs, lowering potential emissions.
6) The thermal oxidizer equipment requires its own safety failure analysis. Equipment like detonation arrestors, back-flow valves, etc. is needed. Vendors of such equipment are well versed in the requirements and design of a specific unit, which is outside to scope of this task.[49]

### 7.1.6 Handling and Storage for the $CO_2$ Capture Process

This section describes the precautions necessary for safe handling and storage of the chemicals used in the $CO_2$ absorption/desorption system. The applicable rules and standards of the Occupational Safety and Health Act (OSHA) are summarized, including safe storage, incompatibilities with other materials, waste treatment and offsite disposal options, accidental release measures, and protective equipment suggestions. The following section provides handling and storage recommendations for GAP-$1_m$, TEG, xylene, methanol, sulfur dioxide, and DDBSA. As discussed in Section C, the toxicity of GAP-$1_m$/$SO_x$ is assumed to be less than or equal to its components, GAP-$1_m$ and $SO_x$. Details of handling and storage of GAP-$1_m$/$SO_x$ is not available but is assumed to be less rigorous than those needed for its components.

a) *GAP-$1_m$ (CAS# 106214-84-0 and 2469-55-8)*

GAP-$1_m$ is classified as a hazardous chemical by the OSHA Standard. It is regulated under both DOT and IATA as a corrosive liquid. Its NFPA Classification is a 3 for health hazard, 1 for flammability, and 0 for reactivity.

1) Storage and Handling Recommendations

GAP-$1_m$ should be stored in a phenolic lined drum or pail and away from acids and oxidizers. When it is burned, it decomposes into carbon monoxide, carbon dioxide, nitrogen oxides, and silicone dioxide. The material should be used in an area with adequate ventilation

2) Accidental Release Measures

When a spill occurs, one should evacuate the area and alert trained spill officials. Those trained to work with spills should wear a respirator when ventilation is not adequate and wear proper personal protect equipment. The spill team should keep those untrained and unprotected from entering the spill area. Also, they should prevent others from touching or walking through the contaminated area. For environmental protection, do not allow the material to be dispersed or come in contact with drains, sewers, soil or any water source. Use an absorbent barrier to prevent contamination into the environment. When or if the material comes in contact with the environment, notify the local authorities immediately.

3) Health Effects and Exposure limits

It is corrosive to the skin, eyes, digestive tract, and respiratory system and may cause burns. Use the material in a well-ventilated area.**Error! Bookmark not defined.** Overexposure to GAP-$1_m$ can cause respiratory irritation, coughing, stomach pains, skin redness, and watering or redness of the eyes. The PEL has not been established for this chemical. Since GAP-$1_m$ has a high boiling point, the amount that vaporizes at ambient conditions is very low.

4) Respiratory Protection Recommendation

If the vapor concentration of GAP-$1_m$ exceeds 2000 ppmv, a full-faced respirator with an olive cartridge is recommended. A cartridge designed for amines is recommended.

5) Hand and Eye Protection Recommendation

When using GAP-$1_m$, chemical resistant gloves should be worn. Butyl rubber and neoprene are recommended. These gloves have an estimated breakthrough time of more than 8 hours. The recommended eye protection is splash goggles or a face shield.

6) Skin and Body Protection Recommendation

The risk of exposure for the production area needs to be evaluated to determine proper body protection. For low risk exposure of only hands, butyl or neoprene gloves are recommended. For high risk exposure, a rubberized acid suit is recommended.,[50]

*b) <u>Triethylene Glycol (CAS# 112-27-6)</u>*

Triethylene Glycol (TEG) is not known as an OSHA hazard. Its NFTP Classification is a 0 for health hazard, 1 for flammability and 0 for reactivity. It is not regulated by the Department of Transportation (DOT) or International Air Transport Association (IATA).

1) Storage and Handling Recommendations

It is recommended that the material be kept in a tightly closed container in a dry, well-ventilated area. Triethylene glycol is hygroscopic, requiring a storage container that minimizes exposure to moisture. Iron can contaminate the material. To avoid contamination from iron, the use of stainless steel, aluminum, phenolic or epoxy resin lined vessels is recommended.[51] Avoid storing this chemical near strong oxidizing agents, strong acids, or bases because triethylene glycol reacts with these materials. An exothermic reaction can take place when TEG mixes with strong acids and oxidizing agents. These reactions often produce a toxic, flammable gas and could lead to an explosion. Special examples of common chemicals that should be avoided are acetic acid and anhydrides.[52] In a fire, triethylene glycol can decompose to carbon monoxide and carbon dioxide.

2) Accidental Release Measures

In the case of a spill or accidental release, evacuate personnel to a safe area. Ensure adequate ventilation and inform trained clean-up professionals of the spill. Only allow these trained officials to enter the spill area wearing the proper protective equipment (including a respirator, if necessary).

Barriers should be placed around the spill to prevent TEG from entering drains or other water sources. Inert absorbent material should be used to cleanup and contain the spill. Contaminated material should be disposed as hazardous waste in closed containers.

3) Health Effects and Exposure Limits

If triethylene glycol is inhaled, it may cause respiratory tract irritation. It may also cause skin and eye irritation. The material is not classified as hazardous under OSHA. No exposure limit data were available.

4)Respiratory Protection Recommendation

At room temperature, exposure to vapor is expected to be small due to low volatility, but at elevated temperatures, vapors may cause irritation of the upper respiratory tract (nose and throat). In such cases, respiratory protection should be worn when exposure to TEG vapors and mists are likely. In misty atmospheres, use an approved air purifying respirator with an organic vapor cartridge and a particulate pre-filter.[53]

5) Hand and Eye Protection Recommendation

Triethylene glycol should be handled with gloves. They should be inspected prior to use. If one is going to be in full contact with TEG, nitrile rubber gloves with a minimum layer thickness of 0.11 mm are recommended. The nitrile gloves have a break through time of >480 min. For splash protection when working with TEG, a nitrile rubber apron should also be worn. For eye protection, safety glasses with side shields are recommended.

6) Skin and Body Protection Recommendation

Prolonged skin contact is unlikely to result in absorption of harmful amounts. Massive contact with damaged skin or of material sufficiently hot to burn skin may result in absorption of potentially lethal amounts. Still, avoid contact with skin and clothing. Wash thoroughly after handling. Use protective clothing chemically resistant to this material, including such items as gloves, face-shields, boots, apron, or a full-body suit, depending upon the task. When handling hot material, protect skin from thermal burns as well as from skin absorption.

*c) Xylene (CAS# 1330-20-7)*

Xylene is classified as a hazardous chemical by the OSHA Standard. It is regulated under both DOT and IATA as a flammable liquid (hazard class 3) with the proper shipping name xylenes. Its NFPA Classification is a 2 for health hazard, 3 for flammability, and 0 for reactivity.

1) Storage and Handling Recommendations

Xylene is a flammable liquid (flash point is 80oF/26.7oC). Handle material away from heat, flames, and sparks. When handling xylene, vessels need to be grounded before transfer or use of material. The material should be used in a cool, dry, and well ventilated area. Xylene should not be handled near alkalis, strong acids, and strong oxidizing agents.

2) Accidental Release Measures

When a spill occurs, spill team authorities should be alerted. All personnel should be evacuated to a safe area away from the spill. Unauthorized individuals should not be allowed to enter the area without proper protective equipment. Xylene is a flammable material; therefore, all sources of ignition (fire, electrical sparks, etc.) should be eliminated. Prevent vapors from building up by providing proper ventilation.

Xylene spills should be contained by non-combustible absorbent materials. Some examples of these materials are sand, vermiculite, and diatomaceous earth. The contaminated absorbent material should be disposed in accordance with national and local regulations pertaining to waste disposal. Xylene should be kept from entering drains and not flushed into the sewer system during the clean-up process. If the material is not able to be contained and gets into the environment, local authorities must be notified immediately.

### 3) Health Effects and Exposure Limits

Xylene may affect the central nervous system leading to dizziness, headache, or nausea. It may cause mild eye irritation with symptoms include stinging, tearing, or redness. It can also cause skin and respiratory tract irritation. Prolonged skin exposure may lead to burns, redness and cracking of the skin. Swallowing the material may lead to lung inflammation or other lung injury. Breathing small amounts (below the permissible exposure limits) of the material will not likely cause any harmful effects. Some symptoms from exposure to xylene include: nausea, vomiting, diarrhea, redness of the skin, inhalation irritation, chest discomfort, shortness and slowness of breath, lack of coordination and memory, irregular heartbeat, narcosis, coma, and central nervous system excitation followed by depression. Exposure to xylene may aggravate pre-existing medical issues relating to the lung, kidney, heart, skin, central nervous system, male reproductive system, and auditory system.

Overexposure to xylene by laboratory animals led to the following effects: testis damage, kidney and liver damage, effects on hearing, cardiac sensitization, and harm to animal fetuses. Also overexposure can lead to effects on the central nervous system. For xylenes, the PEL is 100 ppm or 435 mg/m$^3$ during 8 hrs. The Short Term Exposure Limit (STEL) is 150 ppm or 655 mg/m$^3$ over 15 minutes. The Immediately Dangerous to Life and Health (IDLH) limit is 900 ppm.

### 4) Respiratory Protection Recommendation

Typically, the PEL and IDLH are used to determine the threshold limit for implementation of respirators. From 100 to 900 ppm, an approved air-purifying respirator with an organic vapor cartridge is required. A full-faced respirator with organic cartridges is required when emptying a vessel of xylene, reducing the risk of exposure to vapors and in case of a flash fire. [54]

5) Hand and Eye Protection Recommendation

When working with xylene, one should wear butyl or neoprene gloves which should be inspected prior to use. Wash hands after glove removal. Either a face shield or splash goggles is recommended when working with xylene.

6) Skin and Body Protection Recommendation

Since xylene is a flammable material, one should wear flame resistant protective clothing, especially when handling large quantities. The proper protective attire should be determined by the amount of the chemical being handled and the environment of the plant.

*d) Methanol (CAS# 67-56-1)*

Methanol is classified as a hazardous chemical by the OSHA Standard. It is regulated under both DOT and IATA as a flammable liquid (hazard class 3) with the proper shipping name methanol. Its NFPA Classification is a 2 for health hazard, 3 for flammability, and 0 for reactivity.

1) Storage and Handling Recommendations

Due to the flammability of methanol (flash point is 53.6°F/ 12°C), it should be handled away from hot surfaces, ignition sources, and open flames. When handling methanol, containers storing the material should be grounded or electrically bound before transfer or use of material. The material should be used in a cool, dry, and well ventilated area.

Methanol should not be handled near strong acids, acid anhydrides, acid chlorides, strong bases metals, peroxides, or strong oxidizing agents

2) Accidental Release Measures

When a spill occurs, spill team authorities should be alerted. All personnel should be evacuated to a safe area away from the spill. Unauthorized individuals should not be allowed to enter the area without proper protective equipment. Methanol is a flammable material; therefore, all sources of ignition (fire, electrical sparks, etc.) should be eliminated. Prevent vapors from building up by providing proper ventilation. Methanol spills should be contained by inert absorbent materials. The contaminated absorbent material should be collected and stored in suitable containers for disposal. These containers shall be disposed of in accordance with national and local regulations pertaining to flammable waste disposal. Methanol should be kept from entering drains and not flushed into the sewer system during the clean-up process. If the material is not able to be contained and gets into the environment, local authorities must be notified immediately.

### 3) Health Effects and Exposure Limits

The organs targeted by methanol are the central nervous system, eyes, skin, respiratory system, optic nerve, liver, kidney, spleen, blood, and the gastrointestinal tract (GI). The acute effects are irritation to eyes, skin, and respiratory tract. Research has shown, prolonged exposure (inhalation, dermal, and ingestion) can lead to serious irreversible effects. Methanol has been shown to cause liver and kidney problems along with reproductive toxicity effects.
The PEL is 200 ppm or 260 mg/m$^3$ during 8 hrs. The Short Term Exposure Limit (STEL) is 250 ppm or 325 mg/m$^3$ over 15 minutes. The IDLH level is 6000 ppm.

### 4) Respiratory Protection Recommendation

A full-faced respirator with organic cartridges is recommended.

### 5) Hand and Eye Protection Recommendation

Methanol should be handled with butyl rubber or neoprene gloves. Wash hands after glove removal. Tightly fitting safety goggles or splash goggles are recommended.

### 6) Skin and Body Protection Recommendation

Since methanol is a flammable material, one should wear flame retardant or resistant antistatic protective clothing and boots, especially when handling large quantities. The proper protective attire should be determined by the amount of the chemical being handled. The Methanol Institute recommends the following:

"For routine unloading of methanol where splashing or skin absorption is not anticipated, natural fiber clothing (cotton) is adequate. Avoid wearing synthetic fiber clothing when there is a risk of fire from handling methanol. A chemical resistant apron, butyl or nitrile rubber gloves, and rubber boots, and a full face-shield worn over goggles for additional protection, (but not as a substitute for goggles), may be needed where there is a risk of splashing, such as in coupling and uncoupling hoses or lines. Chemical-resistant clothing/materials should be worn if repeated or prolonged skin contact with methanol is expected. Respiratory protection should be selected based on hazards present and the likelihood of potential exposure. Air purifying respirators with organic vapor (OVA) cartridges are not appropriate protection against methanol vapors due to the very short service life of the OVA cartridge before it becomes saturated, and there are no means of knowing when the vapors break through and the cartridge is no longer offering protection. The use of a supplied air respirator with a full face piece operated in a pressure-demand or other positive-pressure mode is the recommended respiratory protection. Personal protection equipment for the responders should, at a minimum, include chemical splash goggles and face shield, butyl or nitrile gloves, rubber boots, chemical resistance coveralls, and provision for supplied fresh breathing air, such as full face, positive pressure SCBA. Fire resistant clothing is only necessary when fighting a fire. For more information on methanol personal protective equipment consult Chapter 4.2.2 of the Methanol Institute's Methanol Safe Handling Manual."[55]

### *e) <u>DDBSA (CAS# 27176-87-0)</u>*

DDBSA is classified as hazardous by the OSHA Standard based on corrosivity[56]. It is regulated under both DOT and IATA as a corrosive material. Its NFPA Classification is a 3 for health hazard, 0 for flammability, and 0 for reactivity.

#### 1) Storage and Handling Recommendations

This material should be stored in a cool, dry place and the container kept closed when not in use. It should be kept away from oxidizing materials, metals, and alkaline substances. It should be used in a well-ventilated area.

#### 2) Accidental Release Measures

In the case of a spill, personnel should be evacuated to a safe area and trained spill control officials should be notified. The area should be ventilated and the material absorbed with inert materials (e.g. vermiculite, sand or earth). For environmental protection, precautions should be taken to avoid any runoff into drains, storm sewers, or ditches.

#### 3) Health Effects and Exposure Limits

DDBSA causes severe burns to skin and eyes and may cause irreversible eye injury. It is harmful to the digestive tract and respiratory system. The material should be used in a well-ventilated area. No OSHA PEL has been established for this chemical.

4) Respiratory Protection Recommendation

No specific recommendations for exposure limits for respirator usage were available. When risk assessment indicates it is necessary, respirators should meet OSHA 29 CFR 1910.134 and ANSI Z88.2 requirements.

5) Hand and Eye Protection Recommendations

Appropriate gloves and safety glasses/splash goggles should be worn during use.

6) Skin and Body Protection Recommendation

At a minimum, gloves should be worn. The need for additional protective clothing should be evaluated based on the concentration and amount of chemical used.

## 7.2 GAP-$1_m$ Manufacturing Process

### 7.2.1 Air, Water, and Solid Waste Identification

This section describes the potential ancillary or incidental air, water, and solid wastes and estimates their magnitude for the manufacturing process of GAP-$1_m$. In addition to the chemical inputs to the manufacturing process, the potential by-products and waste streams were considered.

The overall manufacturing process is shown in **Figure 93**. For the overall mass balance for the process, both the requirements for the initial fill for the $CO_2$-capture system on a 550 MW power plant (**Table 68**) and for the annual GAP-$1_m$ make-up stream were calculated (**Table 69**). The initial fill for the system used for the calculation was 1785 tons. Based on the mass balance completed for the $CO_2$-capture system (see Section B), the annual requirement for GAP-$1_m$ make-up is 359 tons/year, based on an assumption of 310.25 working days per year.

The first unit operation consists of the reaction of allyl chloride (stream M10) with potassium cyanate (stream M11) in a methanol solvent (stream M12) at elevated temperatures and under pressure to form methyl N-allylcarbamate and potassium chloride. The reaction mixture is cooled and the solid potassium chloride removed by filtration (stream M1). The crude product is stripped to remove methanol which is recycled (stream M5) back to the first step. The crude product is dissolved in xylene (stream M6) and any methylcarbamate by-product formed during the reaction is removed with a water wash (stream M2). The xylene layer is separated from the aqueous layer and the methyl N-allylcarbamate product is isolated by initially stripping off the xylene solvent for reuse (stream M6) and then distilling the product under reduced pressure.

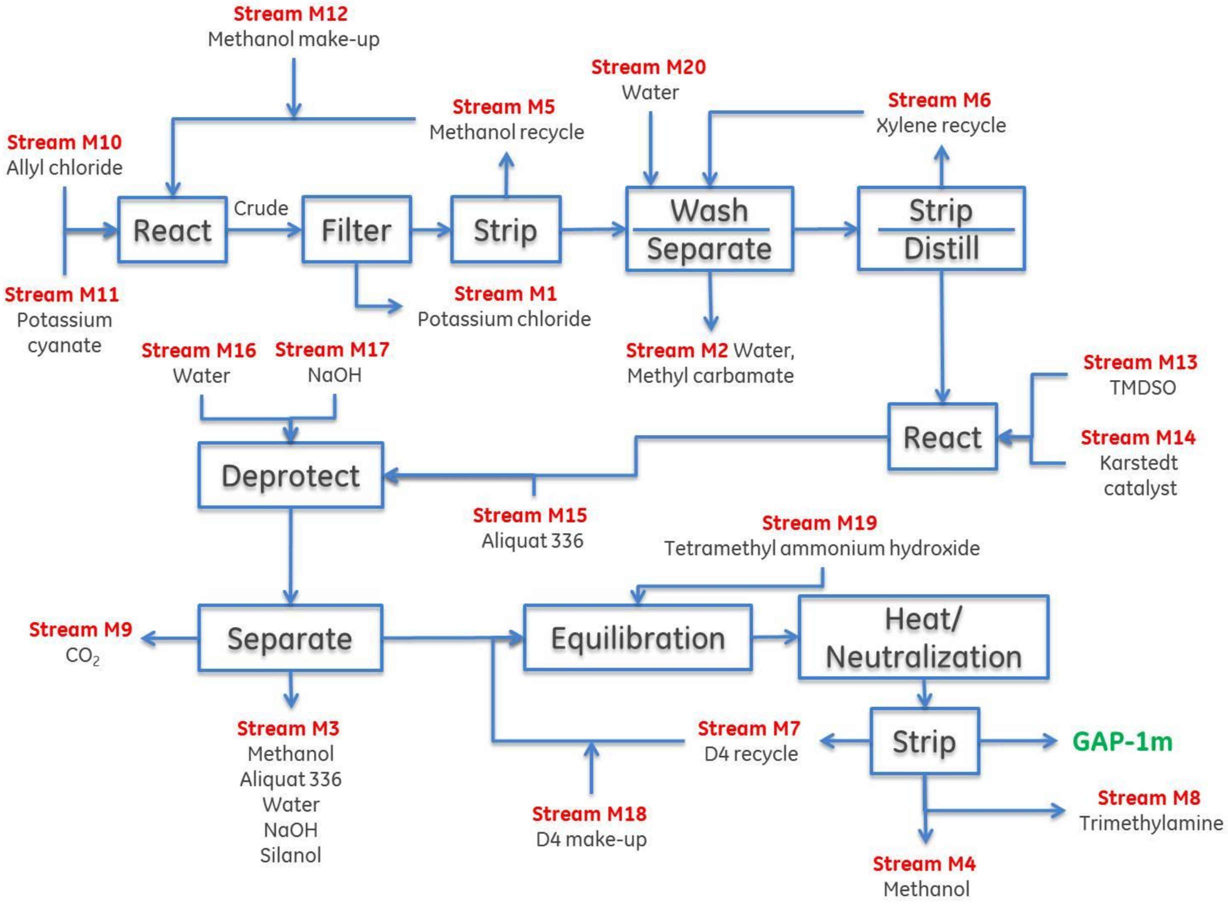


**Figure 93.** Manufacturing process for GAP-$1_m$

The methyl N-allylcarbamate is then contacted with TMSDO (stream M13) and a platinum catalyst (Karstedt's, stream M14) to effect a double hydrosilylation reaction in essentially quantitative yield to give 1,3-bis(3-methylcarbamatopropyl)-1,1,3,3-tetramethyldisiloxane. The carbamate protecting group is then removed by basic aqueous hydrolysis (streams M16 and M17) under phase-transfer catalyst conditions (stream M15) at elevated temperature and pressure. The water layer is then separated (stream M3), the desorbed carbon dioxide vented (stream M9), and the GAP-0 product isolated. This intermediate product is added to $D_4$ (stream M18) and the mixture allowed to undergo an equilibration reaction catalyzed by tetramethylammonium hydroxide (stream M19). When equilibration is complete, the reaction mixture is heated to decompose the catalyst and neutralize the product. The more volatile components (methanol, stream M4 and trimethylamine, stream M8) are removed by scrubbers or condensation. The cyclic siloxanes that are formed during the equilibration reaction can be distilled off (stream M7) and recycled for further use in the equilibration reaction.

**Table 68.** Mass balance for manufacturing of GAP-$1_m$ for initial fill of system

| Stream | Description | Total stream flowrate (lb/hr) | Total stream flowrate (lbmol/hr) | Component | Mol frac | lbmol/hr | MW | lb/hr |
|---|---|---|---|---|---|---|---|---|
| M1 | Waste from filter | 2.59E+02 | 3.47E+00 | Potassium chloride | 1.00E+00 | 3.47E+00 | 7.46E+01 | 2.59E+02 |
| M2 | Waste from Wash/ Separate step | 2.00E+02 | 1.00E+01 | Water | 9.65E-01 | 9.65E+00 | 1.80E+01 | 1.74E+02 |
| | | | | Methyl carbamate | 3.47E-02 | 3.47E-01 | 7.51E+01 | 2.61E+01 |
| M3 | Waste from Separate step | 7.43E+02 | 3.58E+01 | Water | 9.02E-01 | 3.23E+01 | 1.80E+01 | 5.82E+02 |
| | | | | Methanol | 8.72E-02 | 3.12E+00 | 3.20E+01 | 1.00E+02 |
| | | | | Aliquat 336 | 2.42E-03 | 8.68E-02 | 4.04E+02 | 3.51E+01 |
| | | | | NaOH | 4.36E-03 | 1.56E-01 | 4.00E+01 | 6.25E+00 |
| | | | | Silanol | 4.08E-03 | 1.46E-01 | 1.33E+02 | 1.95E+01 |
| M4 | Liquid Waste from Final Strip | 1.74E+00 | 5.42E-02 | Methanol | 1.00E+00 | 5.42E-02 | 3.20E+01 | 1.74E+00 |
| M5 | Recycle stream | 4.45E+02 | 1.39E+01 | Methanol | 1.00E+00 | 1.39E+01 | 3.20E+01 | 4.45E+02 |
| M6 | Recycle stream | 1.74E+02 | 1.64E+00 | Xylene | 1.00E+00 | 1.64E+00 | 1.06E+02 | 1.74E+02 |
| M7 | Recycle stream | 1.67E+01 | 5.62E-02 | D4 | 1.00E+00 | 5.62E-02 | 2.97E+02 | 1.67E+01 |
| M8 | Gas waste stream from final strip | 3.13E+00 | 5.29E-02 | Trimethylamine | 1.00E+00 | 5.29E-02 | 5.91E+01 | 3.13E+00 |
| M9 | Gas waste stream from separate step | 1.38E+02 | 3.13E+00 | CO2 | 1.00E+00 | 3.13E+00 | 4.40E+01 | 1.38E+02 |
| M10 | Allyl chloride input | 2.66E+02 | 3.47E+00 | Allyl chloride | 1.00E+00 | 3.47E+00 | 7.65E+01 | 2.66E+02 |
| M11 | Potassium cyanate input | 2.82E+02 | 3.47E+00 | Potassium cyanate | 1.00E+00 | 3.47E+00 | 8.11E+01 | 2.82E+02 |
| M12 | Methanol make-up stream | 1.08E+02 | 3.38E+00 | Methanol | 1.00E+00 | 3.38E+00 | 3.20E+01 | 1.08E+02 |
| M13 | TMDSO input | 2.10E+02 | 1.56E+00 | TMDSO | 1.00E+00 | 1.56E+00 | 1.34E+02 | 2.10E+02 |
| M14 | Karstedt catalyst input | 8.69E-05 | 2.28E-07 | Karstedt catalyst | 1.00E+00 | 2.28E-07 | 3.81E+02 | 8.69E-05 |
| M15 | Aliquat 336 input | 5.25E+01 | 1.30E-01 | Aliquat 336 | 1.00E+00 | 1.30E-01 | 4.04E+02 | 5.25E+01 |
| M16 | Water input to deprotect step | 5.25E+02 | 2.92E+01 | Water | 1.00E+00 | 2.92E+01 | 1.80E+01 | 5.25E+02 |
| M17 | NaOH input | 1.31E+02 | 3.28E+00 | NaOH | 1.00E+00 | 3.28E+00 | 4.00E+01 | 1.31E+02 |
| M18 | D4 makeup stream | 1.09E+02 | 3.69E-01 | D4 | 1.00E+00 | 3.69E-01 | 2.97E+02 | 1.09E+02 |
| M19 | Tetramethyl ammonium hydroxide input | 4.86E+00 | 5.34E-02 | Tetramethyl ammonium hydroxide | 1.00E+00 | 5.34E-02 | 9.12E+01 | 4.86E+00 |
| M20 | Water input to wash/ separate | 1.74E+02 | 9.65E+00 | Water | 1.00E+00 | 9.65E+00 | 1.80E+01 | 1.74E+02 |

**Table 69.** Mass balance for manufacturing of GAP-$1_m$ for annual GAP-S make-up

| Stream | Description | Total stream flowrate (lb/hr) | Total stream flowrate (lbmol/hr) | Component | Mol frac | lbmol/hr | MW | lb/hr |
|---|---|---|---|---|---|---|---|---|
| M1 | Waste from filter | 5.20E+01 | 6.98E-01 | Potassium chloride | 1.00E+00 | 6.98E-01 | 74.55 | 5.20E+01 |
| M2 | Waste from Wash/ Separate step | 4.02E+01 | 2.01E+00 | Water | 9.65E-01 | 1.94E+00 | 18 | 3.49E+01 |
| | | | | Methyl carbamate | 3.47E-02 | 6.98E-02 | 75.07 | 5.24E+00 |
| M3 | Waste from Separate step | 1.49E+02 | 7.20E+00 | Water | 9.02E-01 | 6.50E+00 | 18 | 1.17E+02 |
| | | | | Methanol | 8.72E-02 | 6.28E-01 | 32.04 | 2.01E+01 |
| | | | | Aliquat 336 | 2.42E-03 | 1.75E-02 | 404.16 | 7.06E+00 |
| | | | | NaOH | 4.36E-03 | 3.14E-02 | 40 | 1.26E+00 |
| | | | | Silanol | 4.08E-03 | 2.94E-02 | 133.1 | 3.91E+00 |
| M4 | Liquid Waste from Final Strip | 3.49E-01 | 1.09E-02 | Methanol | 1.00E+00 | 1.09E-02 | 32.04 | 3.49E-01 |
| M5 | Recycle stream | 8.94E+01 | 2.79E+00 | Methanol | 1.00E+00 | 2.79E+00 | 32.04 | 8.94E+01 |
| M6 | Recycle stream | 3.49E+01 | 3.29E-01 | Xylene | 1.00E+00 | 3.29E-01 | 106.16 | 3.49E+01 |
| M7 | Recycle stream | 3.35E+00 | 1.13E-02 | D4 | 1.00E+00 | 1.13E-02 | 296.62 | 3.35E+00 |
| M8 | Gas waste stream from final strip | 6.29E-01 | 1.06E-02 | Trimethylamine | 1.00E+00 | 1.06E-02 | 59.11 | 6.29E-01 |
| M9 | Gas waste stream from separate step | 2.77E+01 | 6.29E-01 | CO2 | 1.00E+00 | 6.29E-01 | 44 | 2.77E+01 |
| M10 | Allyl chloride input | 5.34E+01 | 6.98E-01 | Allyl chloride | 1.00E+00 | 6.98E-01 | 76.52 | 5.34E+01 |
| M11 | Potassium cyanate input | 5.67E+01 | 6.98E-01 | Potassium cyanate | 1.00E+00 | 6.98E-01 | 81.12 | 5.67E+01 |
| M12 | Methanol make-up stream | 2.18E+01 | 6.80E-01 | Methanol | 1.00E+00 | 6.80E-01 | 32.04 | 2.18E+01 |
| M13 | TMDSO input | 4.21E+01 | 3.14E-01 | TMDSO | 1.00E+00 | 3.14E-01 | 134.32 | 4.21E+01 |
| M14 | Karstedt catalyst input | 1.75E-05 | 4.58E-08 | Karstedt catalyst | 1.00E+00 | 4.58E-08 | 381.48 | 1.75E-05 |
| M15 | Aliquat 336 input | 1.05E+01 | 2.61E-02 | Aliquat 336 | 1.00E+00 | 2.61E-02 | 404.16 | 1.05E+01 |
| M16 | Water input to deprotect step | 1.06E+02 | 5.87E+00 | Water | 1.00E+00 | 5.87E+00 | 18 | 1.06E+02 |
| M17 | NaOH input | 2.64E+01 | 6.60E-01 | NaOH | 1.00E+00 | 6.60E-01 | 40 | 2.64E+01 |
| M18 | D4 makeup stream | 2.20E+01 | 7.42E-02 | D4 | 1.00E+00 | 7.42E-02 | 296.62 | 2.20E+01 |
| M19 | Tetramethyl ammonium hydroxide input | 9.78E-01 | 1.07E-02 | Tetramethyl ammonium hydroxide | 1.00E+00 | 1.07E-02 | 91.15 | 9.78E-01 |
| M20 | Water input to wash/ separate | 3.49E+01 | 1.94E+00 | Water | 1.00E+00 | 1.94E+00 | 18 | 3.49E+01 |

### 7.2.2 Toxicological Effects of Components in the Manufacturing Process of GAP-$1_m$

Toxicological data for both methanol and xylene are provided in the toxicity section for the $CO_2$ capture system and are not included in this section.

In cases where data were not available for a specific endpoint, QSAR modeling with ECOSAR, EPIWIN, TEST, or Toxtree is included, where possible. Some chemicals also had read across data available for chemicals with a similar structure. In all cases where read across data are included, this has been noted in the summary tables. Several tables reference the QSAR Toolbox as the source of toxicological information. This is software resulting from the efforts of OECD countries and provides toxicological and physical property data from several databases.[57] According to the QSAR Toolbox website, the software is "intended to be used by governments, the chemical industry, and other stakeholders to fill gaps in (eco-)toxicity data needed for assessing the hazards of chemicals."

For the acute toxicity endpoints from animal testing (e.g. $LD_{50}$ values), specific durations of the tests were not available for all values, but these tests typically include an observation period of less than or equal to 14 days after the initial dose.

#### Process Inputs

#### Allyl chloride (CAS # 107-05-1) Toxicological Data

The toxicological data for allyl chloride are summarized in **Table 70**. Several toxicological studies have been completed for allyl chloride, given that it is on the original HAP list under the Clean Air Act. Occupational exposures have been documented and effects have included eye/skin irritation, neurotoxicity, and reversible liver/kidney damage.[58, 59]

EPA provides an RfC value based on neurotoxicity in animal studies. EPA applied a 3000 fold uncertainty factor when calculating this value, which indicates that extreme caution should be used when applying the RfC when estimating potential human health risks.

Allyl chloride belongs to the class of compounds known as alkylating agents, which have the capability to interact directly with DNA to form adducts, cause mutations, and, presumably, initiate cancer. This mechanism of action is thought to be widely applicable to many species, including humans. However, species differences in pharmacokinetics and sensitivity can limit the ability to determine that there is a real risk for this endpoint in humans. *In vitro* genotoxicity testing results have been largely positive. This includes the Ames Test (with the exception of one study where the negative result was thought to be due to evaporation of the test article), E. coli reverse mutation, *A. nidulans* chromosome aberration, and yeast gene mutation. However, a cytogenetic assay was negative and two unscheduled DNA synthesis tests reported conflicting results.[60]

In the carcinogenicity evaluation in IRIS, EPA classifies allyl chloride as a Group C carcinogen and IARC classifies it as Group 3. Both of these classifications indicate that adequate data are not available to determine the carcinogenicity of this chemical. In animal testing, some effects on sperm have been observed in mice, but developmental effects have only been observed at maternally toxic doses. Bioconcentration factor testing was completed on *C. carpio* and the results indicated that there is a low risk for bioaccumulation of allyl chloride. The predicted $K_{oc}$ value from the EPIWIN model indicates that high mobility in soils would be expected, since the value is significantly below 500 L/kg.

**Table 70.** Allyl chloride toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Reference concentration (mg/m$^3$) | 1x10$^{-3}$ | N/A | Chronic | EPA IRIS |
| Ingestion LD$_{50}$ (mg/kg b.w.) | 450 to 700 | Rat | 14 days observation after dose | IUCLID |
| Inhalation LC$_{50}$ (mg/m$^3$) | 3,200 to 11,800 | Rat | 2 to 6 hrs | IUCLID |
| Dermal LD$_{50}$ (mg/kg b.w.) | 2,066 | Rabbit | N/A | TOXNET[61] |
| Eye irritation/ skin corrosion | Slightly irritating | Rabbit | N/A | IUCLID |
| Inhalation NOAEL (mg/m$^3$) | 17 | Rabbit | 90 days | Lu, et al 1982[62] |
| Inhalation LOAEL (mg/m$^3$) | 206 | Rabbit | 90 days | Lu, et al 1982[63] |
| Reproductive toxicity | Sperm effects – 124 mg/kg | Mice, subcutaneous injection | 39 days | IUCLID |
| Developmental toxicity | Developmental effects only seen in animals at maternally-toxic doses | N/A | N/A | IUCLID |
| Carcinogenicity | Data not adequate to allow for determination of cancer risks to humans, IARC group 3 and IRIS group C | N/A | N/A | IARC[63] |
| Genotoxicity/ mutagenicity | See discussion of genotoxicity in this section | | | |
| Fish toxicity, acute, LC$_{50}$ (mg/L) | 21 | Carassius auratus (goldfish) | 96 hr | IUCLID |
| Fish toxicity, acute, LC$_{50}$ (mg/L) | 51 | Lebistus reticulates (guppy) | 96 hr | IUCLID |
| Fish toxicity, acute, LC$_{50}$ (mg/L) | 42 | Lepomis macrochirus (bluegill) | 96 hr | IUCLID |
| Fish toxicity, acute, LC$_{50}$ (mg/L) | 20 to 24 | Pimephales promelas (fathead minnow) | 96 hr | IUCLID |

| | | | | |
|---|---|---|---|---|
| Fish toxicity, chronic $LC_{50}$ (mg/L) | 1.2 | Poecilia reticulate (guppy) | 14 day | IUCLID |
| Daphnid toxicity, acute $EC_{50}$ (mg/L) | 250 | Daphnia magna | 24 hr | IUCLID |
| Algae toxicity, chronic NOEC (mg/L) | 8.2 | Microcystis aeruginosa | 8 day | IUCLID |
| Algae toxicity, chronic NOEC (mg/L) | 6.3 | Scenedesmus quadricauda | 8 day | IUCLID[Error! Bookmark not defined.] |
| Octanol Water Partition Coefficient (log $K_{ow}$) | 1.93 | N/A | N/A | Yaws 2003[64] |
| Biodegradability | Readily biodegradable | N/A | N/A | QSAR Toolbox |
| Predicted soil adsorption coefficient, $K_{oc}$ (L/kg) | 39.7 | N/A | N/A | EPIWIN model |
| Bioconcentration factor (L/kg wet weight) | <5.6 | C. carpio | 42 days | QSAR Toolbox |

### Potassium cyanate (CAS# 590-28-3) Toxicological Data

The toxicological data for potassium cyanate are provided in **Table 71**. Genotoxicity test results for this chemical have been negative for the Ames test, chromosomal aberration, and mammalian gene mutation. No information was available for potassium cyanate on skin sensitization, developmental toxicity, or acute algae toxicity. For these values, read-across data has been used for a similar chemical, sodium cyanate (CAS#917-61-3).

Potassium cyanate was found to not be corrosive to skin, but it is irritating to eyes based on rabbit testing. The low predicted $K_{oc}$ value for this chemical indicates that it would have high mobility in subsurface environments. EPIWIN was also used to estimate the BCF, which indicated a low risk of bioaccumulation. ECOSAR modeling could not be completed for this chemical because it is not recommended to use the model for complex organic salts. However, some aquatic toxicity values have been compiled from other sources.

**Table 71.** Potassium cyanate toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Ingestion $LD_{50}$ (mg/kg b.w.) | 567 | Rat | N/A | Sigma Aldrich MSDS[65] |
| Dermal $LD_{50}$ (mg/kg b.w.) | >2000 | Rat | N/A | Sigma Aldrich MSDS[65] |
| Eye irritation/ skin corrosion | No skin irritation, irritating to eyes | Rabbit | N/A | Sigma Aldrich MSDS[65] |
| Skin sensitization | Negative | Mouse (LLNA) | N/A | QSAR Toolbox, read across based on sodium cyanate |
| Developmental LOAEL (mg/kg/day in diet) | 1500 | Mouse | N/A | QSAR Toolbox, read across based on sodium cyanate |
| Genotoxicity/ mutagenicity | Negative for Ames test, chromosomal aberration, and mammalian cell gene mutation | N/A | N/A | QSAR Toolbox |
| Fish toxicity, acute, $LC_{50}$ (mg/L) | 15 | Salmo gairdneri (Rainbow trout) | 96 hr | Sigma Aldrich MSDS65 |
| Fish toxicity, acute, $LC_{50}$ (mg/L) | 24.3 | Salmo gairdneri (Rainbow trout) | 96 hr | TOXNET |
| Daphnid toxicity, acute $EC_{50}$ (mg/L) | 18 | Daphnia magna | 48 hr | Sigma Aldrich MSDS[65] |
| Algae toxicity, acute $EC_{50}$ (mg/L) | >100 | D. subspicatus | 72 hr | QSAR Toolbox, read across based on sodium cyanate |
| Predicted octanol Water Partition Coefficient (log $K_{ow}$) | -4.65 | N/A | N/A | EPIWIN model |

| | | | | |
|---|---|---|---|---|
| Predicted biodegradability | Readily biodegradable | N/A | N/A | EPIWIN model |
| Predicted soil adsorption coefficient, $K_{oc}$ (L/kg) | 0.056 | N/A | N/A | EPIWIN model |
| Predicted bioconcentration factor (L/kg wet weight) | 3.162 (default for compounds with log $K_{ow}$ less than 1) | N/A | N/A | EPIWIN model |

**Sodium hydroxide (CAS #1310-73-2) Toxicological Data**

The toxicological data for sodium hydroxide are summarized in **Table 72**.

Target organ toxicity data following systemic exposure for NaOH is not available or not considered to be reliable, and is considered “scientifically unjustified” by REACH, given its caustic nature. Results from two short term aquatic studies are reported in **Table 72**. The most likely impact of NaOH on the aquatic environment is expected to be due to pH effects, but available studies are not considered of a high enough quality for regulatory support.

The primary human health risk related to NaOH is the corrosive nature of the chemical and potential for severe burns to skin. ECOSAR modeling could not be completed for this compound since the model cannot be used for inorganic compounds. The EPIWIN models for log $K_{ow}$, biodegradability, and $K_{oc}$ are also not valid for inorganic compounds.

**Table 72.** Sodium hydroxide toxicological data.

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Ingestion $LD_{50}$ (mg/kg b.w.) | 140 to 340 | Rat | N/A | TOXNET[66] |
| Dermal $LD_{50}$ (mg/kg b.w.) | 1,350 | Rabbit | N/A | TOXNET[66] |
| Eye irritation/ skin corrosion | Corrosive to eyes and causes severe burns to skin | Rabbit | N/A | Sigma Aldrich MSDS[66] |
| Fish toxicity, acute, $LC_{50}$ (mg/L) | 45.4 | Oncorhynchus mykiss (rainbow trout) | 96 hr | Sigma Aldrich MSDS[66] |
| Daphnid toxicity, acute $EC_{50}$ (mg/L) | 40.4 | Daphnia magna | 48 hr | Sigma Aldrich MSDS[66] |

### TMDSO (CAS# 3277-26-7) Toxicological Data

The toxicological data for TMDSO are summarized in **Table 73**. The results of three Ames tests are available which all provided negative results. Read across data is available for tetramethylcyclotetrasiloxane (CAS# 2370-88-9) for a chromosomal aberration assay in which negative results were obtained. Negative results were also obtained for a mammalian gene mutation chromosomal aberration and in vivo rodent bone marrow cytogenetic assays for a similar chemical, hexamethyldisiloxane (CAS#107-46-0).

Regarding the fate of TMDSO in aquatic environments, it has been shown that TMDSO is rapidly hydrolyzed to dimethylsilanediol (CAS#1066-42-8), with a half-life of 11 minutes at pH 7 and 25°C. Therefore, any effects in an aquatic environment would be due to formation of the dimethylsilanediol and not to the parent compound, TMDSO. Therefore, modeling for environmental fate and transport and aquatic toxicity has been completed for dimethylsilanediol instead of TMDSO. The results are summarized in **Table 73**.

ECOSAR modeling resulted in relatively high $LC_{50}$ and $EC_{50}$ values for aquatic species, which would indicate a relatively low risk to aquatic environments. EPIWIN predicted a very low BCF value, which would indicate a low risk of bioaccumulation. The low predicted $K_{oc}$ value indicates that this would have high mobility in soils.

**Table 73.** TMDSO toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Ingestion $LD_{50}$ (mg/kg b.w.) | >2000 | Rat | 14 days observation after dose | QSAR Toolbox |
| Inhalation $LC_{50}$ ($mg/m^3$) | >5,800 | Rat | 14 days observation after dose | QSAR Toolbox |
| Eye irritation/ skin corrosion | Not irritating to skin or eyes | Rabbits | N/A | QSAR Toolbox |
| Genotoxicity/ mutagenicity | Negative (See discussion in this section | | | |
| Predicted Octanol Water Partition Coefficient (log $K_{ow}$) | 4.154 | N/A | N/A | ECOSAR model |

**Table 74.** Dimethylsilanediol aquatic toxicity predicted data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Water solubility (mg/L) | $1x10^6$ | N/A | N/A | ECOSAR model |
| Predicted fish toxicity, acute, $LC_{50}$ (mg/L) | 10,992 | N/A | 96 hr | ECOSAR model |
| Predicted fish toxicity, chronic $LC_{50}$ (mg/L) | 827 | N/A | N/A | ECOSAR model |
| Predicted daphnid toxicity, acute $LC_{50}$ (mg/L) | 4,998 | Daphnia magna | 48 hr | ECOSAR model |
| Predicted daphnid toxicity, chronic $LC_{50}$ (mg/L) | 263 | Daphnia magna | N/A | ECOSAR model |
| Predicted algae toxicity, acute $EC_{50}$ (mg/L) | 1,485 | Green algae | 96 hr | ECOSAR model |
| Predicted algae toxicity, chronic (mg/L) | 237 | Green algae | N/A | ECOSAR model |
| Predicted Octanol Water Partition Coefficient (log $K_{ow}$) | -0.407 | N/A | N/A | ECOSAR model |
| Predicted biodegradability | Not readily biodegradable | N/A | N/A | EPIWIN model |
| Predicted soil adsorption coefficient, $K_{oc}$ (L/kg) | 0.4403 | N/A | N/A | EPIWIN model |
| Predicted bioconcentration factor (L/kg wet weight) | 3.162 (default for compounds with log $K_{ow}$ less than 1) | N/A | N/A | EPIWIN model |

## Tetramethyl ammonium hydroxide (CAS# 75-59-2) Toxicological Data

Toxicological data for tetramethyl ammonium hydroxide (TMAH) are provided in **Table 75**. Acute human exposure to TMAH solutions (25%) has resulted in severe chemical burns and some deaths.[67] Some aquatic studies have been completed for this material, but, similar to NaOH, the primary concern to aquatic life is expected to be related to pH effects. ECOSAR modeling was not completed for this chemical because it is not recommended to use the model for ammonium salts. TMAH was shown to be corrosive to skin in rabbit testing. Experimental results are available for $K_{oc}$ values. The experiments were conducted for three different soil types and the $K_{oc}$ value increased with increasing % of organic carbon, as expected. However, all measured values are still less than 500 L/kg and would indicate that the chemical would be mobile in a soil environment over a range of soil types. The low predicted BCF value would indicate that little bioaccumulation would be expected with this chemical. Genotoxicity testing has been completed for this chemical and results were negative for Ames test, chromosomal aberration, and mammalian cell gene mutation.

**Table 75.** TMAH toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Ingestion $LD_{50}$ (mg/kg b.w.) | 7.5 to 50 | Rat | 14 day observation after dose | QSAR Toolbox |
| Dermal $LD_{50}$ (mg/kg b.w.) | 12.5 to 50 | Rat | 14 day observation after dose | QSAR Toolbox, TOXNET[68] |
| Eye irritation/ skin corrosion | Corrosive to skin, eye testing not justified given high pH | Rabbit | N/A | QSAR Toolbox |
| Ingestion NOAEL (mg/kg/day) | 5 | Rat | 28 day | QSAR Toolbox |
| Dermal NOAEL (mg/kg/day) | 10 | Rat | 28 day | QSAR Toolbox |
| Reproductive/ developmental toxicity, NOAEL (mg/kg) | ≥20 | Rat | 14 day prior to mating male, 14 day prior to mating through 3 days after delivery female | QSAR toolbox |

| | | | | |
|---|---|---|---|---|
| Genotoxicity/ mutagenicity | Negative for chromosomal aberration, Ames test, and mammalian cell gene mutation test | N/A | N/A | QSAR Toolbox |
| Fish toxicity, acute, $LC_{50}$ (mg/L) | See discussion in this section of report | | | |
| Daphnid toxicity, acute $EC_{50}$ (mg/L) | 3 | Daphnia magna | 48 hr | Sigma Aldrich MSDS[68] |
| Algae toxicity, acute $EC_{50}$ (mg/L) | >251 | D. subspicatus | 72 hr | QSAR Toolbox |
| Cyanobacteria toxicity, acute $EC_{50}$ (mg/L) | 96.3 (in 20% solution in water) | P. subcapitata | 72 hr | QSAR Toolbox |
| Predicted Octanol Water Partition Coefficient (log $K_{ow}$) | -2.47 | N/A | N/A | EPIWIN model |
| Biodegradability | Readily biodegradable | N/A | N/A | QSAR Toolbox |
| Soil adsorption coefficient, $K_{oc}$ (L/kg) | 35 (loamy sand), 258 (sandy loam), 452 (clay) | N/A | N/A | QSAR Toolbox |
| Predicted bioconcentration factor (L/kg wet weight) | 3.162 (default for compounds with log $K_{ow}$ less than 1) | N/A | N/A | EPIWIN model |

### Karstedt catalyst (CAS # 68478-92-2) Toxicological Data

Relatively little toxicity data is available for the pure catalyst and QSAR modeling is not applicable to metal complexes and has not been completed (**Table 76**). This platinum catalyst uses zero valent platinum, which is considered inert and non-hazardous. Some irritation has been reported in occupational settings, but effects from other sources are very rare. This catalyst has been used in silicone breast implants and the FDA considers the Pt catalyst used in the implants not to be a risk,[69] and it has been approved for medical applications.

Since some agencies assume that the catalyst breaks down to platinum and divinyltetramethyldisiloxane (CAS# 2627-95-4) in the environment,[70] toxicological information for the siloxane component is provided in **Table 77**. Genotoxicity testing has been completed for the siloxane component and showed negative results for chromosomal aberration, Ames test, and mammalian cell gene mutation. Aquatic testing has been conducted and most tests showed no effects at the levels measured in the experiments, with the concentrations very close to the water solubility of the material. Experimental testing has shown the material not to be readily biodegradable. The high predicted $K_{oc}$ value indicates that the mobility in a soil environment is expected to be low. The predicted BCF, while below the typical level of concern of 5000, is only a predicted value and is relatively high at 3962 so that could be a potential concern. However, it should be noted that the solubility of this chemical in water is very low.

**Table 76.** Karstedt catalyst toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Ingestion $LD_{50}$ (mg/kg b.w.) | 500 to 5000 | Rat | N/A | NuSil MSDS (inferred from ingredient hazards)[71] |
| Inhalation $LC_{50}$ ($mg/m^3$) | 2 to 20 | Rat | N/A | NuSil MSDS (inferred from ingredient hazards)[71] |
| Dermal $LD_{50}$ (mg/kg b.w.) | 1000 to 2000 | Rabbit | N/A | NuSil MSDS (inferred from ingredient hazards)[71] |
| Eye irritation/ skin corrosion | Moderate irritant | N/A | N/A | Costigan and Tinkler, 2004[72] |
| Genotoxicity/ mutagenicity | Negative in Ames Test | N/A | N/A | Costigan and Tinkler, 2004[72] |
| Predicted genotoxicity | Negative | N/A | N/A | Toxtree model |
| Predicted non-cancer toxicity | Negative | N/A | N/A | Toxtree model |

**Table 77.** Divinyltetramethyldisiloxane toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Ingestion $LD_{50}$ (mg/kg b.w.) | >5000 | Rat | 14 days observation after dose | QSAR Toolbox |
| Inhalation $LC_{50}$ ($mg/m^3$) | >1875 | Rat | 14 days observation after dose | QSAR Toolbox |
| Oral NOAEL (mg/kg/day), liver effects | 150 (males), 50 (females) | Rat | Up to 31 days for males and 34 days for females (14 day recovery for subgroup) | QSAR Toolbox |
| Eye irritation/ skin corrosion | Non-irritating to mild redness to skin, slight redness to eye | Rabbit | N/A | QSAR Toolbox |
| Genotoxicity/ mutagenicity | Negative for Ames test, mammalian cell gene mutation, and in | N/A | N/A | QSAR Toolbox |

| | | | | |
|---|---|---|---|---|
| | vivo chromosomal aberration test | | | |
| Reproductive oral NOAEL (mg/kg/day) | 600 | Rat | N/A | QSAR Toolbox |
| Neonatal oral NOAEL (mg/kg/day) | 150 | Rat | N/A | QSAR Toolbox |
| Fish toxicity, acute $LC_{50}$ (mg/L) | >0.13 | O. mykiss | 96 hr | QSAR Toolbox |
| Daphnia toxicity, acute $EC_{50}$ (mg/L) | >0.1 | Daphnia magna | 48 hr | QSAR Toolbox |
| Daphnia reproductive NOEC (mg/L) | 0.12 | Daphnia magna | 21 day | QSAR Toolbox |
| Algae toxicity, $EC_{50}$ (mg/L) | >0.12 | P. subcapitata | 72 hr | QSAR Toolbox |
| Predicted Octanol-Water Partition Coefficient, log $K_{ow}$ | 5.958 | N/A | N/A | ECOSAR model |
| Water solubility | 0.207 mg/L at 20°C | N/A | N/A | QSAR Toolbox |
| Biodegradability | Not readily biodegradable | N/A | N/A | QSAR Toolbox |
| Predicted soil adsorption coefficient, $K_{oc}$ (L/kg) | 1309 | N/A | N/A | EPIWIN model |
| Predicted bioconcentration factor (L/kg wet weight) | 3962 | N/A | N/A | EPIWIN model |

## Trioctylmethylammonium chloride (CAS# 63393-96-4) Toxicological Data

The toxicological data for trioctylmethylammonium chloride are summarized in **Table 78**. Very little toxicity information is available for this chemical, though some aquatic testing has been completed with $LC_{50}$ values less than 1 mg/L for rainbow trout. Some ECOSAR modeling results are provided in the table. However, the results are not provided for acute fish or acute Daphnid effects because the predicted log $K_{ow}$ is higher than the cutoff for these endpoints. The acute algae result is not provided because it was more than 10 times the solubility of this chemical in water. Based on the very high predicted $K_{oc}$ value, the mobility of this chemical in soils is expected to be low. The low predicted BCF value would also indicate that the risk of bioaccumulation is low. Read across results for genotoxicity testing are provided in the table for didecyl dimethylammonium chloride (CAS#7173-51-5), which showed negative results for mammalian gene mutation, chromosome aberration, and Ames tests.

**Table 78.** Trioctylmethylammonium chloride toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Ingestion $LD_{50}$ (mg/kg b.w.) | 223 | Rat | N/A | Sigma Aldrich MSDS[73] |
| Skin corrosion | Corrosive to skin | N/A | N/A | Sigma Aldrich MSDS[73] |
| Genotoxicity/ mutagenicity (read-across) | Negative for Ames test, mammalian cell gene mutation and chromosome aberration | N/A | N/A | QSAR Toolbox (read across for CAS#7173-51-5) |
| Fish toxicity, acute, $LC_{50}$ (mg/L) | 0.18 to 0.32 | Oncorhynchus mykiss (rainbow trout) | 96 hr | Sigma Aldrich MSDS[73] |
| Predicted fish toxicity, chronic $LC_{50}$ (mg/L) | 0.01 | N/A | N/A | ECOSAR model |
| Predicted daphnid toxicity, chronic (mg/L) | 0.015 | Daphnia magna | N/A | ECOSAR model |
| Predicted algae toxicity, chronic (mg/L) | 0.119 | Green algae | N/A | ECOSAR model |
| Predicted Octanol Water Partition Coefficient (log $K_{ow}$) | 6.131 | N/A | N/A | ECOSAR model |
| Predicted biodegradability | Readily biodegradable | N/A | N/A | EPIWIN model |
| Predicted soil adsorption coefficient, $K_{oc}$ (L/kg) | $1.69 \times 10^4$ | N/A | N/A | EPIWIN model |
| Predicted bioconcentration factor (L/kg wet weight) (read-across) | 70.79 | N/A | N/A | EPIWIN model |

## 1-octanol (CAS# 111-87-5) Toxicological Data

The toxicological data for 1-octanol are provided in **Table 79**. The high dermal and oral $LD_{50}$ values would indicate a low risk for acute toxicity based on testing in rats and rabbits. The

MSDS for this chemical indicates that it is not bioaccumulative, which is consistent with the low BCF value predicted by the EPIWIN model. Genotoxicity testing for this chemical was negative in the Ames test. The low predicted $K_{oc}$ value from EPIWIN indicates that the expected mobility in a soil environment would be high. Experimental results indicate that this material is readily biodegradable.

**Table 79.** 1-octanol toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Ingestion $LD_{50}$ (mg/kg b.w.) | >3,200 | Rat | N/A | Sigma Aldrich MSDS[74] |
| Dermal $LD_{50}$ (mg/kg b.w.) | >5,000 | Rabbit | N/A | TOXNET[74] |
| Eye irritation/ skin corrosion | Skin irritant and moderate eye irritation | Rabbit | N/A | Sigma Aldrich MSDS[74] |
| Genotoxicity/ mutagenicity | Negative for Ames test | N/A | N/A | QSAR Toolbox |
| Fish toxicity, acute, $LC_{50}$ (mg/L) | 17.7 | Oncorhynchus mykiss | 96 hr | Sigma Aldrich MSDS[74] |
| Fish toxicity, acute, $LC_{50}$ (mg/L) | 13.3 | Pimephales promelas | 96 hr | Sigma Aldrich MSDS[74] |
| Fish toxicity, mortality LOEC (mg/L) | 1.19 | Pimephales promelas | 7 day | Sigma Aldrich MSDS[74] |
| Daphnid toxicity, acute $EC_{50}$ (mg/L) | 20 | Daphnia magna | 48 hr | QSAR Toolbox |
| Daphnid toxicity, acute $EC_{50}$ (mg/L) | 26 | Daphnia magna | 24 hr | TOXNET[74] |
| Algae toxicity, acute $EC_{50}$ (mg/L) | 6.5 - 14 | Desmodesmus subpicatus | 48 hr | Sigma Aldrich MSDS[74] |
| Octanol Water Partition Coefficient (log $K_{ow}$) | 3 | N/A | N/A | Yaws 2003[74] |
| Biodegradability, aerobic test | 92%, readily biodegradable | N/A | 28 day | Sigma Aldrich MSDS[74] |
| Predicted soil adsorption coefficient, $K_{oc}$ (L/kg) | 38.3 | N/A | N/A | EPIWIN model |
| Predicted bioconcentration factor (L/kg wet weight) | 44.3 | N/A | N/A | EPIWIN model |

## Trioctylamine (CAS# 1116-76-3) Toxicological Data

The toxicological data for trioctylamine are provided in **Table 80**. Little information is available on the toxicity of this chemical in literature. It is listed as a skin irritant. Predicted genotoxicity, non-cancer toxicity, and mutagenicity for this chemical were negative. ECOSAR modeling is not applicable to this chemical because the predicted log $K_{ow}$ is higher than the log $K_{ow}$ cutoffs for acute and chronic toxicity values for all species included in the model. The water solubility of this chemical is very low. Experimental results have shown that this chemical is not readily biodegradable. The very high predicted $K_{oc}$ value would indicate that it would not be mobile in a soil environment.

**Table 80.** Trioctylamine toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Intraperitoneal $LD_{50}$ (mg/kg b.w.) | 1000 | Rat | N/A | Sigma Aldrich MSDS[75] |
| Eye irritation/ skin corrosion | Irritant to skin | N/A | N/A | Sigma Aldrich MSDS[75] |
| Predicted genotoxicity | Negative | N/A | N/A | Toxtree model |
| Predicted non-cancer toxicity | Negative | N/A | N/A | Toxtree model |
| Predicted mutagenicity | Negative | N/A | N/A | TEST model |
| Predicted Octanol Water Partition Coefficient (log $K_{ow}$) | 10.362 | N/A | N/A | ECOSAR model |
| Water solubility | 0.05 mg/L at 25°C | N/A | N/A | TOXNET[75] |
| Biodegradability | Not readily biodegradable | N/A | N/A | QSAR Toolbox |
| Predicted soil adsorption coefficient, $K_{oc}$ | $2.5 \times 10^6$ | N/A | N/A | EPIWIN model |
| Bioconcentration factor (L/kg wet) | 101 to 143 | C. carpio | N/A | QSAR Toolbox |

## $D_4$ (CAS# 556-67-2) Toxicological Data

The toxicological data for $D_4$ are summarized in **Table 81**. $D_4$ has been classified as PBT (persistent, bioaccumulative, and inherently toxic) by Canada.[76] This is consistent with the high BCF experimental values provided in the table. $D_4$ has been tested for chronic inhalation toxicity in rats and an increase in endometrial adenomas was noted at 700 ppm. The high acute $LD_{50}$ and $LC_{50}$ values would indicate that $D_4$ is not an acute health hazard based on animal testing. Aquatic testing has been completed, which resulted in low chronic toxicity values for rainbow trout and *Daphnia magna*. Biodegradability testing has been completed and showed low biodegradation in sediments and sludge testing. The high measured $K_{oc}$ value for $D_4$ indicates that it would have low mobility in a soil environment. Due the high volatility of $D_4$, it is expected to partition into the atmosphere where it would react with OH radicals to form silanols.[77] Estimated atmospheric lifetimes of approximately 11 days for $D_4$ have been calculated.[78]

**Table 81.** $D_4$ toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Ingestion $LD_{50}$ (mg/kg b.w.) | >4,800 | Rat | 14 day observation after dose | QSAR Toolbox |
| Inhalation $LC_{50}$ (mg/m$^3$) | 36,000 | Rat | 14 day observation after dose | QSAR Toolbox |
| Dermal $LD_{50}$ (mg/kg b.w.) | >2,000 | Rat | 14 day observation after dose | QSAR Toolbox |
| Eye irritation/ skin corrosion | Not irritating to skin or eyes | Rabbit | N/A | QSAR Toolbox |
| Reproductive/ developmental NOAEL (ppm) | 300 | Rat | N/A | QSAR Toolbox |
| Carcinogenicity | See discussion in this section | | | QSAR Toolbox |
| Genotoxicity/ mutagenicity | Negative for Ames test, mammalian cell gene mutation, and chromosomal aberration test | N/A | N/A | QSAR Toolbox |
| Fish toxicity, acute, $LC_{50}$ (mg/L) | >0.0063 | C. variegatus | 96 hr | QSAR Toolbox |
| Fish toxicity, chronic $LC_{50}$ (mg/L) | 0.01 | O. mykiss | 14 day | QSAR Toolbox |
| Daphnid toxicity, acute $EC_{50}$ (mg/L) | >0.015 | Daphnia magna | 48 hr | QSAR Toolbox |
| Daphnia reproduction NOEC (mg/L) | 0.0079 | Daphnia magna | 21 day | QSAR Toolbox |
| Daphnia toxicity, chronic (mg/L) | >0.015 | Daphnia magna | 21 day | QSAR Toolbox |
| Water solubility | 0.07 mg/L at 25°C | N/A | N/A | Sigma Aldrich MSDS[79] |
| Octanol Water Partition Coefficient (log $K_{ow}$) | 6.49 | N/A | N/A | QSAR Toolbox |
| Soil adsorption coefficient, $K_{oc}$ (L/kg) | 16,596 | N/A | N/A | QSAR Toolbox |
| Bioconcentration factor (L/kg wet weight) | 12,400 to 13,400 | P. promelas | 28 days | QSAR Toolbox |

## Potential Byproducts

### Methyl carbamate (CAS# 598-55-0) Toxicological Data

The toxicological data for methyl carbamate are provided in **Table 82**. Genotoxicity testing has been completed for methyl carbamate, with negative results obtained for chromosome aberration and mammalian cell gene tests. Of the 38 test results provided for the Ames test from the QSAR toolbox databases, only two of the results were positive. NIH, EPA, and IARC do not classify the carcinogenicity of methyl carbamate given that limited testing has been conducted. However, California does list methyl carbamate as a known carcinogen under Prop 65 and it is listed as a concern in Maine and Minnesota. California provides a no significant risk level (NSRL) of 160 µg/day at a $10^{-5}$ cancer risk level and a cancer potency value of 0.0044 (mg/kg/day) [80]

No aquatic test results were found for this chemical so ECOSAR modeling was completed and is summarized in the table. The predicted BCF is very low, which would indicate that the risk of bioaccumulation should be low for this chemical. The low predicted $K_{oc}$ value indicates a potential for high mobility in a soil environment.

**Table 82.** Methyl carbamate toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Ingestion $LD_{50}$ (mg/kg b.w.) | 2500 | Rat | N/A | Sigma Aldrich MSDS[81] |
| Dermal $LD_{50}$ (mg/kg b.w.) | >2000 | Rabbit | N/A | Sigma Aldrich MSDS[81] |
| Eye irritation/ skin corrosion | Irritant to eyes and skin | Rabbit | N/A | Sigma Aldrich MSDS |
| Genotoxicity/ mutagenicity | See discussion in this section | | | |
| Predicted Fish toxicity, acute, $LC_{50}$ (mg/L) | 293.4 | N/A | 96 hr | ECOSAR model |
| Predicted fish toxicity, chronic (mg/L) | 37.4 | N/A | N/A | ECOSAR model |
| Predicted daphnid toxicity, acute $LC_{50}$ (mg/L) | 798 | Daphnia magna | 48 hr | ECOSAR model |
| Predicted daphnid toxicity, chronic (mg/L) | 1123 | Daphnia magna | N/A | ECOSAR model |
| Predicted algae toxicity, acute $EC_{50}$ (mg/L) | 505.5 | Green algae | 96 hr | ECOSAR model |
| Predicted algae toxicity, chronic (mg/L) | 57.4 | Green algae | 96 hr | ECOSAR model |
| Predicted Octanol Water Partition Coefficient (log $K_{ow}$) | -0.51 | N/A | N/A | ECOSAR model |
| Predicted biodegradability | Not readily biodegradable | N/A | N/A | EPIWIN model |
| Predicted soil adsorption coefficient, $K_{oc}$ (L/kg) | 3.003 L/kg | N/A | N/A | EPIWIN model |
| Predicted bioconcentration factor (L/kg wet weight) | 3.162 (default for compounds with log $K_{ow}$ less than 1) | N/A | N/A | EPIWIN model |

## Potassium chloride (CAS# 7447-40-7) Toxicological Data

The toxicological data for potassium chloride are summarized in **Table 83**. Potassium chloride is a gastrointestinal irritant in humans at high doses (greater than 31 mg/kg/day).[82] A 2 year oral chronic rat study yielded no tumors related to exposure up to 1820 mg/kg/day in food. There have been mixed results from genotoxicity/mutagenicity testing, with positive results at high KCl concentrations and increased chromosomal aberrations in ovary cells. EPIWIN modeling could not be completed for this compound because the modeling is not valid for inorganic compounds. The low predicted BCF value indicates that the risk of bioaccumulation is very low.

**Table 83.** Potassium chloride toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Ingestion $LD_{50}$ (mg/kg b.w.) | 2600 to 3020 | Rat | N/A | TOXNET, OECD Report[3] |
| Repeated dose oral NOAEL (mg/kg/day) | 1820 | Rat | 2 year | OECD Report[83] |
| Eye irritation | Not irritating | | | Sigma Aldrich MSDS[83] |
| Genotoxicity/ mutagenicity | See discussion in this section | | | |
| Developmental NOAEL (mg/kg/day) | 235 | Mouse | N/A | OECD Report[83] |
| Developmental NOAEL (mg/kg/day) | 310 | Rat | N/A | OECD Report[83] |
| Fish toxicity, acute, $LC_{50}$ (mg/L) | 880 | Pimephales promelas (fathead minnow) | 96 hr | OECD Report[83] |
| Fish toxicity, acute, $LC_{50}$ (mg/L) | 720 | Ictalurus punctatus (catfish) | 48 hr | OECD Report[83] |
| Fish toxicity, chronic, $LC_{50}$ (mg/L) | 700 to 1200 | O. mykiss | 7 days | QSAR Toolbox |
| Daphnid toxicity, acute $EC_{50}$ (mg/L) | 177 to 660 | Daphnia magna | 48 hr | OECD Report[83] |
| Daphnid toxicity, chronic $EC_{50}$ (mg/L) | 130 | Daphnia magna | 21 day | OECD Report[83] |
| Algae toxicity, acute $EC_{50}$ (mg/L) | 1337 | Nitzschia linearis | 120 hr | OECD Report[83] |
| Calculated Octanol Water Partition Coefficient (log $K_{ow}$) | -0.46 | N/A | N/A | OECD Report[83] |
| Predicted bioconcentration factor (L/kg wet weight) | 3.162 (default for compounds with log $K_{ow}$ less than 1) | N/A | N/A | EPIWIN model |

**Silanol, (3-aminopropyl)dimethyl- (CAS# 180051-45-0) Toxicological Data**

No experimental toxicity data are available for this chemical so the QSAR modeling results are summarized in **Table 84**. It should be noted that this material will not be used as a pure chemical in the manufacturing process, but it will be present in very dilute concentrations in one waste stream that will be disposed of as non-hazardous waste under RCRA Subpart D (Section K). The predicted genotoxicity, non-cancer toxicity, and mutagenicity for this chemical were all negative. The modeled aquatic toxicity data are summarized in the table. The EPIWIN model predicts that this chemical would not be readily biodegradable. The very low predicted BCF value indicates a low potential for bioaccumulation and the low predicted $K_{OC}$ value indicates a high potential for mobility in a soil environment.

**Table 84.** Silanol toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Predicted genotoxicity | Negative | N/A | N/A | Toxtree model |
| Predicted non-cancer toxicity | Negative | N/A | N/A | Toxtree model |
| Predicted mutagenicity | Negative | N/A | N/A | TEST model |
| Predicted fish toxicity, acute, $LC_{50}$ (mg/L) | 196.3 | N/A | 96 hr | ECOSAR model |
| Predicted fish toxicity, chronic, $LC_{50}$ (mg/L) | 18.4 | N/A | N/A | ECOSAR model |
| Predicted daphnid toxicity, acute $EC_{50}$ (mg/L) | 20 | Daphnia magna | 48 hr | ECOSAR model |
| Predicted daphnid toxicity, chronic $EC_{50}$ (mg/L) | 1.4 | Daphnia magna | N/A | ECOSAR model |
| Predicted algae toxicity, acute $EC_{50}$ (mg/L) | 22.5 | Green algae | 96 hr | ECOSAR model |
| Predicted algae toxicity, chronic $EC_{50}$ (mg/L) | 6.7 | Green algae | 96 hr | ECOSAR model |
| Predicted Octanol Water Partition Coefficient (log $K_{ow}$) | 0.654 | N/A | N/A | ECOSAR model |
| Predicted biodegradability | Not readily biodegradable | N/A | N/A | EPIWIN model |
| Predicted soil adsorption coefficient, $K_{oc}$ (L/kg) | 18.32 | N/A | N/A | EPIWIN model |
| Predicted bioconcentration factor (L/kg wet weight) | 3.162 (default for compounds with log $K_{ow}$ less than 1) | N/A | N/A | EPIWIN model |

### Trimethylamine (CAS# 75-50-3) Toxicological Data

The toxicological data for trimethylamine are provided in **Table 85**. At ambient temperature and pressure, trimethylamine is in the gas phase and is expected to be released in the gas phase from the manufacturing process, which will be handled with the proper engineering controls (Section L). Trimethylamine has been shown to be highly irritating to skin and destructive to eyes in rabbit testing. Genotoxicity testing has been completed and negative results were obtained for the Ames test, in vitro mammalian chromosomal aberration, and mammalian gene mutation tests. The very high acute inhalation $LC_{50}$ value indicates that it is a low acute risk via this exposure pathway. Aquatic testing has been completed for trimethylamine in solution and the results are summarized in the table. The low predicted BCF value indicates a low risk for bioaccumulation and the low measured $K_{oc}$ value would indicate a high potential for mobility in soil if this chemical were in a subsurface environment.

**Table 85.** Trimethylamine toxicological data

| | Value | Species | Time | Resource |
|---|---|---|---|---|
| Ingestion $LD_{50}$ (mg/kg b.w.) | 397 to 766 | Rat | 14 days observation after dose | QSAR Toolbox, Sigma Aldrich MSDS[84] |
| Inhalation $LC_{50}$ ($mg/m^3$) | >5,900 | Rat | N/A | TOXNET |
| Dermal $LD_{50}$ (mg/kg b.w.) | >5,000 | Rat | 14 days observation after dose | QSAR Toolbox |
| Eye irritation/ skin corrosion | Highly irritating to skin and destructive to eyes | Rabbit | N/A | QSAR Toolbox |
| Reproductive/ developmental toxicity, NOAEL (mg/kg/day) | 200 | Rat | N/A | QSAR Toolbox |
| Genotoxicity/ mutagenicity | Negative in Ames test, in vitro mammalian chromosome aberration test, and mammalian gene mutation assay | N/A | N/A | QSAR Toolbox |
| Fish toxicity, acute, $LC_{50}$ (mg/L) | 1000 | Oryzias latipes (Japanese rice fish) | 48 hr | QSAR Toolbox |
| Fish toxicity, acute, $LC_{50}$ (mg/L) | 25 | Leuciscus idus | 48 hr (non-neutralized sample) | QSAR Toolbox |
| Fish toxicity, acute, $LC_{50}$ (mg/L) | 610 | Leuciscus idus | 48 hr (neutralized sample) | QSAR Toolbox |
| Daphnid toxicity, acute $EC_{50}$ (mg/L) | 140 (trimethylamine in 45% solution) | Daphnia magna | 48 hr | QSAR Toolbox |
| Algae toxicity, acute, $EC_{50}$ (mg/L) | 90.6 to 150 (trimethylamine in 45% solution) | Scenedesmus subspicatus | 72 hr | QSAR Toolbox |
| Octanol Water Partition Coefficient (log $K_{ow}$) | 0.16 | N/A | N/A | Yaws 2003 |
| Biodegradability | Readily biodegradable | N/A | N/A | QSAR Toolbox |
| Soil adsorption coefficient, $K_{oc}$ (L/kg) | 2.4 to 4.7 | N/A | N/A | QSAR Toolbox |
| Predicted bioconcentration factor (L/kg wet weight) | 3.162 (default for compounds with log $K_{ow}$ less than 1) | N/A | N/A | EPIWIN model |

### 7.2.3 Physical Properties of the Chemicals in the Manufacturing Process of $GAP_{-1m}$

The physical properties for the inputs to the manufacturing process are summarized in **Table 86** and **Table 87**. The physical properties for the potential by-products are summarized in **Table 88**. Since the physical properties for both methanol and xylene were summarized in the section on the $CO_2$ capture process (Section D), that information is not duplicated here.

Unfortunately, physical property data were not available for the silanol material. Some properties were modeled, so it should be noted that there is uncertainty around the properties listed in the table. This chemical is part of an aqueous waste stream in low concentrations (2.6 wt%) and will not be handled in pure form. Allyl chloride, TMDSO, $D_4$, 1-octanol, and trimethylamine are all classified as flammable chemicals. Of these, only trimethylamine has an NFPA rating of 4. Allyl chloride and TMDSO are rated as 3 and $D_4$ and 1-octanol are rated as 2.

Of the inputs and potential byproducts reviewed, allyl chloride, sodium hydroxide, tetramethyl ammonium hydroxide, and trioctylmethyl ammonium chloride are considered corrosive. Allyl chloride and TMDSO have high volatility. Though $D_4$ has a lower vapor pressure relative to allyl chloride and TMDSO, it is classified as a cyclic volatile methylsiloxane and is expected to volatilize under ambient temperature and pressure conditions. Information on volatility was not available for trioctylmethyl ammonium chloride or the silanol material so the vapor pressures were modeled for these two chemicals. In both cases, the predicted volatility is low, with trioctylmethyl ammonium chloride significantly lower. No volatility information was available for the Karstedt catalyst and no modeling could be completed for the metal complex.

Regarding reactivity of the chemicals, in all cases, strong oxidizing agents should be avoided and the MSDS for most chemicals also warn that strong acids should be avoided. The MSDS' for TMDSO, Karstedt catalyst, and $D_4$ all warn that strong bases should be avoided, so these chemicals need to be stored separately from such chemicals as sodium hydroxide and tetramethyl ammonium hydroxide.

The MSDS for trimethylamine lists certain types of metals that need to be avoided. These metals include brass, zinc, magnesium, copper, mercury and mercury oxides, and tin and tin oxides. This should be considered when handling the gaseous waste stream that includes this chemical.

Of the materials reviewed, only trimethylamine is a gas at ambient temperature and pressure. Given the concerns regarding flammability and corrosivity of this chemical, care needs to be taken that the control device for vapor containment for the waste stream that includes this chemical is always operational while the process is running.

**Table 86.** Physical properties for inputs to manufacturing process

| | Allyl Chloride[85, 86] | Potassium Cyanate | NaOH[87] | TMDSO[88, 89, 90] | Tetramethyl ammonium hydroxide[91, 92] |
|---|---|---|---|---|---|
| Volatility (evap. rate) | 7 | Not applicable | Not applicable | >1 | Not available |
| Flash point | -32°C | Not flammable | Not applicable | -26°C | >100°C |
| Lower explosion limit/ upper explosion limit | 3.2% (V)/ 11.2%(V) | Not flammable | Not combustible | 0.8% (V)/ 62.9%(V) | Not available |
| Auto-ignition temperature | 391°C | Not available | Not combustible | 240°C | Not available |
| Chemical reactivity | Avoid strong oxidizing agents, boron trifluoride, sulfuric acid, nitric acid, ethylene | Avoid strong oxidizing agents | Avoid strong oxidizing agents, strong acids and organic materials | Avoid strong acids, strong bases and strong oxidizing agents | Avoid aluminium, alkali metals, strong oxidizing agents, acids, acid chlorides, acid anhydrides, halogens |
| Corrosivity | Corrosive | Not corrosive | Corrosive | Not corrosive | Corrosive |
| State, STP | Liquid | Powder, chunks | Pellets | Liquid | Liquid |
| Color | Colorless, yellow or purple | White | white | Colorless | Colorless to pale yellow |
| Odor | Garlic-like odor | Odorless | Odorless | Musty | Strong ammonia-like |
| Melting point | -134.5°C | 315°C | 318°C | < -78°C | 63°C |
| Boiling point | 44-45°C | Not applicable | 1,390°C | 70°C | 102°C |
| Vapor pressure | 295 mm Hg at 20°C | Not available | < 18 mmHg at 20°C | 112.5 mmHg at 20°C | 17.5 mmHg at 20°C |
| Vapor density | 2.64 (Air = 1.0) | Not available | 1.38 (Air = 1) | >1 (Air = 1) | 3.14 (Air = 1) |
| Density | 0.939 g/cm$^3$ at 25°C | 2.056 g/cm$^3$ at 25°C | 2.13 g/cm$^3$ at 25°C | 0.76 g/mL at 25°C | 1.014 g/cm$^3$ at 20°C |
| Water solubility | 4000 mg/L at 25°C | 6.3X10+5 mg/L @ 10 deg C | 1260 g/L at 20°C | Insoluble | Fully miscible |
| Solubility properties | Miscible with alcohol, chloroform, ether and petroleum ether | Very slightly soluble in alcohol | Soluble in alcohol | Soluble in chloroform, THF, toluene, and acetone | Soluble in methanol |
| Viscosity, dynamic | 0.32 cP at 25°C | Not applicable | 4.0 cP at 350°C | 0.5 cP | Not available |

**Table 87.** Physical properties for inputs to manufacturing process (continued)

| | Karstedt catalyst[93] | Trioctylmethylammonium chloride[94, 95, 96] | 1-octanol [97, 98, 99] | Trioctylamine [100] | $D_4$ [101] |
|---|---|---|---|---|---|
| Volatility (evap. rate) | Not available | Not available | 0.007 | Not available | <1 |
| Flash point | >110°C | 132°C | 80°C | 163°C | 55°C |
| Lower explosion limit/ upper explosion limit | Not available | Not available | 0.9% (V)/ 6.4% (V) | Not available | 0.75%(V)/ 7.4%(V) |
| Auto-ignition temperature | Not available | Not available | 270°C | 315° | 384°C |
| Chemical reactivity | Avoid oxidizing agents, acids and bases | Avoid strong oxidizing agents | Avoid Acids, acid chlorides, oxidizing agents | Avoid Strong oxidizing agents, acids, Acid chlorides, | Avoid strong oxidizing agents, acids, Bases |
| Corrosivity | Not corrosive | Corrosive | Not corrosive | Not corrosive | Not corrosive |
| State, STP | Liquid | Viscous liquid | Liquid | Liquid | Liquid |
| Color | Colorless | Amber | Colorless | Colorless | Colorless |
| Odor | Not available | Mild | Orange-rose odor | Amine-like | Odorless |
| Melting point | Not available | -20°C | -15°C | -34°C | 17°C |
| Boiling point | >200°C | 240°C | 196°C | 357°C | 175°C |
| Vapor pressure | Not available | 2E-12 mmHg (EPIWIN) | 0.14 mmHg at 25°C | <0.01 hPa at 20°C | 0.99 mmHg at 25°C |
| Vapor density | Not available | Not available | 4.5 (air = 1) | Not available | 10.24 |
| Density (25 C) | 0.98 g/cm$^3$ | 0.88 g/mL | 0.827 g/cm$^3$ at 25°C | 0.803 g/cm$^3$ | 0.956 g/mL |
| H2O solubility | Not available | 10 g/L | 540 mg/L at 25°C | 0.05 mg/L | 0.07 g/L at 25 |
| Solubility properties | Not available | Not available | Miscible in ethanol, ether, chloroform and carbon tetrachloride, | Soluble in chloroform | Soluble in carbon tetrachloride |

**Table 88.** Physical properties for potential byproducts from manufacturing process

| | Methyl carbamate | Potassium chloride | Silanol, (3-aminopropyl) dimethyl- | Trimethylamine[102, 103] |
|---|---|---|---|---|
| Volatility (evap. rate) | Not available | Not available | Not available | >1 |
| Flash point | Not available | Not available | Not available | -7°C |
| Lower explosion limit/ upper explosion limit | Not available | Not available | Not available | 2%(V)/ 11.6%(V) |
| Auto-ignition temperature | Not available | Not available | Not available | 190°C |
| Chemical reactivity | Avoid Strong oxidizing agents, Strong bases, Phosphorus halides | Avoid Strong acids, strong oxidizing agents | Not available | Avoid strong oxidizing agents, brass, magnesium, zinc, copper, mercury/mercury oxides., yin/tin oxides |
| Corrosivity | Not corrosive | Not corrosive | Not available | Corrosive |
| State, STP | Crystalline | Crystalline powder | liquid | Gas |
| Color | White | White | Not available | Colorless |
| Odor | Not available | Odorless | Not available | Fish-like |
| Melting point | 56°C | 770°C | Not available | -117°C |
| Boiling point | 176°C | 1500°C | 178°C (modeled)[104] | 3°C |
| Vapor pressure | Not available | Not available | 0.045 to 0.064 mmHg at 25°C (modeled)[105] | 1366 mmHg at 20°C |
| Vapor density | Not available | Not available | Not available | 2.04 (Air = 1) |
| Density | 1.1361 g/cm$^3$ at 25°C | 1.98 g/mL at 25°C | 0.89 g/mL at 25°C (modeled) | 0.63 g/cm$^3$ at 20°C |
| Water solubility | 6.91X10+5 mg/l at 15.5 deg C | Soluble | Not available | 8.9X10+5 mg/L at 30 deg C |
| Solubility properties | Soluble in ether | Soluble in glycerin, slightly soluble in alcohol, | Not available | Readily absorbed by alcohol with which it is miscible; also soluble in ether, benzene, toluene, xylene, ethylbenzene, chloroform. |
| Viscosity, dynamic | Not available | Not available | Not available | 0.185 cP at 25°C |

### 7.2.4 U.S. EH&S Law Compliance and Regulation Implications for the Manufacturing Process of GAP-$_{1m}$

The relevant regulations for the materials in the manufacturing process are summarized in **Table 89**. The applicable regulations that were considered are the same as those reviewed in Section E of this report for the $CO_2$ capture system. In the table, all entries are marked as being regulated by RCRA. This indicates that all materials in the process should be considered in the RCRA evaluation, but it does not indicate if these are considered hazardous or non-hazardous wastes. That classification will be discussed in detail in the RCRA section of this report for the manufacturing process. This section does not include a regulatory review of GAP-$1_m$ because this material is addressed in the section for the $CO_2$ capture system and it is not present in waste streams for the manufacturing process.

All materials reviewed have an MSDS available, with the exception of the silanol material. It should be noted that the silanol material will not be handled in pure form and will only be present in dilute concentrations in an aqueous waste stream. This waste stream is discussed in more detail within the RCRA section of the regulatory review.

**Table 89.** Regulatory overview for materials in manufacturing process

| Chemical | TSCA | CERCLA RQ (lbs) | CWA | CAA HAP | CAA VOC | SARA 302 EHS | SARA 311/312 | SARA 313 | OSHA | RCRA |
|---|---|---|---|---|---|---|---|---|---|---|
| Methanol | Y | Yes – 5000 lb RQ | N | Y | Y | N | Acute<br>Chronic<br>Fire | Y | Y | Y |
| Xylene | Y | Yes – 100 lb RQ | Yes – 100 lb RQ | Y | Y | N | Acute<br>Chronic<br>Fire | Y | Y | Y |
| Allyl chloride | Y | Yes – 1000 lb RQ | Yes – 1000 lb RQ | Y | Y | N | Acute<br>Chronic<br>Fire | Y | Y | Y |
| KOCN | Y | N | N | N | Y | N | Acute | N | Y | Y |
| NaOH | Y | Yes – 1000 lb RQ | Yes – 1000 lb RQ | N | N | N | Acute | N | Y | Y |
| TMDSO | Y | N | N | N | Y | N | Fire | N | Y | Y |
| Tetramethyl ammonium hydroxide | Y | N | N | N | Y | N | Acute | N | Y | Y |
| Karstedt's catalyst | Y | N | N | N | Y | N | Acute | N | Y | Y |
| D4 | Y | N | N | N | Y | N | Chronic<br>Fire | N | Y | Y |
| **Aliquat 336 components:** | | | | | | | | | | |
| Trioctylmethylammonium chloride | Y | N | N | N | Y | N | Acute<br>Chronic | N | Y | Y |
| 1-octanol | Y | N | N | N | Y | N | Acute<br>Chronic<br>Fire | N | Y | Y |
| trioctylamine | Y | N | N | N | Y | N | Acute | N | Y | Y |
| **Potential byproducts:** | | | | | | | | | | |
| Methyl carbamate | Y | N | N | N | Y | N | Acute<br>Chronic | N | Y | Y |
| Potassium chloride | Y | N | N | N | N | N | Chronic | N | Y | Y |
| Silanol, (3-aminopropyl)dimethyl- | Unknown | N | N | N | Y | N | Unknown | N | Y | Y |
| Trimethylamine | Y | Yes – 100 lb RQ | Yes – 100 lb RQ | N | Y | N | Acute<br>Fire<br>Sudden release of pressure | N | Y | Y |

## TSCA

With the exception of the silanol material, all chemical inputs to and potential byproducts from the manufacturing process are on EPA's TSCA inventory. However, it should be noted that only the non-confidential TSCA registrations could be searched to determine if the silanol material was TSCA registered.

## CERCLA

Of the chemicals associated with the manufacturing process, methanol, xylene, allyl chloride, and sodium hydroxide are listed as CERCLA hazardous substances. The minimum reportable quantities are 5000 lbs/day, 100 lbs/day, 1000 lbs/day, and 1000 lbs/day for methanol, xylene, allyl chloride, and sodium hydroxide, respectively.

## Clean Water Act

Xylene, allyl chloride, and sodium hydroxide are designed as hazardous substances to the water supply in accordance with CWA (40 CFR §116.4). The minimum reportable quantities for these chemicals are the same as those for CERCLA.

## Clean Air Act

All chemicals associated with the manufacturing process, with the exception of potassium chloride and sodium hydroxide, are considered to be VOCs by EPA's definition. Methanol, xylene, and allyl chloride are also regulated HAPs.

Trimethylamine is also on the CAA 112r list with a limit of 10,000 lbs. The specific concern for this chemical is based on the high flammability. For this process, trimethylamine will not be stored onsite and is only present as a gaseous waste stream that will be handled with the proper engineering controls (Section L). The worst case release for this system would not approach 10,000 lbs and this material would not be stored in significant quantities on-site. Given the flammable and corrosive nature of trimethylamine, the manufacturing process should not be run if the necessary engineering controls are not in the proper working condition for this waste stream.

The manufacturer could also be subject to additional regulatory requirements under 40 CFR 63 Subpart FFFF National Emission Standards for Hazardous Air Pollutants: Miscellaneous Organic Chemical Manufacturing if the manufacturing units are located at or part of a major source of hazardous air pollutants as defined in section 112(a) of the CAA. Section 112(a) states that a major source has the potential to emit 10 tons per year or more of an individual hazardous air pollutant or 25 tons per year or more of any combination of hazardous air pollutants. Methanol, xylene, and allyl chloride would not be emitted above these levels under normal process conditions, but these regulations could still be relevant if the manufacturing process is part of a larger site that would be classified as a major source.

Different state regulatory agencies have different requirements for Title V air permits, so these requirements would need to be reviewed on a case by case basis. The determination of whether a site is considered a major source is dependent on the facility's potential to emit VOCs and HAPs under normal process conditions. Some states also require different types of permits for minor and major sources so the detailed requirements in the location of manufacturing would need to be consulted to determine what would be required. If the relevant jurisdiction calculates the potential to emit post-engineering controls and it is not co-located with a facility that is already classified as a major source, this is not expected to be classified as a major source.

## SARA

None of the chemicals are on the SARA 302 list, which indicates that EPA does not consider these chemicals to pose an immediate hazard to a community upon release. With the exception of TMDSO, $D_4$, potassium chloride, and the silanol material, all of the chemicals are considered to be acute hazards under SARA 311/312. Methanol, xylene, allyl chloride, $D_4$, trioctylmethylammonium chloride, 1-octanol, methyl carbamate, and potassium chloride are all listed as chronic hazards. Methanol, xylene, allyl chloride, TMDSO, $D_4$, 1-octanol, and trimethylamine are listed as fire hazards. Trimethylamine is also listed as a hazard for sudden release of pressure when in its compressed gas state, which is not relevant for this process.

Chemical releases of methanol, xylene, or allyl chloride would need to be reported to public and government officials under SARA 313.

## **OSHA**

As was the case for the $CO_2$ capture process, all of the chemicals would be regulated by OSHA and require the MSDS and proper handling, shipping, and storage. These requirements are discussed in further detail in Section M of this report.

## **RCRA**

A review of the RCRA requirements was provided in Section E of this report. As in Section E, this RCRA review focuses only on the federal regulations. A detailed review of state regulations was considered outside the scope of this document. Since regulations can vary depending on the relevant jurisdiction, this would need to be reviewed on a case-by-case basis to ensure that compliance is maintained.  Streams M1 through M9 are discussed individually in the following section of the report and the results are summarized at the end of this section in Table 48. Streams M10 through M20 are not discussed in this section because they are inputs to the process and not potential waste streams.

### Stream M1

Stream M1 contains potassium chloride from the filter after reaction of allyl chloride, potassium cyanate, and methanol.

*Question 1:* Is the material a solid waste?
Yes the material is solid waste because it will not be recycled back to the process and would require disposal.
*Question 2*: Is the material excluded from the definition of solid waste or hazardous waste?
No this material is not excluded from the definition of solid or hazardous waste.

*Question 3*: Is the material a listed or characteristic hazardous waste?
Potassium chloride is not a listed waste and does not exhibit any of the characteristics necessary to be considered a hazardous waste. Therefore, this stream would be considered industrial, non-hazardous waste and would be disposed of under RCRA Subpart D.

Stream M2

Stream M2 contains primarily water with 13% methyl carbamate (by weight).

*Question 1*: Is the material a solid waste?
Yes the material is a solid waste because it will not be recycled back to the process and would require disposal.

*Question 2:* Is the material excluded from the definition of solid waste or hazardous waste?
No this material is not excluded from the definition of solid or hazardous waste.

*Question 3:* Is the material a listed or characteristic hazardous waste?
The materials in this stream are not listed wastes under RCRA. The mixture will also not exhibit any of the characteristics necessary to be considered a hazardous waste under RCRA. It would, therefore, be considered industrial, non-hazardous waste and be disposed of under Subpart D.

Stream M3

Stream M3 contains methanol (13% weight), Aliquot 336 (4.7% weight), water (78% weight), sodium hydroxide (0.8% weight), and silanol (2.6% weight).

*Question 1*: Is the material a solid waste?
Yes the material is a solid waste because it will not be recycled back to the process and would require disposal.

*Question 2*: Is the material excluded from the definition of solid waste or hazardous waste?

No this material is not excluded from the definition of solid or hazardous waste.

*Question 3*: Is the material a listed or characteristic hazardous waste?
Methanol is a listed waste under RCRA, with the designation of F003. However, F003 materials are only listed based on the characteristic of ignitability. According to RCRA, if the waste no longer exhibits the characteristic for which it was listed, it is no longer considered a listed hazardous waste. Aqueous wastes containing less than 24% alcohol by volume are not considered ignitable (40 CFR §261.21(a)(1)). Since methanol is approximately 16.3% by volume in this waste stream, the stream is not considered ignitable. Methanol is also on the U list, which is only relevant for unused chemicals and does not apply to this waste stream. The stream also does not exhibit any other characteristics that would classify the stream as hazardous. This stream would therefore not be a listed or characteristic hazardous waste and would be disposed of under Subpart D.

Stream M4

Stream M4 contains methanol from the final stripping step in the process.

*Question 1*: Is the material a solid waste?
Yes the material is a solid waste because it will not be recycled back to the process and would require disposal.

*Question 2*: Is the material excluded from the definition of solid or hazardous waste?
No this material is not excluded from the definition of solid or hazardous waste.

*Question 3*: Is the material a listed or characteristic hazardous waste?
Yes, methanol is a listed waste under RCRA with a F003 designation.

*Question 4:* Is the waste delisted?

No this waste is not delisted. This stream would therefore require disposal as a RCRA hazardous waste under Subpart C. The Subpart C requirements are discussed in more detail later in this section as they apply to this process.

Stream M5

Stream M5 is a methanol recycle stream.

*Question 1*: Is the material a solid waste?
No this material is not a solid waste because it is recycled directly back to the process without reclamation.

Stream M6

Stream M6 is the xylene recycle stream.

*Question 1*: Is the material a solid waste?
No this material is not a solid waste because it is recycled directly back to the process without reclamation.

Stream M7

Stream M7 is a $D_4$ recycle stream.

*Question 1*: Is the material a solid waste?
No this material is not a solid waste because it is recycled directly back to the process without reclamation.

Stream M8

Stream M8 is a gaseous trimethylamine amine stream from the final stripping step in the process.

*Question 1*: Is the material a solid waste?
Yes this material is a considered a solid waste because it is not returned to the process.

*Question 2*: Is the material excluded from the definition of solid waste or hazardous waste?
No this material is not excluded from the definition of solid or hazardous waste.

*Question 3*: Is the material a listed or characteristic hazardous waste?
No this material is not a listed waste under RCRA. It also does not exhibit the characteristics necessary to classify as a hazardous waste. It would therefore fall under Subpart D.

Stream M9

Stream M9 is a gaseous $CO_2$ stream from the separate step after the deprotect step.

*Question 1*: Is the material a solid waste?
Yes this material is considered a solid waste because it is not returned to the process.

*Question 2*: Is the material excluded from the definition of solid waste or hazardous waste?
No this material is not excluded from the definition of solid or hazardous waste.

*Question 3*: Is the material a listed or characteristic hazardous waste?
No this material is not a listed waste under RCRA. It also does not exhibit the characteristics necessary to classify as a hazardous waste. It would therefore fall under Subpart D.

**Table 90.** Summary of RCRA classifications

| Stream Number | Materials | Classification and other relevant RCRA Information |
|---|---|---|
| M1 | Potassium chloride | Industrial, non-hazardous solid waste to be disposed of under Subpart D |
| M2 | Methyl carbamate and water | Industrial, non-hazardous solid waste to be disposed of under Subpart D |
| M3 | Methanol, Aliquot 336, sodium hydroxide, silanol and water | Industrial, non-hazardous solid waste to be disposed of under Subpart D |
| M4 | Methanol | Listed hazardous waste based on F003 designation to be disposed of under Subpart C |
| M5 | Methanol | Not considered solid waste since directly recycled back to the process without reclamation |
| M6 | Xylene | Not considered solid waste since directly recycled back to the process without reclamation |
| M7 | $D_4$ | Not considered solid waste since directly recycled back to the process without reclamation |
| M8 | Trimethylamine (gas) | Industrial, non-hazardous solid waste in gas phase to be disposed of under Subpart D. |
| M9 | $CO_2$ gas | Industrial, non-hazardous solid waste in gas phase to be disposed of under Subpart D. |

## RCRA Subpart C requirements

### Generator requirements

Specific requirements for hazardous waste handling depend on the generator classification based on the quantity of hazardous waste generated per month. The only stream from this process for which the Subpart C requirements are relevant is stream M4. Requirements for CESQG, SQG, and LQG are summarized briefly in Section E of this report.

### *Classification for annual GAP-1$_m$ make-up*

The quantity of methanol generated based on the mass balance for stream M4 is estimated to be 216.7 lbs per month (calculated based on 310.25 working days per year), or 98.5 kg per month for the manufacturing of GAP-1$_m$ to account for annual GAP-1$_m$ make-up for the system. This would classify this process as a CESQG based on the RCRA definition. However, it is very close to the cutoff for SQG classification (more than 100 kg per month).

*Classification for initial fill of system*

The quantity of methanol generated based on the mass balance for stream M4 is estimated to be 1078 lbs per month (calculated based on 310.25 working days per year), or 490 kg per month for the manufacturing of GAP-$1_m$ for the initial fill of the system. This would classify this process as a SQG based on the RCRA definition. If this manufacturing process is co-located with other processes that generate RCRA hazardous waste in sufficient quantities, it could potentially be subject to LQG requirements. A facility is classified as LQG if it generates greater than or equal to 1000 kg/month.

### 7.2.5 Engineering Analysis and Controls for the Manufacturing Process of GAP-$1_m$

Controls of vapor emissions will be necessary in this process, given the use of three chemicals on the HAP list (methanol, xylene, and allyl chloride). In order to comply with 40 CFR 63, which regulates equipment leaks, all emissions from equipment leaks at this facility would be vented through a closed-vent system to a control device, in accordance with the requirements of 40 CFR §63.172. These requirements are summarized briefly in this section.

If a closed-vent system is not in place at the facility in question, then the specific requirements outlined in 40 CFR §63.163 through §63.171, §63.173, and §63.174 would apply in order to ensure compliance with equipment leak regulations. These requirements are not summarized in detail in this report.

Requirements for the closed-vent systems and control devices (40 CFR §63.172) include:

- Recovery or recapture devices (such as condensers or absorbers) need to operate with an efficiency of 95% or greater, or to an exit concentration of 20 $ppm_v$, whichever is less stringent.
- Enclosed combustion devices also need to operate with an efficiency of 95% or greater, or to an exit concentration of 20 $ppm_v$, whichever is less stringent, or to provide a

minimum residence time of 0.5 seconds at a minimum temperature of 760°C. In this case, the 20 $ppm_v$ is on a dry basis and is corrected to 3% oxygen.

- Control devices need to be monitored, including an initial inspection and annual inspections. Specific requirements for these inspections are detailed in the regulations.
- Leaks are indicated by either an instrument reading greater than 500 $ppm_v$ or by visual inspections and need to be repaired as soon as practicable.

A control device should also be designed that will reduce trimethylamine emissions from waste stream M8. Though this chemical is not on the HAP list, it is a corrosive and flammable gas and the need for safe handling of this stream should be considered in designing a vapor mitigation and control strategy for the facility.

### 7.2.6 Handling and Storage for the Manufacturing Process of $GAP_{-1m}$

The following section provides handling and storage recommendations for allyl chloride, potassium cyanate, sodium hydroxide, TMDSO, tetramethylammonium hydroxide, Karstedt's catalyst, $D_4$, trioxtylmethylammonium chloride, 1-octanol, trioctylamine, methyl carbamate, potassium chloride, and trimethylamine. There is no MSDS with safety and handling information for the silanol material. However, this material will only be present as part of a waste stream that will be handled safely in accordance with RCRA Subpart D regulations. Methanol and xylene were discussed earlier in this report for the $CO_2$ capture system (Section G) and the information is not duplicated here.

a) Allyl chloride (CAS # 107-05-1)

Allyl chloride is classified as a hazardous chemical by the OSHA standard. It is regulated under both DOT and IATA as a flammable liquid. The NFPA rating for allyl chloride is 2 for health hazard, 3 for flammability, and a 0 for reactivity.

1) Storage and Handling Recommendations

Allyl chloride needs to be stored in a closed container in a dry area with adequate ventilation. The recommended storage temperature is 2-8°C. It should be used in explosion proof equipment and kept away from ignition sources. Contact with skin and eyes and inhalation of vapors or mist need to be avoided. Allyl chloride should be stored separately from strong oxidizing agents. Additional chemicals that should be stored separately from allyl chloride are listed in Section J of this report.

2) Accidental Release Measures

In the event of a spill, personnel should be evacuated to a safe area and all sources of ignition removed. PPE should be worn, including respiratory protection to avoid breathing vapors. Precautions should be taken due to the high volatility, corrosivity, and flammability of allyl chloride. If it is safe to do so, further leakage or spillage should be prevented and discharge to the environment avoided. The spill should be contained and the material collected with an electrically protected vacuum cleaner or by wet-brushing.

3) Health Effects and Exposure Limits

ACGIH provides TLV-TWA (threshold limit value – time weighted average) of 1 $ppm_v$ and a TLV-STEL (threshold limit value – short-term exposure limit) of 2 $ppm_v$. Both of these exposure limits are based on eye and upper respiratory tract irritation and liver and kidney damage. Both NIOSH and OSHA provide a TWA of 1 $ppm_v$ (3 $mg/m^3$) and a STEL of 2 $ppm_v$ (6 $mg/m^3$). OSHA classifies this chemical as being harmful by ingestion and skin absorption, an irritant, a carcinogen, and a mutagen. Symptoms of exposure to allyl chloride include spasm, inflammation and edema of the larynx and bronchi, pneumonitis, pulmonary edema, burning sensation, coughing, headache, nausea, and vomiting.

4) Respiratory Protection Recommendation

If the risk assessment indicates that a respirator is necessary, use a full-face respirator with either multi-purpose combination or type ABEK (EN 14387) respirator cartridges in addition to engineering controls. If the respirator is the only protection available, use a full-face supplied air respirator.

5) Hand and Eye Protection Recommendation

This material should be handled with gloves. Fluorinated rubber gloves with a minimum layer thickness of 0.7 mm are recommended. Face shield and safety glasses are the recommended eye protection. Eye protection must be approved under appropriate government standards, such as NIOSH or EN 166.

6) Skin and Body Protection Recommendation

When complete suit protection is required, wear flame retardant antistatic protective clothing. The need for this type of protection is determined based on the concentration and amount of material in the workplace in question.

b) Potassium Cyanate (CAS# 590-28-3)

Potassium cyanate is classified as a hazardous chemical by the OSHA standard. It is not regulated by either DOT or IATA as dangerous goods. The NFPA rating for potassium cyanate is 2 for health hazard, 0 for flammability, and a 0 for reactivity.

1) Storage and Handling Recommendations

Potassium cyanate should be kept in a closed container in a dry area with adequate ventilation. Contact with skin and eyes should be avoided. The formation of dust and aerosols can also pose a risk and may result in the formation of combustible dusts. Potassium cyanate should be stored separately from strong oxidizing agents.

2) Accidental Release Measures

Proper PPE should be worn when dealing with spills of this material. Dust formation should be avoided and proper ventilation should be provided in the area of the spill. If it is safe to do so, further leakage or spillage should be prevented and discharge to the environment avoided. The spill should be cleaned in such a way so as to avoid the creation of dust and the material kept in suitable, closed containers for disposal.

3) Health Effects and Exposure Limits

OSHA classifies potassium cyanate as an acute toxicity hazard in the case of ingestion and an eye irritant. No OSHA, ACGIH, or WEEL (Workplace Environmental Exposure Levels) exposure limit values are provided for this material.

4) Respiratory Protection Recommendation

Use type P95 or type P1 particle respirator for nuisance exposures. Use type OV/AG/P99 or ABEK-P2 respirator cartridges for higher level exposures.

5) Hand and Eye Protection Recommendation

This material should be handled with gloves. Nitrile rubber gloves with a minimum layer thickness of 0.11 mm are recommended. Safety glasses and side-shields should be worn for eye protection. Eye protection needs to be approved under such standards as NIOSH or EN 166.

6) Skin and Body Protection Recommendation

The need for complete suit protective clothing against chemicals should be determined based on the concentration and amount of the substance in the workplace in question.

c) Sodium hydroxide (CAS# 1310-73-2)

Sodium hydroxide is classified as a hazardous chemical by the OSHA standard. It is regulated under both DOT and IATA as a corrosive material. The NFPA rating for sodium hydroxide is 3 for health hazard, 0 for flammability, and a 0 for reactivity.

1) Storage and Handling Recommendations

Sodium hydroxide should be kept in a closed container in a dry area with adequate ventilation. The formation of dusts and aerosols should be avoided. This material is a strong base and should not be stored with certain types of incompatible chemicals, including strong acids and organic materials. Specific chemicals involved in this process that should be stored separately include TMDSO, Karstedt catalyst, and D4.

2) Accidental Release Measures

In the event of a spill, personnel should be evacuated to safe areas. The use of proper PPE is necessary when dealing with a spill of this material, including respiratory protection. When handling this material, the corrosivity should be considered and contact with skin avoided. Dust formation should be avoided and adequate ventilation provided in the location of the spill. If it is safe to do so, further leakage or spillage should be prevented and discharge to the environment avoided. The spill should be cleaned in such a way so as to avoid the creation of dust and the material kept in suitable, closed containers for disposal.

3) Health Effects and Exposure Limits

Sodium hydroxide is extremely corrosive and will cause damage to skin and eyes. ACGIH provides a TLV-C (threshold limit value – ceiling limit) value of 2 mg/m$^3$. OSHA also provides TWA and C (ceiling limit) values of 2 mg/m$^3$. These values are based on eye, skin, and upper respiratory tract irritation.

4) Respiratory Protection Recommendation

If the risk assessment determines that a respirator is necessary, use a full-face particle respirator with type N100 or type P3 cartridges in addition to engineering controls. If the respirator is the only means of protection, use a full-face supplied air respirator.

5) Hand and Eye Protection Recommendation

This material needs to be handled with gloves. Nitrile rubber gloves with a minimum layer thickness of 0.11 mm are recommended. A face shield and safety glasses are recommended. All eye protection needs to be approved under such standards or NIOSH or EN 166.

6) Skin and Body Protection Recommendation

The need for complete suit protective clothing against chemicals should be determined based on the concentration and amount of the substance in the workplace in question.

d) <u>TMDSO (CAS# 3277-26-7)</u>

TMDSO is classified as a hazardous chemical by the OSHA standard. It is regulated under both DOT and IATA as a flammable liquid. The NFPA rating for TMDSO is 0 for health hazard, 3 for flammability, and a 0 for reactivity.

1) Storage and Handling Recommendations

TMDSO should be stored in a closed container in a dry area with adequate ventilation. It should also be stored under inert gas given its moisture sensitivity. It should be used in explosion proof equipment and kept away from ignition sources. Contact with skin and eyes and inhalation of vapors or mist need to be avoided. TMDSO should be stored separately from strong acids, bases, and oxidizing agents.

2) Accidental Release Measures

In the event of a spill, personnel should be evacuated to a safe area and all sources of ignition removed. PPE should be worn, including respiratory protection to avoid breathing vapors. Precautions should be taken due to the flammability of TMDSO. If it is safe to do so, further leakage or spillage should be prevented and discharge to the environment avoided. The spill should be contained and the material collected with an electrically protected vacuum cleaner or by wet-brushing.

3) Health Effects and Exposure Limits

This material may form a siloxane polymer when in contact with skin, eyes, or in the lungs and may cause irritation, dizziness, or headache. No specific information on target organ effects was available. No OSHA, ACGIH, or WEEL exposure limit values are provided for this material.

4) Respiratory Protection Recommendation

If the risk assessment indicates that respiratory protection is necessary, a full-face respirator with multi-purpose combination of type ABEK respirator cartridges should be used in addition to engineering controls. If a respirator is the only means of protection, use a full-face supplied air respirator.

5) Hand and Eye Protection Recommendation

This material needs to be handled with gloves. Nitrile rubber gloves with a minimum thickness of 0.11 mm are recommended. A face shield and safety glasses are recommended for eye protection. All equipment used for eye protection needs to be approved under the appropriate standard such as NIOSH or EN 166.

6) Skin and Body Protection Recommendation

Impervious, flame retardant, antistatic protective clothing is recommended. The type of protective clothing necessary would be determined based on the concentration and amount of the material in the workplace in question.

e) Tetramethyl ammonium hydroxide (CAS# 75-59-2)

Tetramethyl ammonium hydroxide is classified as a hazardous chemical by the OSHA standard. It is regulated under both DOT and IATA as a corrosive liquid. The NFPA rating for tetramethylammonium hydroxide is 3 for health hazard, 0 for flammability, and a 0 for reactivity.

1) Storage and Handling Recommendations

Tetramethyl ammonium hydroxide needs to be stored in a closed container in a dry area with adequate ventilation. Contact with skin and eyes and inhalation of vapors or mist need to be avoided. Tetramethyl ammonium hydroxide should be stored separately from alkali metals, strong oxidizing agents, acids, acid chlorides, acid anhydrides, and halogens.

2) Accidental Release Measures

In the event of a spill, personnel should be evacuated to safe areas. Proper PPE should be worn when dealing with the spill, including respiratory protection, given the corrosive nature of this material. Adequate ventilation should be provided. If it is safe to do so, further leakage or spillage should be prevented and discharge to the environment avoided. To clean the spill, soak with an inert absorbent material and dispose of as hazardous waste.

3) Health Effects and Exposure Limits

OSHA classifies this chemical as hazardous based on acute oral toxicity, acute dermal toxicity, skin corrosion, and eye damage. It is listed as being fatal if swallowed or if in contact with skin. It is destructive to mucous membranes and upper respiratory tract, eyes, and skin. Symptoms of exposure include burning sensation, coughing, shortness of breath, headache, nausea, and vomiting. Symptoms of inhalation exposure may include pulmonary edema, spasm, inflammation, and edema of bronchi and larynx. No OSHA, ACGIH, or WEEL exposure limit values are provided for this material.

4) Respiratory Protection Recommendation

If the risk assessment indicates that respiratory protection is needed, use a full-face respirator with multi-purpose combination or type ABEK cartridges in addition to engineering controls. If a respirator is the only means of protection, use a full-face supplied air respirator.

5) Hand and Eye Protection Recommendation

This material should be handled with gloves. Nitrile rubber gloves with a minimum layer thickness of 0.11 mm are recommended. Tightly fitting safety goggles and an 8" minimum faceshield are recommended eye protection. All eye protection equipment needs to be approved by the appropriate standards, such as NIOSH or EN 166.

6) Skin and Body Protection Recommendation

The need for complete suit protective clothing against chemicals should be determined based on the concentration and amount of the substance in the workplace in question.

f) Karstedt catalyst (CAS# 68478-92-2)

Karstedt catalyst when prepared in vinyl terminated polydimethylsiloxane (PDMS) is not classified as a hazardous chemical by the OSHA standard. It is not regulated by either DOT or IATA as dangerous goods. The NFPA rating for Karstedt catalyst is 2 for health hazard, 0 for flammability, and a 0 for reactivity.

1) Storage and Handling Recommendations

Karstedt catalyst needs to be stored in a closed container in a dry area with adequate ventilation. It should be stored separately from oxidizing agents, acids, and bases, such as NaOH and tetramethyl ammonium hydroxide.

2) Accidental Release Measures

In the event of a spill, proper PPE should be worn. Adequate ventilation should be provided. To clean the spill, soak with an inert absorbent material and dispose of as hazardous waste.

3) Health Effects and Exposure Limits

No specific data on target organs or health effects is available on the MSDS. It should be noted that this catalyst has been approved by the FDA for use in medical applications (Section I). No OSHA, ACGIH, or WEEL exposure limit values are provided for this material.

4) Respiratory Protection Recommendation

If the risk assessment indicates that respiratory protection is required, use a full-face respirator with multi-purpose combination or type ABEK cartridges in addition to engineering controls. If the respirator is the only means of protection, use a full-face supplied air respirator.

5) Hand and Eye Protection Recommendation

This material should be handled with gloves. Safety glasses with side-shields are recommended for eye protection. Any eye protection equipment needs to be approved under the appropriate standard, such as NIOSH or EN 166.

6) Skin and Body Protection Recommendation

Impervious clothing should be worn if protective clothing is necessary. The need for protective clothing would be determined based on the concentration and amount of the material in the workplace in question.

g) $D_4$ (CAS# 556-67-2)

$D_4$ is classified as a hazardous chemical by the OSHA Standard. It is regulated under both DOT and IATA as a flammable liquid. The NFPA rating for D4 is 1 for health hazard, 2 for flammability, and a 0 for reactivity.

1) Storage and Handling Recommendations

$D_4$ should be stored in a closed container in a dry area with adequate ventilation away from ignition sources. Contact with skin and eyes and inhalation of vapors or mist need to be avoided. It should be stored separately from strong oxidizing agents, acids, and bases, such as NaOH and tetramethyl ammonium hydroxide.

2) Accidental Release Measures

In the event of a spill, personnel should be evacuated to a safe area and all sources of ignition removed. PPE should be worn, including respiratory protection to avoid breathing vapors. Precautions should be taken due to the flammability of $D_4$. If it is safe to do so, further leakage or spillage should be prevented and discharge to the environment avoided. The spill should be contained and the material collected with an electrically protected vacuum cleaner or by wet-brushing.

3) Health Effects and Exposure Limits

$D_4$ is classified as hazardous by OSHA based on reproductive toxicity (category 2), it is suspected of potentially damaging fertility or the unborn child based on testing in rats. It does not cause skin or eye irritation. No OSHA, ACGIH, or WEEL exposure limit values are provided for this material.

4) Respiratory Protection Recommendation

If the risk assessment indicates that a respirator is necessary, a full-face respirator with multi-purpose combination or type ABEK cartridges should be used in addition to engineering controls. If the respirator is the only protection, a full-face supplied air respirator should be used.

5) Hand and Eye Protection Recommendation

This material should be handled with gloves. Nitrile gloves with a minimum thickness of 0.11 mm are recommended for splash contact. If there is potential for full contact with the chemical, nitrile gloves with a minimum layer thickness of 0.4 mm should be used. A face shield and safety glasses are the recommended eye protection. All eye protection equipment needs to be approved under the appropriate standards, such as NIOSH or EN 166.

6) Skin and Body Protection Recommendation

If protective clothing is needed, it should be impervious, flame retardant, and anti-static. The need for protective clothing would be determined based on the concentration and amount of the material in the workplace in question.

h) Trioctylmethylammonium chloride (CAS# 63393-96-4)

Trioctylmethylammonium chloride is classified as a hazardous chemical by the OSHA Standard. It is regulated under both DOT and IATA as a toxic substance. The NFPA rating for trioctylmethylammonium chloride is 2 for health hazard, 0 for flammability, and a 0 for reactivity.

1) Storage and Handling Recommendations

Trioctylmethylammonium chloride should be stored in a closed container in a dry area with adequate ventilation. Contact with skin and eyes and inhalation of vapors or mist need to be avoided. This material is hygroscopic so care should be taken to limit exposure to moisture. It should be stored separately from strong oxidizing agents.

2) Accidental Release Measures

In the event of a spill, evacuate personnel to safe areas. When dealing with the spill, proper PPE needs to be worn, including respiratory protection and adequate ventilation provided. If it is safe to do so, further leakage or spillage should be prevented and discharge to the environment avoided. To clean the spill, soak up with inert absorbent material and dispose of as a hazardous waste.

3) Health Effects and Exposure Limits

OSHA classifies this as hazardous based on acute oral toxicity, skin corrosion, and serious eye damage. Potential effects upon exposure include burning sensation, cough, shortness of breath, headache, nausea, vomiting, and narcosis. No OSHA, ACGIH, or WEEL exposure limit values are provided for this material.

4) Respiratory Protection Recommendation

If the risk assessment indicates that a respirator would be necessary, wear a full-face respirator with multi-purpose combination or type ABEK cartridges in addition to engineering controls. If the respirator is the only source of protection, use a full-face supplied air respirator.

5) Hand and Eye Protection Recommendation

This material needs to be handled with gloves. Nitrile gloves with a minimum layer thickness of 0.11 mm are recommended. Tightly fitting safety goggles and an 8" minimum faceshield are the recommended eye protection. All eye protection equipment needs to be approved under the appropriate standard, such as NIOSH or EN 166.

6) Skin and Body Protection Recommendation

The need for protective clothing would be determined based on the concentration and amount of the material in the workplace in question.

i) <u>1-octanol (CAS# 111-87-5)</u>

1-octanol is classified as a hazardous chemical by the OSHA Standard. It is not regulated under DOT or IATA as dangerous goods. The NFPA rating for 1-octanol is 2 for health hazard, 2 for flammability, and a 0 for reactivity.

1) Storage and Handling Recommendations

1-octanol should be stored in a closed container in a dry area with adequate ventilation away from ignition sources. Contact with skin and eyes and inhalation of vapors or mist need to be avoided. It should be noted that this material is a component of Aliquat 336 and would not be present on-site in its pure form.

2) Accidental Release Measures

In the event of a spill, personnel should be evacuated to a safe area and all sources of ignition removed. PPE should be worn, including respiratory protection to avoid breathing vapors. Precautions should be taken due to the flammability of 1-octanol. If it is safe to do so, further leakage or spillage should be prevented and discharge to the environment avoided. The spill should be contained and the material collected with an electrically protected vacuum cleaner or by wet-brushing.

3) Health Effects and Exposure Limits

OSHA classifies this chemical as hazardous based on skin and eye irritation. It can cause central nervous system depression, nausea, headache, vomiting, and narcosis. WEEL provides a TWA of 50 $ppm_v$ for this chemical.

4) Respiratory Protection Recommendation

If the risk assessment indicates that a respirator is necessary, use a full-face respirator with multi-purpose combination or type ABEK cartridges in addition to engineering controls. If the respirator is the only source of protection, use a full-face supplied air respirator.

5) Hand and Eye Protection Recommendation

This material needs to be handled with gloves. For splash contact, nitrile gloves with a minimum layer thickness of 0.11 mm are recommended. For full contact, nitrile gloves with a minimum layer thickness of 0.4 mm are recommended. Safety glasses with side-shields are the recommended eye protection. All eye protection equipment needs to be approved under the appropriate standard, such as NIOSH or EN 166.

6) Skin and Body Protection Recommendation

If protective clothing is necessary, it should be impervious. The need for protective clothing would be determined based on the concentration and amount of material in the workplace.

j) Trioctylamine (CAS# 1116-76-3)

Trioctylamine is classified as a hazardous chemical by the OSHA Standard. It is not regulated under DOT or IATA as dangerous goods. The NFPA rating for trioctylamine is 2 for health hazard, 1 for flammability, and a 0 for reactivity.

1) Storage and Handling Recommendations

Trioctylamine needs to be stored in a closed container in a dry area with adequate ventilation. Contact with skin and eyes and inhalation of vapors or mist need to be avoided. It should be noted that this material is a component of Aliquat 336 and would not be present on-site in its pure form.

2) Accidental Release Measures

In the event of a spill, personnel should be evacuated to safe areas. When dealing with the spill, proper PPE should be worn and adequate ventilation provided to avoid breathing vapors. To clean the material, soak up with inert absorbent material and dispose of as hazardous waste.

3) Health Effects and Exposure Limits

OSHA classifies this chemical as hazardous based on skin and eye irritation and for respiratory irritation. No OSHA, ACGIH, or WEEL exposure limit values are provided for this material.

4) Respiratory Protection Recommendation

If the risk assessment indicates that a respirator is needed, a full-face respirator with multi-purpose combination or type ABEK cartridge should be used in addition to engineering controls. If the respirator is the only means of protection, a full-face supplied air respirator should be used.

5) Hand and Eye Protection Recommendation

This material should be handled with gloves. Nitrile gloves with a minimum layer thickness of 0.11 mm are recommended. Safety glasses with side-shields are the recommended eye protection. All eye protection equipment needs to be approved under the appropriate standard, such as NIOSH or EN 166.

6) Skin and Body Protection Recommendation

If protective clothing is necessary, it should be impervious. The need for protective clothing would be determined based on the concentration and amount of material in the workplace.

### k) Methyl carbamate (CAS# 598-55-0)

Methyl carbamate is classified as a hazardous chemical by the OSHA Standard. It is not regulated under DOT or IATA as dangerous goods. The NFPA rating for methyl carbamate is 2 for health hazard, 0 for flammability, and a 0 for reactivity.

#### 1) Storage and Handling Recommendations

Methyl carbamate needs to be stored in a closed container in a dry area with adequate ventilation. Contact with skin and eyes needs to be avoided. The formation of dust and aerosols should also be avoided. This material should be stored separately from strong oxidizing agents, strong bases, and phosphorous halides.

#### 2) Accidental Release Measures

In the event of a spill, evacuate personnel to safe areas. When dealing with the spill, proper PPE should be worn and adequate ventilation provided to avoid breathing vapors. Dust formation should be avoided. If it is safe to do so, further leakage or spillage should be prevented. When cleaning, the creation of dust should be avoided and the material stored in closed containers for disposal.

#### 3) Health Effects and Exposure Limits

OSHA classifies this chemical as hazardous based on eye irritation and carcinogenicity. For carcinogenicity, it is category 2, which means they suspect it causes cancer. No OSHA, ACGIH, or WEEL exposure limit values are provided for this material.

#### 4) Respiratory Protection Recommendation

If the risk assessment indicates that a respirator is necessary, a full-face particle respirator with type N100 or P3 cartridge should be used in addition to engineering controls. If the respirator is the only means of protection, a full-face supplied air respirator should be used.

#### 5) Hand and Eye Protection Recommendation

This material should be handled with gloves. Safety glasses with side-shields are the recommended eye protection. All eye protection must be approved under the appropriate standard, such as NIOSH or EN 166.

6) Skin and Body Protection Recommendation

If protective clothing is needed, it should be impervious. The need for protective clothing would be determined based on the concentration and amount of material in the workplace in question.

l) Potassium chloride (CAS# 7447-40-7)

Potassium chloride is classified as a hazardous chemical by the OSHA Standard. It is not regulated under DOT or IATA as dangerous goods. The NFPA rating for potassium chloride is 0 for health hazard, 0 for flammability, and a 0 for reactivity.

1) Storage and Handling Recommendations

Potassium chloride should be stored in a closed container in a dry area with adequate ventilation. Formation of dusts and aerosols should be avoided. This material is hygroscopic so care should be taken to limit exposure to moisture. It should be stored separately from strong acids and oxidizing agents.

2) Accidental Release Measures

In the event of a spill, proper PPE should be worn and adequate ventilation provided to avoid breathing vapors. Dust formation should be avoided. If it is safe to do so, further leakage or spillage should be prevented and discharge to the environment avoided. When cleaning, the creation of dust should be avoided and the material stored in closed containers for disposal.

3) Health Effects and Exposure Limits

Potassium chloride is a gastrointestinal irritant after ingestion of high doses. Potential symptoms of exposure include hyperkalemia, nausea, vomiting, abdominal pain, diarrhea, constipation, thirst, dizziness, rash, weakness, and muscle cramps. No OSHA, ACGIH, or WEEL exposure limit values are provided for this material.

4) Respiratory Protection Recommendation

Respiratory protection for this chemical is not required. If protection from nuisance levels is desired, use type N95 or P1 dust masks.

5) Hand and Eye Protection Recommendation

This material should be handled with gloves. Nitrile gloves with a minimum layer thickness of 0.11 mm are recommended. No specific eye protection is recommended on the MSDS for this material, but, if eye protection is used, it should be approved under the appropriate standard, such as NIOSH or EN 166.

6) Skin and Body Protection Recommendation

The need for protective clothing would be determined based on the concentration and amount of material in the workplace in question. No specific requirements are listed on the MSDS.

m) Trimethylamine (CAS# 75-50-3)

Trimethylamine is classified as a hazardous chemical by the OSHA Standard. It is regulated under both DOT and IATA as a flammable gas. The NFPA rating for trimethylamine is 2 for health hazard, 4 for flammability, and a 0 for reactivity.

1) Storage and Handling Recommendations

Trimethylamine needs to be stored in a closed container in a dry area with adequate ventilation. The recommended storage temperature is 2-8°C. It should be used in explosion proof equipment and kept away from ignition sources. Contact with skin and eyes and inhalation of vapors or mist need to be avoided. It should be stored separately from oxidizing agents. Specific metals that should be avoided when storing or handling this chemical are listed in Section J of this report.

2) Accidental Release Measures

In the event of a spill, personnel should be evacuated to a safe area and all sources of ignition removed. PPE should be worn, including respiratory protection to avoid breathing vapors, given the corrosive nature of the material. Precautions should be taken due to the flammability of trimethylamine. If it is safe to do so, further leakage or spillage should be prevented and discharge to the environment avoided.

### 3) Health Effects and Exposure Limits

OSHA classifies this chemical as hazardous based on acute oral toxicity, acute inhalation toxicity, skin irritation, eye damage, and respiratory irritation. It is destructive to mucous membranes and the upper respiratory tract, eyes, and skin. Potential symptoms of exposure include cough, shortness of breath, headache, and nausea. ACGIH provides a TWA of 5 ppm$_v$ and a STEL of 15 ppm$_v$. These levels are based on respiratory tract irritation. Both OSHA and NIOSH provide a TWA of 10 ppm$_v$. OSHA provides a STEL of 15 ppm$_v$. NIOSH provides a ST (short-term) value of 15 ppm$_v$. WEEL provides a TWA of 1 ppm$_v$.

### 4) Respiratory Protection Recommendation

If the risk assessment indicates that respiratory protection is necessary, a full-face respirator with multi-purpose combination or type ABEK cartridge should be used in addition to engineering controls. If the respirator is the only source of protection, a full-face supplied air respirator should be used.

### 5) Hand and Eye Protection Recommendation

This material needs to be handled with gloves. Fluorinated rubber gloves with a minimum layer thickness of 0.7 mm are recommended. Tightly fitting safety goggles and an 8" minimum face shield are the recommended eye protection. All eye protection equipment needs to be approved under the appropriate standard, such as NIOSH or EN 166.

### 6) Skin and Body Protection Recommendation

If protective clothing is necessary, it should be flame retardant and anti-static. The need for protective clothing would be determined based on the concentration and amount of material in the workplace in question.

# 8 Bibliography

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104. Modeled using TEST model

105. Modeled using EPIWIN model

# 9 Acronyms

| | |
|---|---|
| BCF | Bio-Concentration Factor |
| CCF | Capital Charge Factor |
| CERCLA | Comprehensive Environmental Response and Liability Act |
| CEPCI | Chemical engineering plant cost index |
| COE | Cost of electricity |
| CESQG | Conditionally Exempt Small Quantity Generator |
| CSTR | Continuous Stirred Tank Reactor |
| CWA | Clean Water Act |
| $D_4$ | Octamethylcyclotetrasiloxane |
| DDBSA | Sodium dodecylbenzenesulfonate |
| ECOSAR | Ecological Structure Activity Relanship |
| EPIWIN | Estimations Programs Interface for Windows |
| FGD | Flue Gas Desulfurizer |
| hi | Individual film heat-transfer coefficients shell and tube heat exchanger |
| $H_{CO2}$ | Henry constant of $CO_2$ |
| HPA | Hazardous Air Pollutants |
| HSS | Heat stable salts |
| GAP-1 | (1,5-Bis(3-aminopropyl 1,1,3,3,5,5-hexamethyl trisiloxane)) |
| IATA | International Air Transport Association |

| | |
|---|---|
| IARC | International Agricultural Research Center |
| ICP-OES | Inductively coupled plasma-optical emission spectroscopy |
| IDLH | Immediately Dangerous to Life and Health |
| IOU | Investor owned utilities |
| $K_{ow}$ | octanol/water partition coefficient |
| $Keq$ | Equilibrium constant |
| MEA | Mono-ethanol amine |
| NCCC | National Carbon Capture Center |
| NFPA | National Fire Protection Association |
| Nu | Nusselt number |
| OECD | Organization for Economic Co-operation and Development |
| PC | Pulverized coal |
| PEL | Permissible Exposure Limit |
| $R_{do}$ | Fouling resistances shell and tube heat exchanger |
| RCRA | Resource Conservation and Recovery Act |
| REACH | Regulation on Registration, Evaluation, Authorization and Restriction of Chemicals |
| QSAR | Quantitative Structure Activity Relationships |
| SCR | Selective Catalytic Reduction |
| Sh | Sherwood Number |
| SARA | Superfund Amendments and Reauthorization Act (SARA) Title III |

| | |
|---|---|
| SSC | Steam Stripper Column |
| SQG | Small quantity generator |
| STEL | Short Term Exposure Limit |
| $U_o$ | Heat transfer coefficient for shell and tube heat exchangers |
| TEG | Triethylene glycol |
| TSCA | Toxic Substances Control Act, , the Occupational Safety and Health Act (OSHA) |
| TMDSO | Tetramethyldisiloxane |
| TMAH | Tetramethyl ammonium hydroxide |
| TOXNET | Toxicology data network |
| TS&M | Transportation, storage, and monitoring |
| TSDF | Transport, storage, and disposal facilities |
| VOC | Volatile Organic Compounds |