



**Pacific Northwest**  
NATIONAL LABORATORY

*Proudly Operated by Battelle Since 1965*

# Accelerating the Development of “Transformational” Solvents for CO<sub>2</sub> Separations

Quarterly Progress Report, Budget Period  
2, Q5, 2015

**May 2016**

DJ Heldebrant  
PK Koech

RJ Rousseau  
V Glezakou



## DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor Battelle Memorial Institute, nor any of their employees, makes **any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights.** Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or Battelle Memorial Institute. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

PACIFIC NORTHWEST NATIONAL LABORATORY

*operated by*

BATTELLE

*for the*

UNITED STATES DEPARTMENT OF ENERGY

*under Contract DE-AC05-76RL01830*

Printed in the United States of America

Available to DOE and DOE contractors from the  
Office of Scientific and Technical Information,  
P.O. Box 62, Oak Ridge, TN 37831-0062;  
ph: (865) 576-8401  
fax: (865) 576-5728  
email: [reports@adonis.osti.gov](mailto:reports@adonis.osti.gov)

Available to the public from the National Technical Information Service,  
U.S. Department of Commerce, 5285 Port Royal Rd., Springfield, VA 22161  
ph: (800) 553-6847  
fax: (703) 605-6900  
email: [orders@ntis.fedworld.gov](mailto:orders@ntis.fedworld.gov)  
online ordering: <http://www.ntis.gov/ordering.htm>



This document was printed on recycled paper.

(9/2003)



**Submitted to:** U.S. Department of Energy (DOE)  
Office of Fossil Energy

**FWP Award:** FWP-65872

**Project Title:** Accelerating the Development of “Transformational” Solvents  
for CO<sub>2</sub> Separations

**Quarterly Progress Report, Budget Period 2, Q6, 2015**

**Principal Investigators:**

**Dr. David J. Heldebrant**  
Phone: 509-372-6359  
[david.heldebrant@PNNL.gov](mailto:david.heldebrant@PNNL.gov)

**Dr. Phillip K. Koech**  
Phone: 509-372-6891  
[phillip.koech@PNNL.gov](mailto:phillip.koech@PNNL.gov)

**Dr. Roger Rousseau**  
Phone: 509-372-6092  
[roger.rousseau@PNNL.gov](mailto:roger.rousseau@PNNL.gov)

**Dr. Vassiliki-Alexandra Glezakou**  
Phone: 509-375-6961  
[vanda.glezakou@PNNL.gov](mailto:vanda.glezakou@PNNL.gov)

**Submitting Official:** Contracting Officer

**Date Submitted:** January 29, 2016

**Recipient Organization:** Pacific Northwest National Laboratory  
P.O. Box 999, MS K2-44  
Richland, WA 99352

**Project Period:** May 1, 2014 through September 30, 2016

**Reporting Period End Date:** December 31, 2015

**Reporting Term:** Quarterly

**Signature:** *kevin ghirardo*

## I. Accomplishments and Milestone Update

### Synopsis of Accomplishments

The team has continued to make consistent progress in all prior Tasks and Subtasks in Q6 in addition to beginning the new added scope for the General Electric Company (GE) aminosilicone solvent system. The program is on budget and on track to achieve all relevant Milestones for the program by the end of FY16. The theory team has begun to develop models and simulations on GE's new GAP-1 solvent platform, while the synthesis team continues to synthesize the candidate molecules from the modeling team. The testing team has been focused on measuring viscosity and vapor-liquid equilibria curves of candidate molecules to provide relevant process data in Task 4 for the performance projections in Task 5. More detailed descriptions of each accomplishment are provided below.

### Milestones

With the addendum and revised scope of work, the Milestones for this project have been revised. Table 1 identifies the revised target or actual completion times for the program Milestones. Completed Milestones are denoted with underlined text. The project team completed Milestones 1-5 and 7. The project team is continuing synthesis and testing for Milestone 6, with the goal of far exceeding the 400 cP reduction identified in Milestone 7. The team has also started on the scope of work for GE in Milestone 10, beginning the model construction of the carbamate chemistry.

**Table 1.** Major Milestones Relevant to BP1.

<b>Milestone Number</b>	<b>Milestone Description</b>	<b><u>Actual or Revised Completion Time</u></b>
1	Updated Project Management Plan (PMP)	<u>June, 2014</u>
2	Construct physical property model	<u>December, 2014</u>
3	Synthesize and characterize 13 candidate CO <sub>2</sub> BOL molecules	<u>May, 2015</u>
4	Viscosity reduction of 200 cP demonstrated	<u>April, 2014</u>
5	Go no-go presentation at NETL	<u>May, 2015</u>
6	Synthesize and characterize second round of 13 candidate CO <sub>2</sub> BOL Molecules	February, 2016
7	Viscosity reduction of 400 cP demonstrated	<u>December, 2015</u>
10	Construct first-generation molecular dynamics (MD) model for carbamates. Initial assessment of viscosity reduction for GE aminosilicones via additives & blends	March, 2016
11	Model 50 carbamate derivatives and identify 3 new candidate molecules for synthesis & characterization	June, 2016

12	Synthesis & characterization of 3 carbamate solvent variants from MD simulations	August, 2016
8	Synthetic methodology of optimal CO <sub>2</sub> BOLs demonstrated at \$10/kg	May, 2016
9	Final report provided to NETL	October, 2016

## **Project Accomplishments by Task**

### **Task 1. Project Management**

#### **Subtask 1.1 General project management**

The PMP was updated and sent to DOE as required.

### **Task 2. Molecular Development**

#### **Subtask 2.1 Design 100 candidate molecules based on variations of current formulation**

Subtask 2.1 was completed.

#### **Subtask 2.2 Construct physical property prediction model**

Subtask 2.2 was completed.

#### **Subtask 2.3 Predict physical and thermodynamic properties of first 100 molecules**

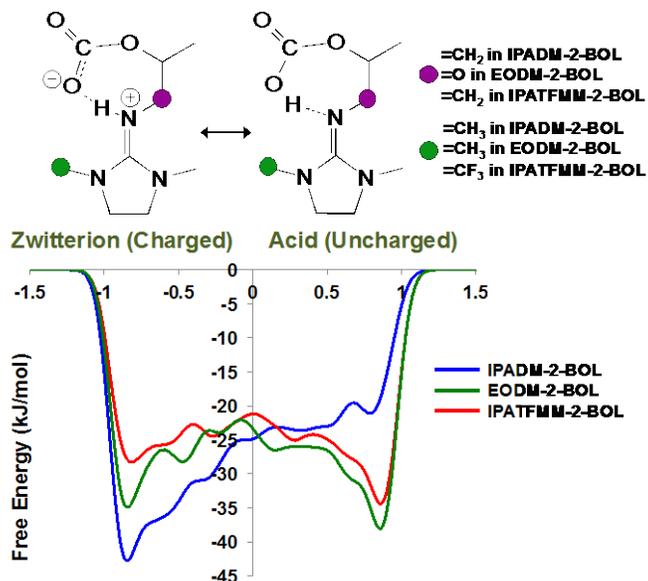
Subtask 2.3 was completed.

#### **Subtask 2.4 Revise performance targets and design the second 100 molecules**

In the last quarter, we examined the hypothesis of neutral CO<sub>2</sub> capture that results from a dynamic equilibrium between the charged (zwitterionic) and non-charged (acid) state of CO<sub>2</sub>-bound CO<sub>2</sub>BOLs. Given that viscosity in CO<sub>2</sub>BOLs is a direct result of agglomerating charged molecular species, we explored the molecular modification that would shift this equilibrium toward the non-charged acid state. *Ab initio* molecular dynamics (AIMD) simulations with the metadynamics technique to accelerate the proton transfer event were performed to obtain the free energy surface of the acid/zwitterion equilibrium. Three different compounds with different acidities were used to demonstrate proof of principle: (i) IPADM-2-BOL (Koechanol), (ii) a molecule with an oxime group to reduce the acidity of the alkanol group (EODM-2-BOL), and (iii) a fluorinated guanidium core to decrease the basicity at the N site (IPATFMM-2-BOL). The oxime and fluorinated BOLs are currently based on simple, theoretical molecular models chosen to test a hypothesis, but we are also examining their synthesis, or that of close equivalents.

We found that making the alkanol group (green in the upper portion of Figure 1) less

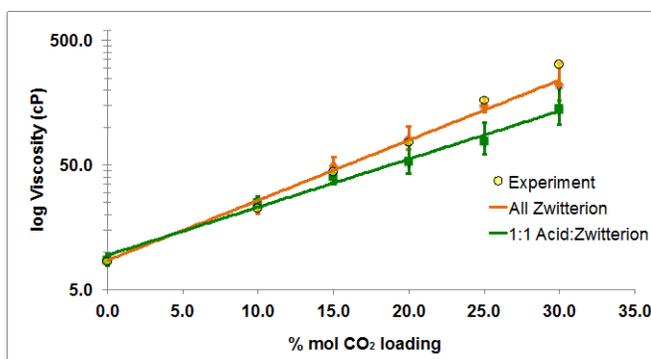
acid, or the guanidinium core (pink) less basic can result in the acid state being favored over the zwitterionic state, as shown in the relative energies of the two states in the lower portion of Figure 1. The zwitterionic state is favored for IPADM-2-BOL (blue), confirming known observations.



**Figure 1:** Free Energy Profiles of the Acid-Zwitterion Equilibrium for IPADM-2-BOL, the Oxime Derivative (EODM-2-BOL), and the Fluoro-Substituted Derivative (IPATFMM-2-BOL).

With the metadynamics AIMD simulations, we were also able to calculate the energy barriers required to cross to/from acid/zwitterion states. These barriers were found to be low enough that at carbon capture conditions, an equilibrium between the two states will exist, resulting in ~1:1 acid:zwitterion populations of the CO<sub>2</sub>BOL molecules that are CO<sub>2</sub>-bound.

We further explored the impact of such an acid/base equilibrium on the viscosity with two independent sets of classical MD simulations on the IPADM-2-BOL system at varying CO<sub>2</sub> loadings: (i) one with all CO<sub>2</sub>-bound molecules in zwitterionic form, and (ii) another with 1:1 acid:zwitterion populations. Figure 2 shows very good agreement between the computed (orange) and experimental (yellow circles) viscosities for IPADM-2-BOL, as we had previously shown for other examples. However, the hypothetical 1:1 mixture (green) shows a pronounced drop in viscosity, on the order of 30–50%, for the higher loadings (over 25% mol). This appreciable viscosity reduction, while not altering the CO<sub>2</sub> storage capacity, points to a potential for viable, nonionic CO<sub>2</sub> capture solvent systems that can be brought about with simple molecular modifications once the fundamental reaction drivers are taken into account.



**Figure 2:** IPADM-2-BOL Viscosities: Experimental Data Points (yellow), All Zwitterions (orange), and CO<sub>2</sub>-Loaded Molecules in 1:1 Acid:Zwitterion (green).

This work formed part of a manuscript that is under review by *Nature Communications*.

### **Subtask 2.5 Predict physical and thermodynamic properties of second 100 molecules**

Modeling of the next 100 candidates has started; the properties of these compounds have not yet been predicted.

### **Subtask 2.6 Construct physical property model for carbamate derivative (GE aminosilicone) [new\*]**

The project team began electronic structure calculations on a library of siloxane-based compounds for CO<sub>2</sub> capture provided by GE. The Si-O-Si group does not have known force field parameters that will allow us to perform classical MD simulations necessary to determine the bulk properties, as was done with the CO<sub>2</sub>BOLs. To this effect, a set of molecular calculations are currently in progress, including ~25 siloxane compounds, to obtain the missing parameters. These will be completed in January 2016, and classical MD simulations will be started in the same month to obtain siloxane properties, such as density and viscosity, for the library.

### **Subtask 2.7 Predict initial viscosity reduction options for GE aminosilicone solvent [new\*]**

No work has begun on this subtask to date.

## **Task 3. Synthesis and Characterization of Candidate Molecules**

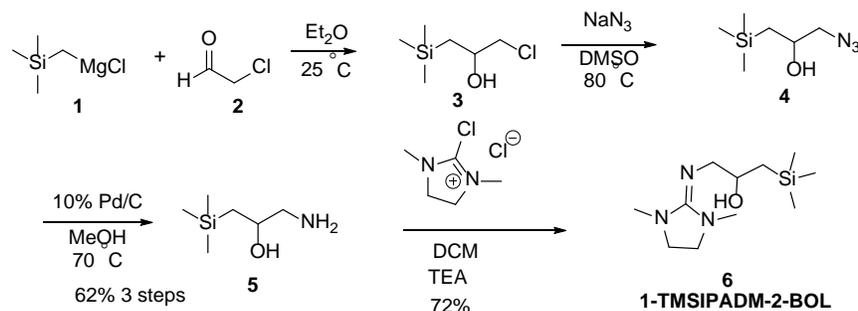
### **Subtask 3.1 Synthesize 12–13 promising derivatives from first 100 molecules library**

Subtask 3.1 was completed.

### **Subtask 3.2 Synthesize 12-13 promising derivatives from second 100 molecule library**

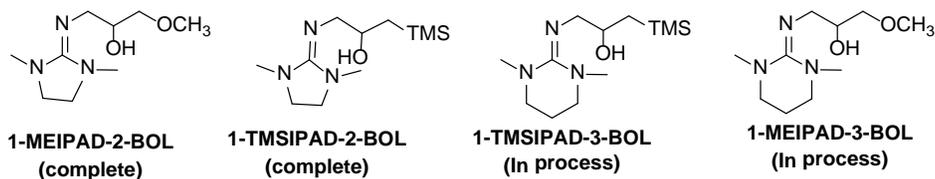
In the last quarter, we reported an economical and environmentally friendly route for the synthesis of the ether derivative, 1-MEIPAD-3-BOL. Using the same methodology, we designed the synthesis of the ether-based silane CO<sub>2</sub>BOL, 1-TMSIPAD-2-BOL (Figure 3). This

synthesis involved the addition of trimethylsilylmethyl magnesium chloride (**1**) to chloroacetaldehyde (**2**) to generate chlorotrimethylsilyl alcohol (**3**) at room temperature. The trimethylsilylchloro hydrin (**3**) was reacted with sodium azide to furnish the corresponding azido alcohol (**4**), which underwent reduction, catalyzed by palladium on carbon, to generate a silylamino alcohol (**5**). The silylamino alcohol (**5**) underwent condensation with Vilsmeier salt to afford 1-TMSIPADM-2-BOL (**6**).



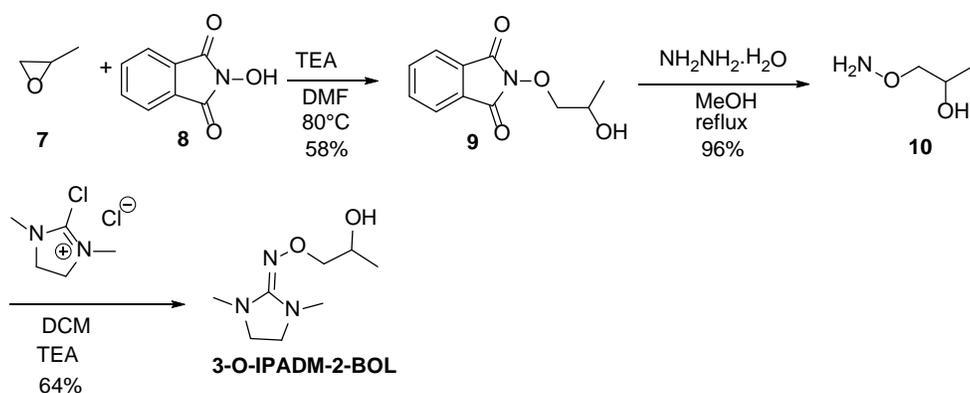
**Figure 3.** Synthesis of 1-TMSIPAD-2-BOL using the New Synthetic Strategy.

To date, using our newly developed strategy, we have completed the scale-up of ether CO<sub>2</sub>BOL, 1-MEIPAD-2-BOL and silane-based CO<sub>2</sub>BOL, 1-TMSIPAD-2-BOL to obtain 40 mL of pure materials, which are being tested for material property measurements such as viscosity, kinetics, and thermodynamics. In order to further explore the impact of incorporating sterics and stacking, our efforts are currently focused on completing the synthesis of six-membered ring tetrahydropyrimidine analogues of silane, i.e., TMSIPAD-3-BOL, and ether, i.e., 1-MEIPAD-2-BOL (Figure 4).



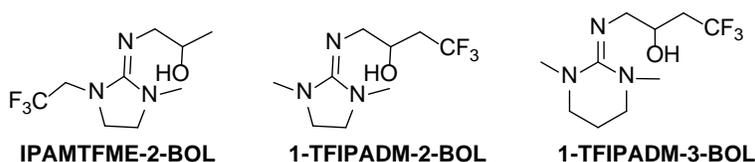
**Figure 4.** CO<sub>2</sub>BOL Molecules being Scaled Up using New Synthetic Route.

In order to explore the effect of solvation of charges towards viscosity reduction, we have also investigated the synthesis of an oxime derivative of CO<sub>2</sub>BOL 3-O-IPADM-2-BOL (Figure 5). This synthesis was performed by the nucleophilic attack of N-hydroxyphthalimide (**7**) on propylene oxide (**8**) to afford hydroxypropoxy isoindolinedione (**9**) followed by the treatment with hydrazine hydrate under reflux conditions. The corresponding aminoxy alcohol (**10**) was subjected to our standard Vilsmeier salt chemistry, i.e., condensation of aminoxy alcohol (**10**) with Vilsmeier salt to yield 3-O-IPADM-2-BOL with 64% yield. In the future, the CO<sub>2</sub> capture ability of 3-O-IPADM-2-BOL will be evaluated gravimetrically by bubbling CO<sub>2</sub> through a neat sample, and depending on the viscosity results, the substrate will be scaled up for material property testing.



**Figure 5.** Synthesis of the Oxime Derivative of CO<sub>2</sub>BOL 3-O-IPADM-2-BOL.

In order to reduce the electrostatic cation-anion interaction in CO<sub>2</sub>-rich solvent we have designed CO<sub>2</sub>BOL derivatives based on fluorine motifs. To this end, our future synthetic targets are based on incorporating a fluorine motif in the ring as well as in the side chain to understand its best placement for designing less-viscous materials (Figure 6). The fundamental understanding of sterics, stacking, and solvation of charges developed through synthetic efforts coupled with computational studies will help us design less-viscous, energetically viable CO<sub>2</sub>BOLs.



**Figure 6.** Future Targets Containing a Fluorine Motif.

### Subtask 3.3 Laboratory property testing completed for model validation

Shakedown of the new pressure-volume temperature (PVT) cell was completed and a total of four compounds have made it through testing at 40 °C. All four revised formulations from Subtask 3.1 that were made at scale showed lower viscosity than our previous formulation, IPADM-2-BOL. The most promising candidate, 1-MEIPAD-2-BOL, was subjected to further testing at 40, 56, and 71 °C for a complete range of isotherms in order to get more detailed information regarding its performance. At a rich solvent loading (0.5 mol CO<sub>2</sub>/mol BOL), 1-MEIPAD-2-BOL projects a viscosity of only 1,100 cP at 40 °C, far lower than the 3,000 cP of IPADM-2-BOL at 40 °C. This finding meets Milestone 7, far surpassing the 400 cP reduction in viscosity required.

## Task 4. Measurement of Key Physical/Thermodynamic Data

### Subtask 4.1 Key CO<sub>2</sub>BOL process data measured for process performance projections

1-MEIPAD-2-BOL shows marked performance with respect to viscosity, though it should

be cautioned that the vapor-liquid equilibrium (VLE) behavior needs more detailed analysis as its heat of reaction and CO<sub>2</sub> sorption behavior needs to be modeled the same way as IPADM-2-BOL was in our previous work. We are reaching out to Dr. Paul Mathias from Fluor to provide a more detailed thermodynamic analysis of the 1-MEIPAD-2-BOL to validate acceptable performance. Analysis of the heat of solution (enthalpy of CO<sub>2</sub> binding) and kinetics at a given loading and temperature are currently underway by Dr. Mathias. Kinetic data from the absorption rates of each point in the measured VLE curves is being analyzed, by taking the peak absorption rate of the absorption curves. VLE curves are being modeled to extrapolate the heat of solution. This analysis should be available for at least one derivative in next quarter's report.

**Subtask 4.2 Key carbamate process data measured for process performance projections [new\*]**

No work has been performed on this task to date.

**Task 5. Process Performance Projections**

No work has been performed on this subtask to date.

**Subtask 5.1 Project reboiler heat duty, regeneration temperatures and net power outputs for candidate molecules**

No work has been performed on this subtask to date.

**Subtask 5.2 Project equipment sizing and costing for candidate molecules**

No work has been performed on this subtask to date.

**Task 6. Alternative Synthetic Methodology Identified**

No work has been performed on this subtask to date.

**Task 7. Translation of Development Capabilities to Other Transformational Solvent Systems**

No work has been performed on this subtask to date.

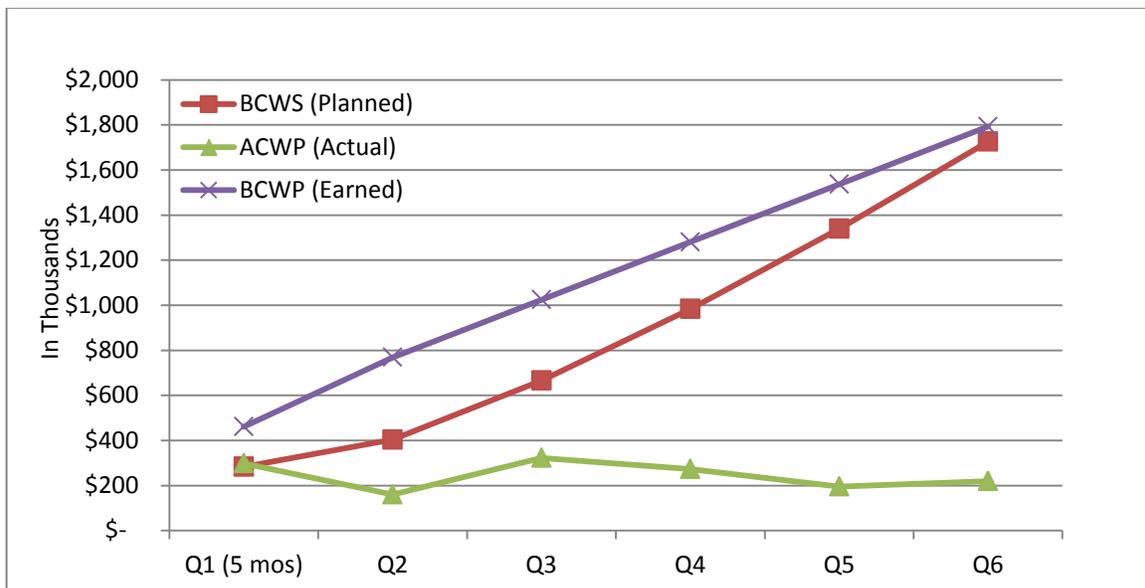
**Cost Status:**

The budget of the program through Q6 can be found in Table 2. All project accruals are through 12/31/15. Table 6 has been revised from prior versions to reflect the additional scope and budget as described above. Total accrued costs for the program are \$1,469,966 with \$4,864 in commitments for purchases, chemicals and supplies. The project has a remaining balance of \$1,086,170 through the end of FY16.

**Table 2.** Total Project Budget Summary to Date (12/31/15)

Project Summary	Total Project Budget	Total Cost to Date (12/31/2015)	Commitments	Balance Remaining
Federal Share	\$2,561,000	\$1,469,966	\$4,864	\$1,086,170
Totals	\$2,561,000	\$1,469,966	\$4,864	\$1,086,170

Quarter 6 comprised the months of October through December 2015. Continuing with our previous reporting, all of the planned and earned value costs for Q5 are provided both graphically in Figure 7 and tabulated in Table 3. Actual value costs (ACWP) were \$220K, with a planned cost (BCWS) of \$1,726K and an earned cost (BCWP) of \$1,793. Spending for the remaining quarters is expected to continue at this spend rate. Cumulative costs and schedule variances were 88% and 4%, respectively.



**Figure 7.** Performance Measurement Graph for BP1

**Table 3.** BP1 Cost and Schedule Variance by Quarter

Job to Date All BP	Q1 (5 mos)	Q2	Q3	Q4	Q5	Q6
Quarterly Amounts	\$ 283	\$ 121	\$ 262	\$ 318	\$ 356	\$ 387
BCWS (Planned)	\$ 283	\$ 404	\$ 666	\$ 984	\$ 1,339	\$ 1,726
ACWP (Actual)	\$ 299	\$ 160	\$ 322	\$ 273	\$ 196	\$ 220
BCWP (Earned)	\$ 461	\$ 768	\$ 1,024	\$ 1,281	\$ 1,537	\$ 1,793
Cum Cost Variance	162.28	608.08	702.00	1007.20	1340.86	1573.11
Cum Scheduled Variance	177.77	364.49	358.86	296.98	197.45	66.67
Cum % Cost Var	35%	79%	69%	79%	87%	88%
Cum % Sch Var	63%	90%	54%	30%	15%	4%

Detailed project costing by quarter is listed in Table 4, which is complemented by cost breakdowns by Task in Table 5. Task 1 had minimal charging; \$73,075 was used for modeling in Task 2, \$85,632 for synthesis in Task 3, and \$59,904 for data collection on the PVT cell in Task 4.

**Table 4. Project Costing by Quarter (BP2)**

Baseline Reporting Quarter	Budget Period 2 (05/01/2015–09/30/2016)							
	FY15		FY16		FY16		FY16	
	Q5	Project Total	Q6	Project Total	Q7	Project Total	Q8	Q9
<b>Total Planned</b>	\$355,633	\$1,339,150	\$386,883	\$1,726,033	\$491,550	\$2,217,583	\$196,500	\$146,917
<b>Quarterly Cost</b>	\$195,745	\$1,250,380	\$219,586	\$1,469,966		\$1,469,966		
<b>Plan/Actual Variance</b>	\$159,888	\$88,770	\$167,297	\$256,067	\$491,550	\$747,617	\$196,500	

**Table 5. Project Costing by Task (BP2)**

Task	Task Title	BP1					BP2			TOTAL ALL BPs
		Q1 (5 mos)	Q2	Q3	Q4	Total BP1	Q5	Q6	Total BP2	
1	Project Management	\$ 49,002	\$ 27,782	\$ 11,439	\$ 19,772	\$ 107,995	\$ 14,280	\$ 975	\$ 15,255	\$ 123,250
2	Molecular Development	\$ 145,636	\$ 69,639	\$ 214,965	\$ 86,261	\$ 516,502	\$ 103,114	\$ 73,075	\$ 176,189	\$ 692,691
3	Synthesis & Characterization of Candidate Mole	\$ 104,066	\$ 62,802	\$ 96,000	\$ 116,163	\$ 379,032	\$ 54,452	\$ 85,632	\$ 140,084	\$ 519,116
4	Measurement of Key Physical/Thermodynamic P	\$ -	\$ -	\$ -	\$ 51,105	\$ 51,105	\$ 23,899	\$ 59,904	\$ 83,803	\$ 134,908
5	Process Performance Projections	\$ -	\$ -	\$ -	\$ -	\$ -			\$ -	\$ -
6	Alternative Synthetic Methodology Identified	\$ -	\$ -	\$ -	\$ -	\$ -			\$ -	\$ -
7	Translation of Development Capabilities to Othe	\$ -	\$ -	\$ -	\$ -	\$ -			\$ -	\$ -
	<b>TOTAL - ALL TASKS</b>	\$ 298,705	\$ 160,223	\$ 322,404	\$ 273,302	\$ 1,054,634	\$ 195,745	\$ 219,586	\$ 415,331	\$ 1,469,965

## **Schedule Status**

### **II. Issues, Risks, and Mitigation**

There are no currently identified risks or issues identified for the project.

#### ***Risk 1: Program budget***

The program has sufficient funds to complete the remaining scope of work, with a projected spend rate at ~100K per month.

### **III. Changes in Approach**

The additional scope of work for incorporating GE's aminosilicone solvent chemistry was added. Key subtasks added are 2.6 and 2.7, and Milestones 10–12. This work will be used to further validate the accuracy and precision of the modeling efforts.

### **IV. Key Personnel**

There are no changes in personnel, though Dr. Paul Mathias is being consulted to perform thermodynamic analysis of the new derivatives tested in the PVT cell.

### **V. Project Output**

A manuscript from our previous program on kinetic analysis of the CO<sub>2</sub> capture by CO<sub>2</sub>BOL solvents was accepted by *Energy and Fuels* and is currently in press. A second manuscript on the mechanism of CO<sub>2</sub> capture and of the acid/base behavior of CO<sub>2</sub>BOL capture solvents was submitted to *Nature Communications*. A third manuscript is being drafted for the PVT cell's operation and precision/accuracy of other cells used for analysis (e.g., PTx cell, wetted-wall column).

## **Project Schedule Status**

The revised project timeline is shown in Table 6. The Gantt chart identifies the Tasks and Subtasks broken out by quarter with revised completion dates. Task 1, was completed (quarterly report). Milestones 1–5 and 7 were completed, and Subtasks 2.1–2.4 and Subtask 3.1 have been completed. Subtask 2.6 was started in this quarter, with Subtask 2.7 slated to begin in the next quarter. Subtask 4.1 has been started, and more information regarding the key process data is expected to be available in the next quarter.

**Table 6. Project Timeline**

		BP1 (5/1/14- 4/28/15)				BP2 (5/1/15-9/30/16)			
<b>Task 1. Project Management</b>									
1.1	General project management								
	<b>Milestone 1 Updated Project Management Plan</b>								
<b>Task 2. Molecular Development</b>									
2.1	Design 100 candidate molecules based on variations of current formulation								
2.2	Construct physical property prediction model								
	<b>Milestone 2 Construct physical property model for CO2BOL derivatives</b>								
2.3	Predict physical and thermodynamic properties of first 100 molecules								
	<b>Milestone 3 synthesize and characterize 13 candidate CO2BOL molecules</b>								
	<b>Milestone 4 Viscosity reduction of 200 cP demonstrated</b>								
2.4	Revise technology performance targets and design the second 100 molecules								
2.5	Predict physical and thermodynamic properties of the second 100 molecules								
	<b>Milestone 5 Go/No-Go decision from initial feasibility study</b>								
2.6	Construct physical property model for carbamate derivative (GE aminosilicone)								
2.7	Predict initial viscosity reduction options for GE aminosilicone solvent (focus not on molecular modifications - additives and blends only)								
	<b>Milestone 10 Construct first-generation MD model for carbamates. Initial assessment of viscosity reduction for GE aminosilicones via additives &amp; blends</b>								
2.8	Predict physical and thermodynamic properties of 50 variations of carbamate molecules (focus on molecular modifications)								
	<b>Milestone 11 Model 50 carbamate derivatives and identify 3 new candidate molecules for synthesis &amp; characterization</b>								
<b>Task 3. Synthesis and Characterization of Candidate Molecules</b>									
3.1	Synthesize 12-13 promising derivatives from first 100 molecule library								
3.2	Synthesize 12-13 promising derivatives from second 100 molecule library								
3.3	Laboratory property testing completed for model validation (e.g., B.P., viscosity, CO <sub>2</sub> capacity)								
	<b>Milestone 6 Synthesize and characterize 13 candidate CO2BOL molecules</b>								
3.4	Characterize 1-2 top additive/blend options for reducing carbamate solvent (GE's aminosilicone) viscosity								
3.5	Synthesis and characterize 3 top candidate formulations based on improved molecular design of a carbamate solvent								
	<b>Milestone 12 Synthesis &amp; characterization of 3 carbamate solvent variants from molecular dynamics simulations</b>								
<b>Task 4. Measurement of Key Physical/Thermodynamic Data</b>									
4.1	Key process data measured for process performance projections (e.g., VLE, kinetics)								
	<b>Milestone 7 Viscosity reduction of 400 cP demonstrated for CO2BOLs solvent</b>								
4.2	Measure VLE and adsorption kinetics for baseline carbamate solvent and 3 new synthesized variants								
<b>Task 5. Process Performance Projections</b>									
5.1	Project reboiler heat duty, regen temp, and net power output for candidate molecules								
<b>Task 6. Alternative Synthetic Methodology Identified</b>									
6.1	Provide alternative synthetic methodology (& projected costs) for optimal candidate solvents for CO2BOLs solvent								
	<b>Milestone 8 Synthetic methodology for candidate molecules demonstrated at</b>								

