Development of a Novel Biphasic CO_2 Absorption Process with Multiple Stages of Liquid–Liquid Phase Separation for Post-Combustion Carbon Capture

(DOE/NETL Agreement No. DE-FE0026434)

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Illinois State Geological Survey

University of Illinois at Urbana-Champaign

Project Review Meeting

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Team Members

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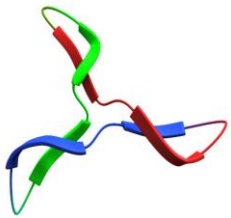

Presentation outline:

- Project Overview
- Technical Background
- Budget Period (BP) 1 Work and Budget Status
- BP1 Technical Activities and Major Findings
- BP2 Work and Budget Plan

Project Overview

- Project objectives
  - Develop new biphasic solvents
  - Generate engineering and scale-up data
  - Demonstrate process concept via lab/bench column testing
  - High-level process and techno-economic analysis (TEA)

- Project duration
  - BP1: 10/1/15 to 06/30/17 (21 months)
  - BP2: 07/1/17 to 12/31/18 (18 months)

- Funding profile

DOE funding	**1,999,996**
BP1	1,079,663
BP2	920,333
Recipient cost share	**501,052**
BP1	269,920
BP2	231,132
Total	**2,501,048**

Project Participants

- **University of Illinois**
  - **Illinois State Geological Survey**
    - Solvent development
    - Solvent equilibria, kinetics & properties measurements
    - Absorption and desorption column testing
    - Process modeling
  - **Illinois Sustainable Technology Center**
    - Assessment of solvent stability and corrosion impacts
  - **Applied Research Institute**
    - Molecular dynamics simulation study for solvent screening
- **Trimeric Corporation**
    - Process feasibility and high-level TEA

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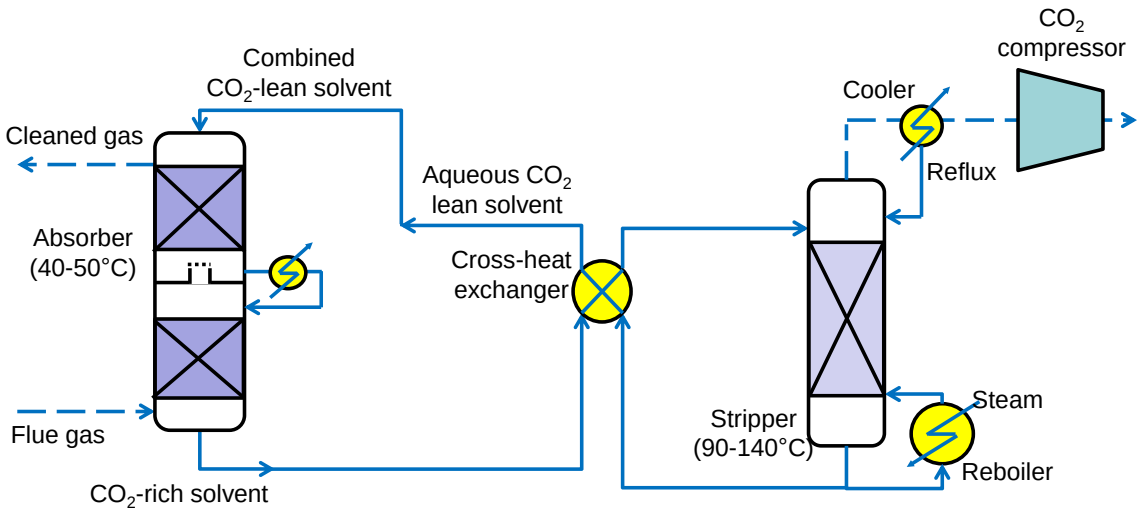
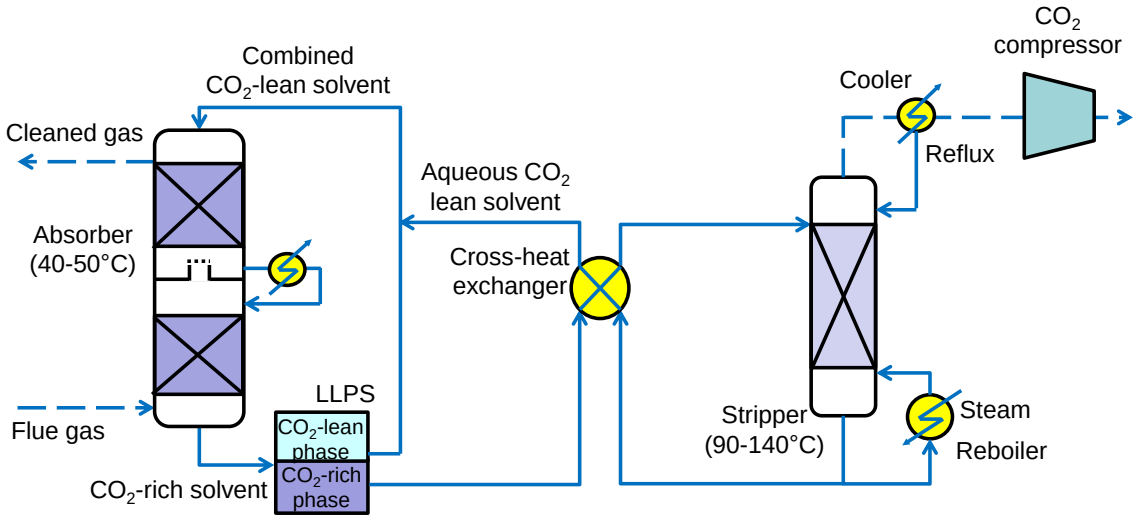
Biphasic vs. Monophasic Absorption Process



Monophasic Absorption Process (e.g., MEA)

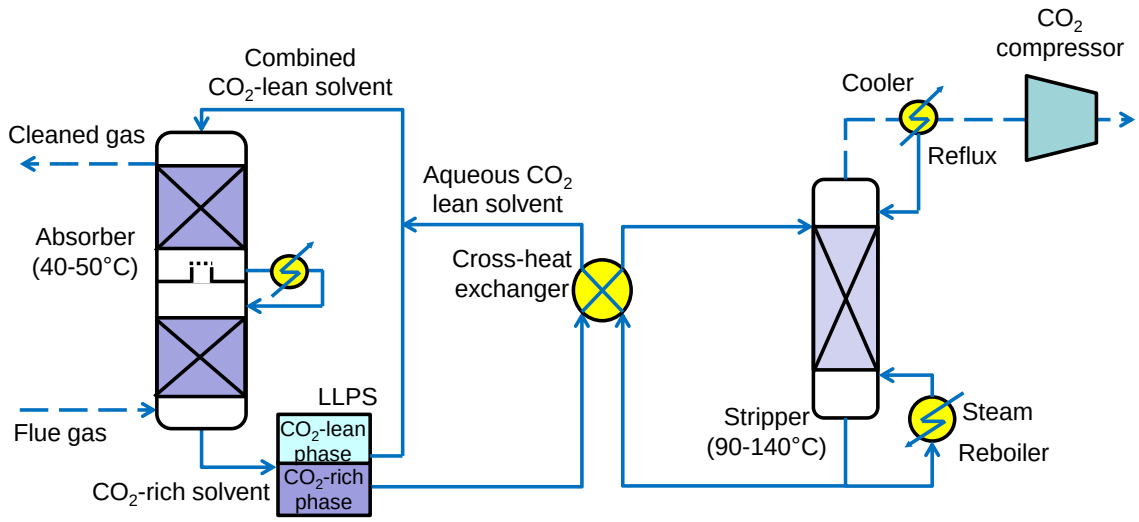


Biphasic Absorption Process

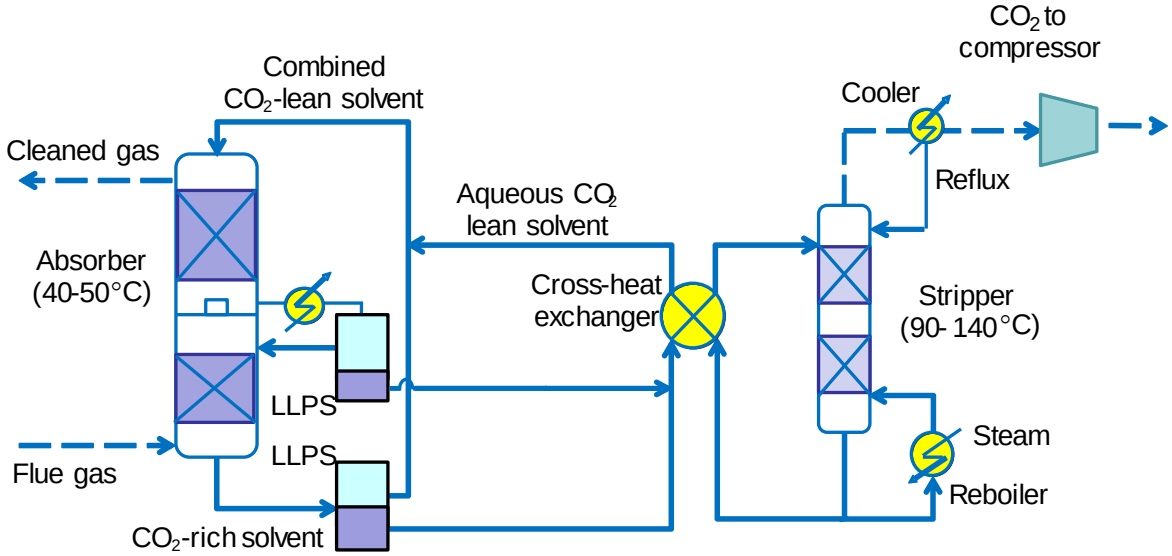
Benefits of biphasic process in stripper:

- Reduced equipment size due to reduced mass of solvent to be regenerated in stripper
- Reduced energy use and compression requirement due to enriched CO_2 loading in feed solvent, reduced mass of solvent, and elevated stripping pressure

Staged vs. Non-Staged Biphasic Absorption Process



Non-Staged

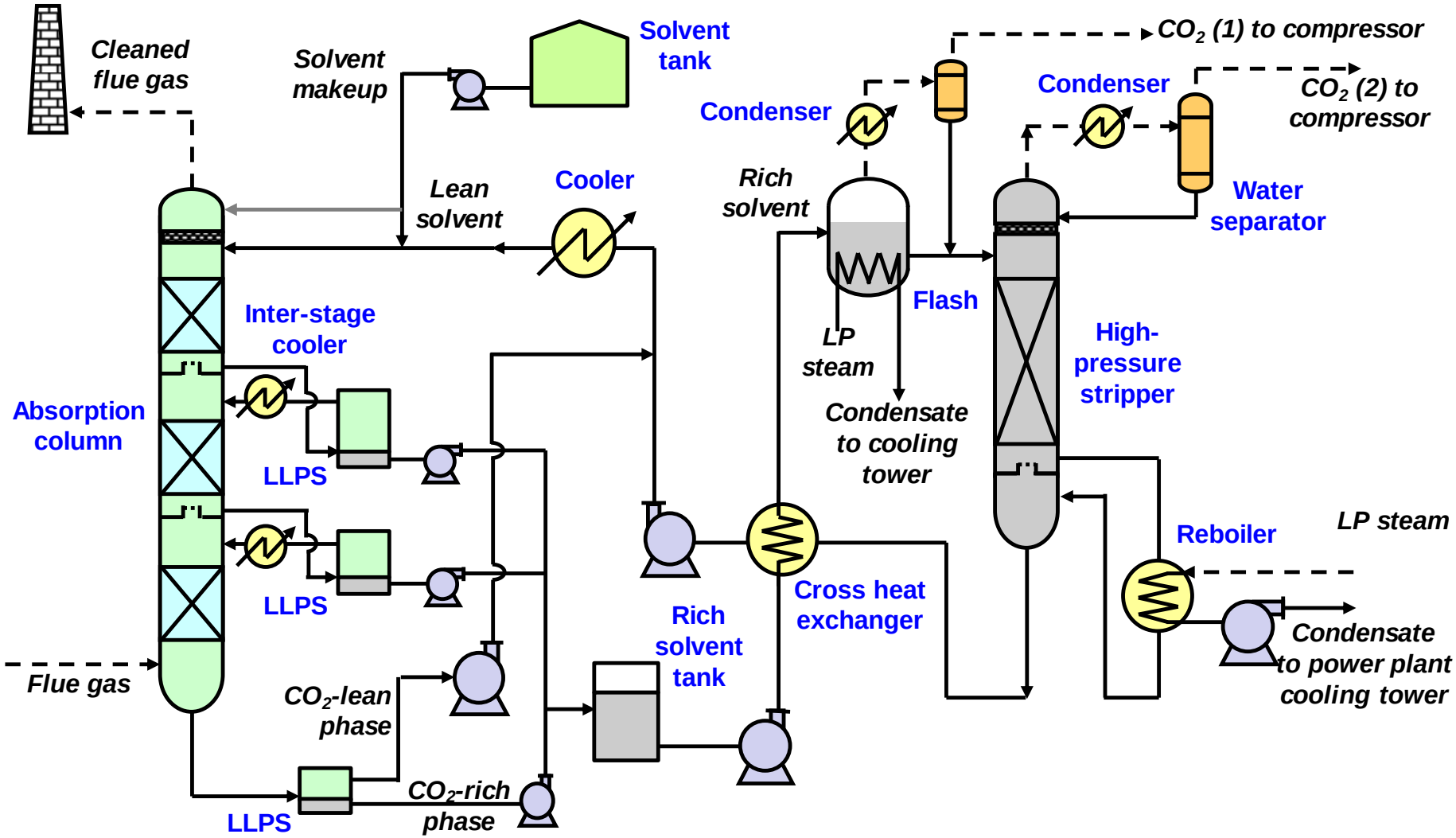


Staged (2 Stages for Illustration)

Benefits in absorber via phase separation:

- Reduced viscosity with separation of rich, viscous phase improves mass transfer rate and allows a wider selection of biphasic solvents
- Effect of leaner solvent mixture on kinetics to next packed section to be assessed
- Effect of reduced mass of solvent to next packed section to be assessed

Proposed Biphasic CO_2 Absorption Process with Multi-Stages of Liquid-Liquid Phase Separation

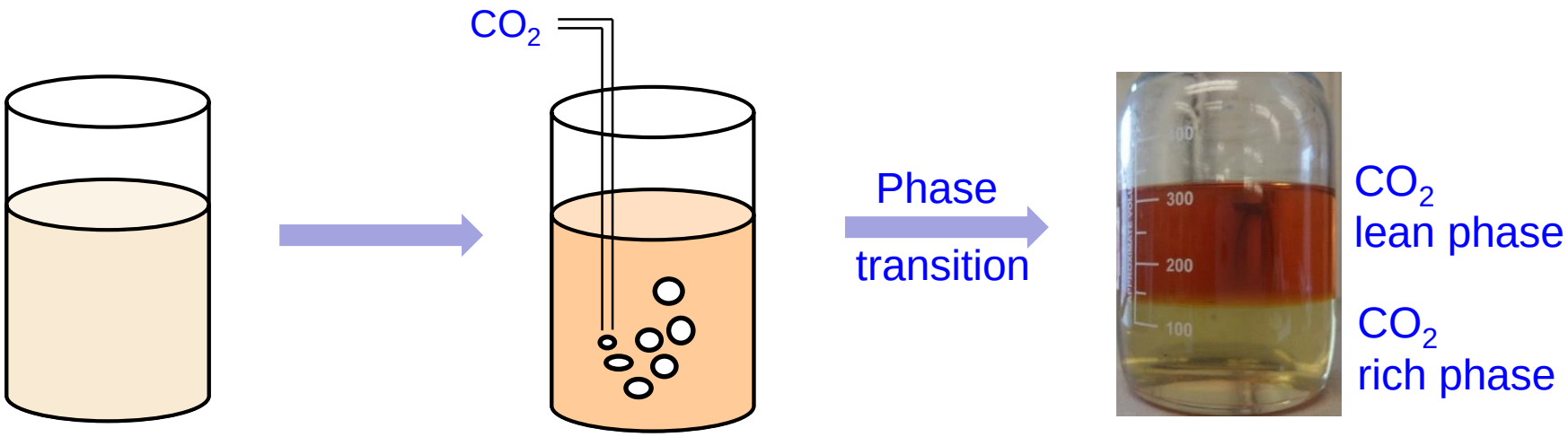


Proposed Biphasic CO_2 Absorption Process (BiCAP)

Newly Developed Biphasic Solvents

Amine-based solvent blends:

- Phase transition behavior is tunable
- Consider multi-criteria (capacity, rate, CO_2 enrichment level, viscosity, desorption pressure, stability, and corrosion)
- Allow multiple steps of phase separation
- In aqueous form suitable for humid flue gas application



Lean solvent in a single phase

Phase transition induced by CO_2 loading

Two-phase system (w/ tunable phase vol.%)

BiCAP vs. MEA and Other Biphasic Processes

Biphasic processes vs MEA

- Biphasic solvents have higher loading capacity for CO_2 stripping due to absorbed CO_2 enriched in one phase as feed solution to the stripper
- Reduced mass of rich solvent and elevated pressure for CO_2 stripping
  - Reduced heat use (lower sensible heat & stripping heat)
  - Reduced CO_2 compression work requirement

BiCAP vs. other biphasic processes

- ***Absorption process:***
  Multi-LLPS in BiCAP allows for lower viscosity and CO_2 loading throughout the absorber, resulting in a fast mass transfer rate
- ***Solvent***:
  Phase transition behavior of BiCAP solvents is tunable, facilitated with the use of a unique solubilizer(s), allowing for a wide range of solvent selection;
  Extremely stable with O_2 & temperature
- ***Desorption process:***
  Desorption with a flash step to obtain high-pressure stripping and reduce compression requirements

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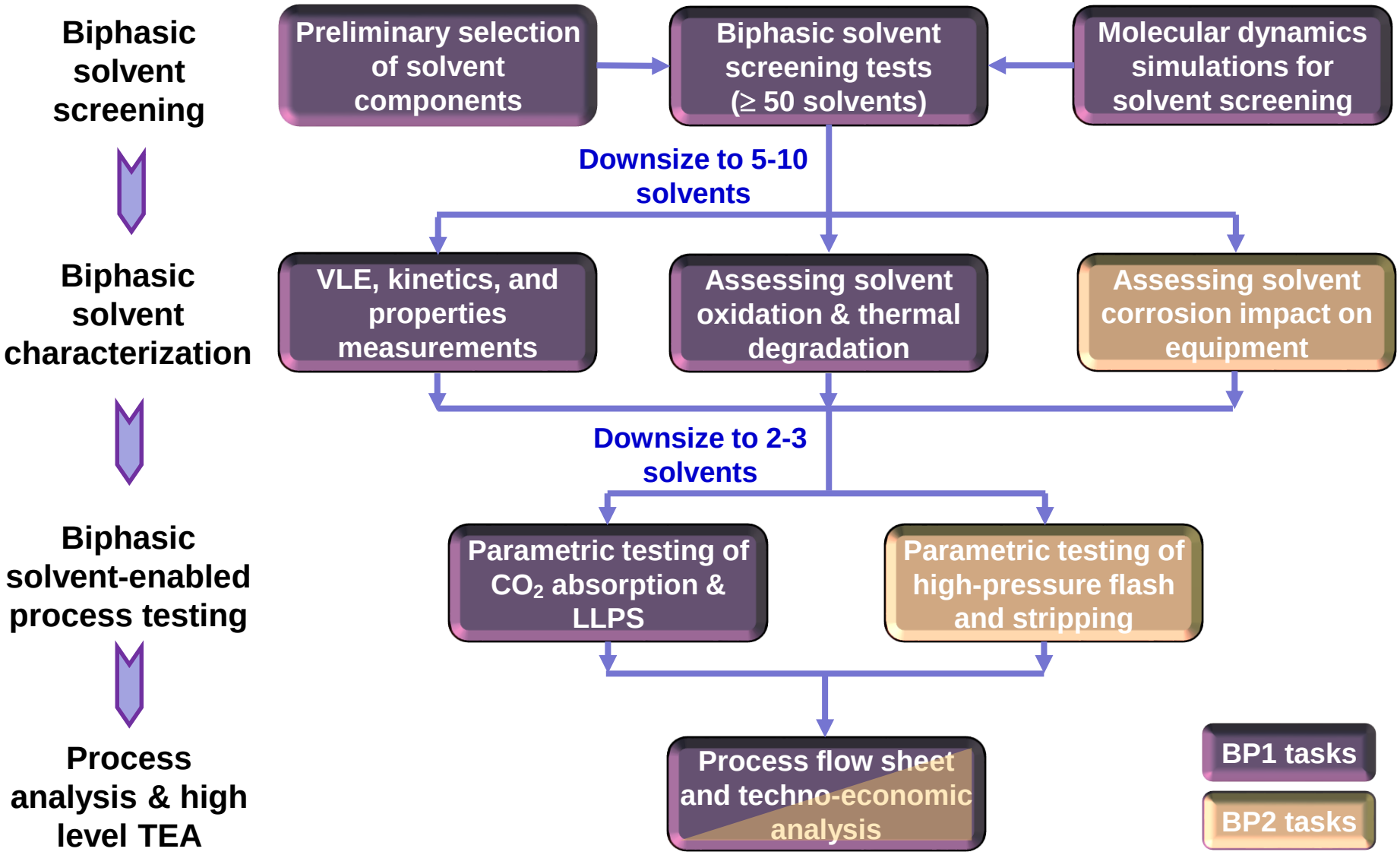
Planned Work for BP1 (10/1/15 – 6/30/17)



Tasks Completed on Schedule

Project Tasks	Progress to date
Task 1. Project planning & management	In process
2. Screening & characterization of biphasic solvents (~50 solvents) • Screening on CO_2 absorption & phase transition Screening on CO_2 desorption • Molecular dynamics simulation studies	Complete (>80 formulations evaluated)
3. Phase equilibria, absorption kinetics, and solvent properties (5-10 solvents) • VLE measurement • Absorption kinetics measurement • Solvent properties measurement	Complete (VLE for 10 solvents; kinetics for 6 solvents; viscosity/density for ~80 solvents, heat capacity for 11 solvents; heat of absorption for 10 solvents)
4. Determining thermal & oxidation stabilities of solvents (5-10 solvents) • Oxidation stability • Thermal stability	Complete (Oxidation stability for 6 solvents for 2 weeks; thermal stability at 120-150 °C for 10 solvents for up to 8 weeks)
5. Testing CO_2 absorption & phase separation in a multi-stage packed-bed column (2-3 solvents) • Fabrication of experimental system • Parametric testing	In progress, expected to complete by BP1 end (parametric testing completed for 1st solvent and underway for 2nd)
6. Development of a process sheet and preliminary techno-economic analysis • Conceptual process flow sheets • Preliminary techno-economic analysis	In progress, expected to complete by BP1 end (flow sheets completed, preliminary TEA in progress)

Milestones Achieved in BP1

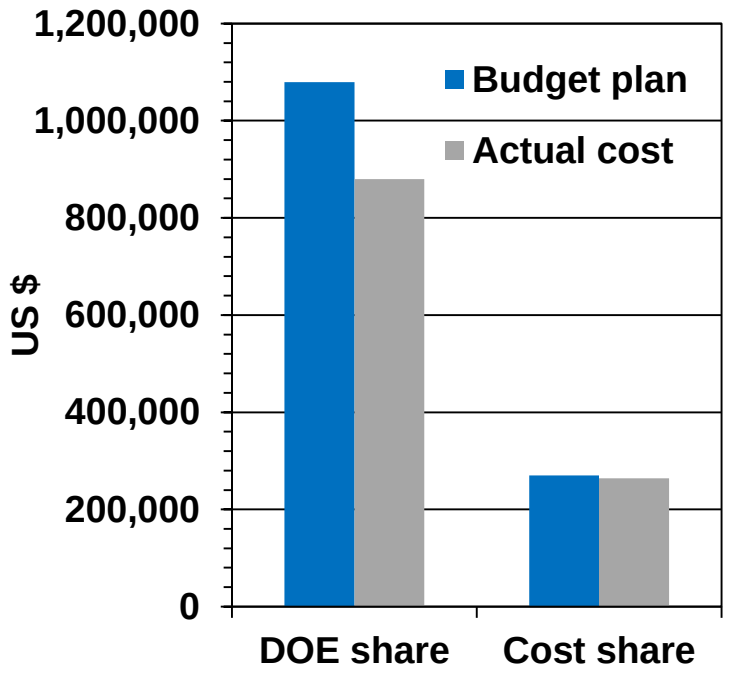
ID	Task	Milestone title/description	Planned completion	Actual completion	Verification method	Status/ comments
	1	Submit updated PMP	10/31/2015	10/07/15	PMP file	Completed
	1	Project kickoff meeting convened	12/31/2015	12/11/15	Presentation file	Completed
a	2.1/ 2.2	Down-select 5–10 biphasic solvents based on capacity, phase transition & CO_2 enrichment behavior, and CO_2 desorption pressure	06/30/16	06/15/16	Results in quarterly report (QR)	Completed
b	2.3	Complete MD simulations and predictions	06/30/16	06/30/16	Results in QR	Completed
c	3	Down-select 2–3 biphasic solvents based on VLE results, absorption kinetics, heat of reaction, and solvent viscosity	09/30/16	09/30/16	Results in QR	Completed
d	5.1	Complete modification of the existing packed-bed CO_2 absorption column to include 2–3 stages of LLPS	09/30/16	09/30/16	Description and photographs in QR	Completed
e	4	Complete comprehensive assessment of biphasic solvent oxidation and thermal stability	12/31/16	12/31/16	Results in QR	Completed
f	5.2	Complete simulated flue gas testing of 2–3 down-selected biphasic solvents using the modified absorption-LLPS column system	06/30/17	06/30/17 (projected)	Results in QR	In progress
g	6	Complete a preliminary process analysis and develop a conceptual process flow sheet	06/30/17	06/30/17 (projected)	Results in QR	In progress

7 milestones in BP1:

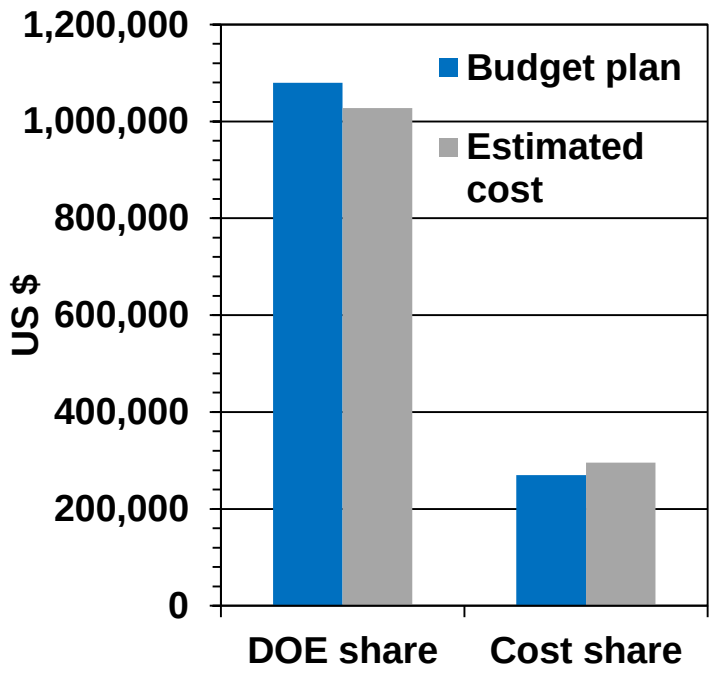
- 5 milestones completed
- 2 milestones (f & g) in progress expected to be completed by the end of BP1
- Project extended for 3 months for Milestone (f) due to additional time taken to improve solvent stabilities and to purchase bulk solvent components (~100 LB)

Project Costs on Track at the Close of BP1

BP1 budget and actual costs as of 3/31/17



BP1 budget and estimated costs by 6/30/17 (end of BP1)



- Costs by the end of BP1 are close to the budget plan
  - Estimated DOE cost 4.8% < budget plan
  - Estimated cost share 9.5% > budget plan

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Summary of BP1 Work Activities

Task 2: Screening and Characterization of Biphasic Solvents

- >80 solvent formulations screened for CO_2 absorption and phase transition
- Desorption pressure of 17 rich phase solvents measured at 100 and 120°C
- MD simulation methodology established and used for solvent analysis

Task 3: Measuring Phase Equilibria, Absorption Kinetics, & Solvent Properties

- VLE measured for 10 solvents at 30–50°C and for 6 rich solvents at 100-130°C
- Absorption kinetics of 6 solvents at 3 loadings tested with WWC at 25-50°C
- Viscosity, density, heat of absorption, heat capacity determined for multiple solvents

Task 4: Determining Thermal and Oxidative Stabilities of the Selected Solvents

- Oxidation of 6 solvents in 96% O_2 (+4% or 400 ppm CO_2) for 2 weeks at 50°C
- Thermal stability of 10 rich-phase solvents at 120,135, 150°C for up to 8 weeks

Task 5: Testing CO_2 Absorption & Phase Separation in a Multistage Packed-Bed Column

- An absorption system with 3 stages of columns and phase separators fabricated (each stage with a 4-in ID, 7-ft high packed bed & a 3- or 1-gallon LLPS unit)
- Parametric experiments completed for 1st solvent; ongoing for 2nd solvent

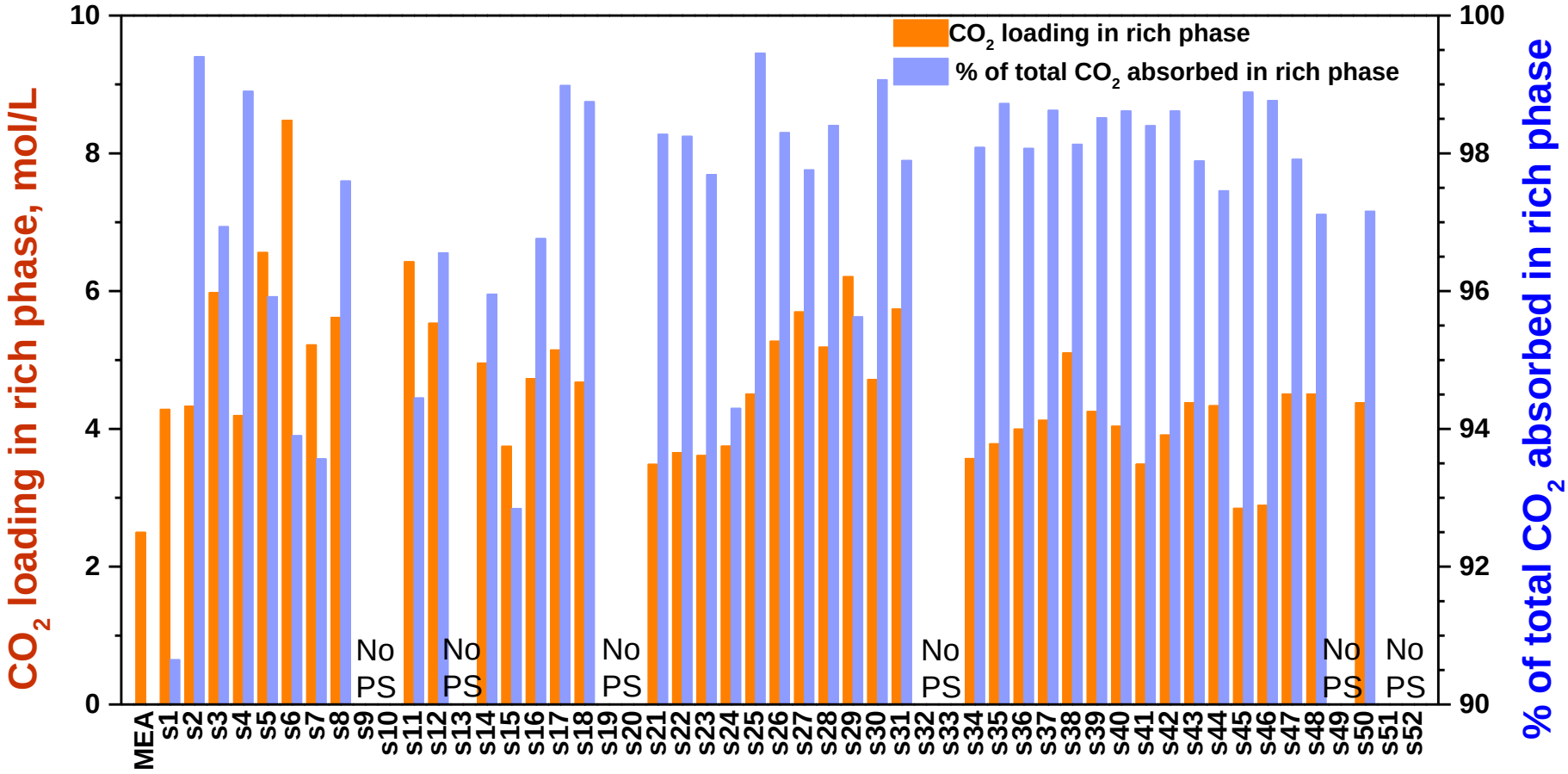
Task 6: Development of a Process Sheet and Preliminary Process Analysis

- Conceptual PFDs of BiCAP system developed
- Preliminary MEB calculations performed with Aspen Plus
- Initial high-level analysis of equipment and operating costs in progress

Fulfillment of BP1 Success Criteria

Criteria	Outcome
Identify 2-3 top-performing solvents (based on phase transition & CO_2 enrichment behavior, CO_2 loading capacity, absorption kinetics, and viscosity)	**This criterion has been satisfied:** Two top-performing solvents were identified based on screening tests and properties assessment (loading capacity, VLE, absorption kinetics, thermal & oxidative stability, heat of absorption, viscosity, etc.)
Complete lab testing of 2-3 solvents using a multi-stage absorption & LLPS system (CO_2 capacity and kinetics ≥5 M MEA; each LLPS stage ≤ 5 min; ≥ 80% CO_2 enrichment in rich liquid phase)	**This criterion expected to be satisfied by the end of BP1 (Testing of 1st solvent completed and 2nd one in progress):** (1) CO_2 loading capacity and removal rate for 1st solvent ≥ 5M MEA under comparable conditions; (2) Lean and rich phases able to separate in <0.5 min; (3) ~98% of absorbed CO_2 enriched in rich phase (4) Rich phase is only ~40% of liquid leaving the absorber
The multi-stage absorption and LLPS configuration demonstrates **reliable operability** during lab-scale testing and the optimal number of LLPS stages is determined for process design	**This criterion has been satisfied:** (1) Reliable operation achieved with any portion of rich phase withdrawal from individual inter-stage phase separators; (2) The system able to operate with either 1, or 2, or 3 stages; (3) Current results indicate 1-stage LLPS operation suited for low viscosity solvents (e.g., <50 cP) and 2/3-stage LLPS operation could suit for high viscosity solvents (>50 cP)

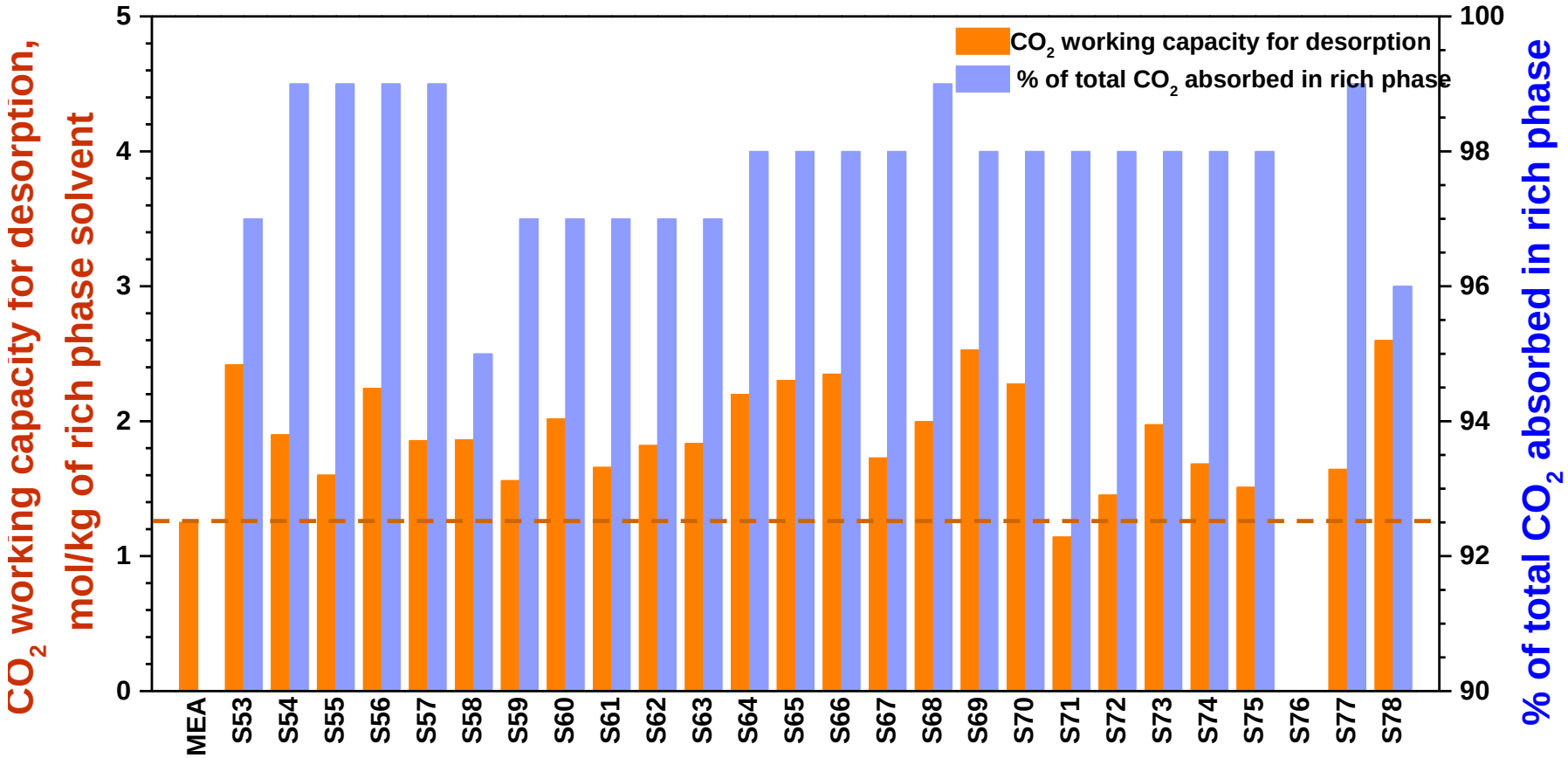
Task 2. Solvent Screening: Capacity and Phase Separation



Initial screening tests in 1-bar CO_2 for 60 min at 40°C:

- Occurrence of dual phases and rich-lean volumetric ratio are controllable
- CO_2 loading highly concentrated in rich phase (91-99% of total loading)
- CO_2 capacity of rich phase solution 1.5-3 time > 5M MEA

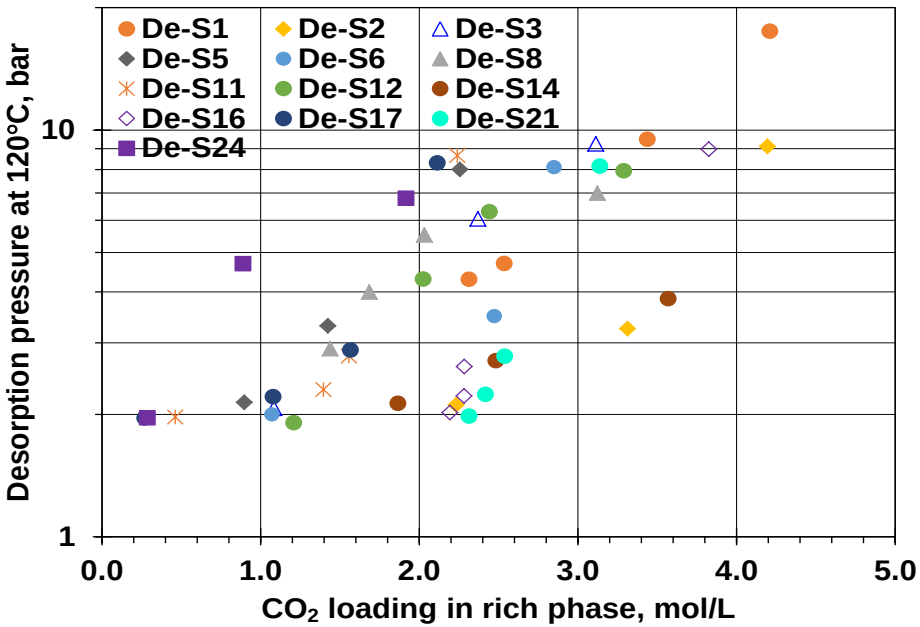
Capacity and Phase Separation under Flue Gas Conditions



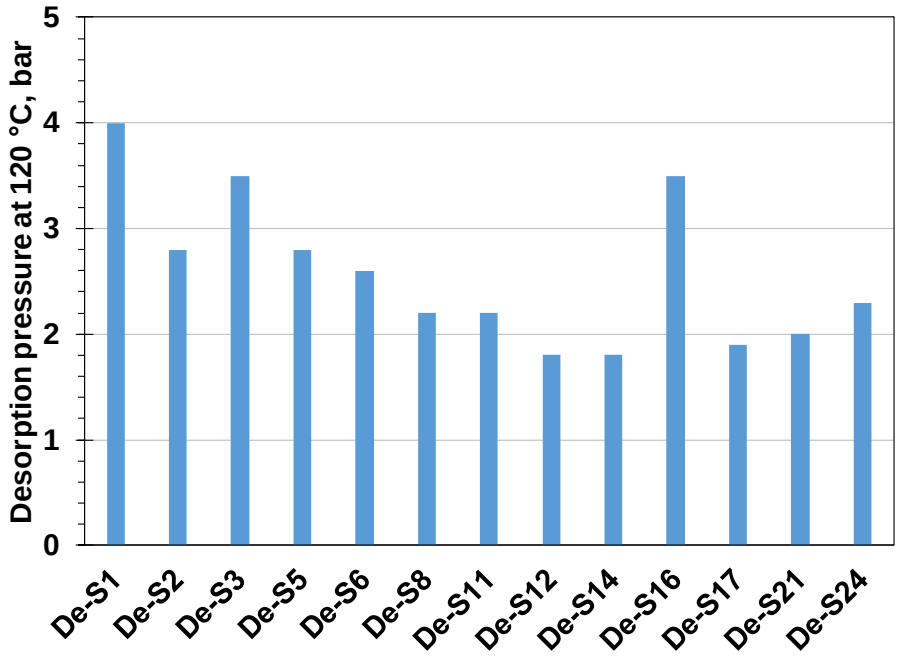
Later screening on CO_2 working (cyclic) capacity under 5 and 0.1 kPa CO_2 at 40°C:

- ~98% of CO_2 concentrated in rich phase for most solvents
- CO_2 working capacity of rich phase solvent (equivalent to P^*_{CO2}=5.0 / 0.1 kPa at absorber outlet / inlet at 40°C) for CO_2 desorption 1.5-2 times > 5M MEA

CO_2 Stripping Pressure



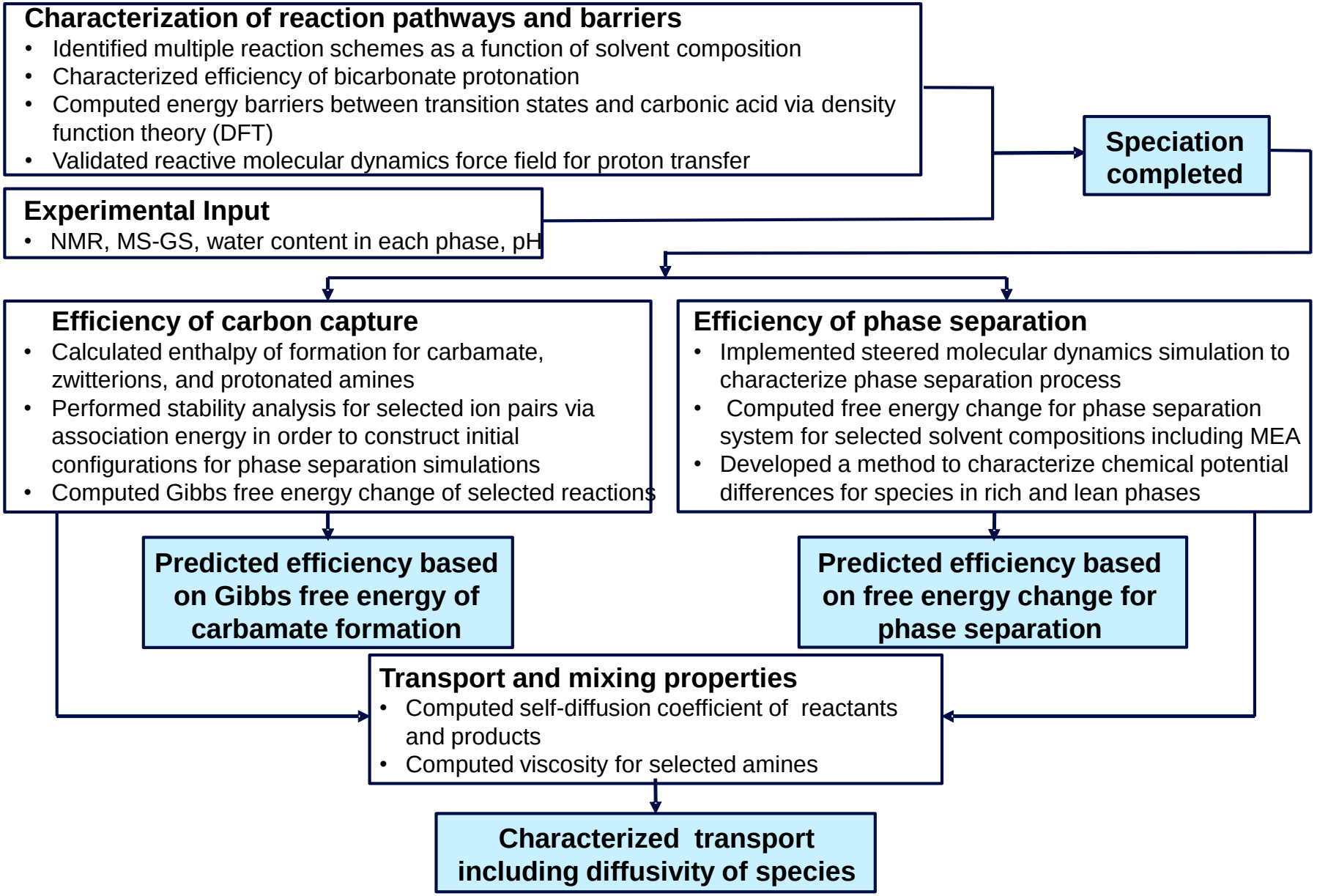
120°C data for illustration



Stripping P of <u>regenerated</u> rich phase at 120°C (CO_2 loading of mixture returning to absorber equivalent to P^*_{CO2}=0.1 kPa at 40°C)

- CO_2 stripping pressure screened for 17 rich phase solvents at 100, 120, 130°C
- At lean CO_2 loading (equiv. to P^*_{CO2}=0.1 kPa at 40°C), total stripping pressure reached 2-4 bar at 120°C vs. 1.5-2 bar for 5M MEA

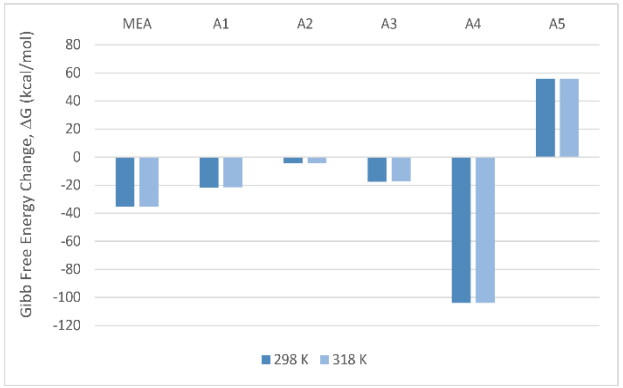
MD Modeling for Solvent Screening: Methodology Flowchart

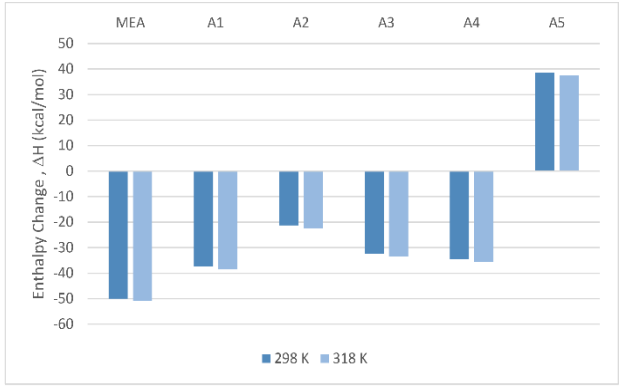


MD Modeling of Carbon Capture Efficiency and Phase Separation

- Carbon capture efficiency screening is performed via thermodynamic calculations using semi-empirical molecular orbital theory (18 reactions considered). Below is one example for the carbamate formation:

$$Am + CO_2 + Am \rightarrow AmCO_2^- + AmH^+$$

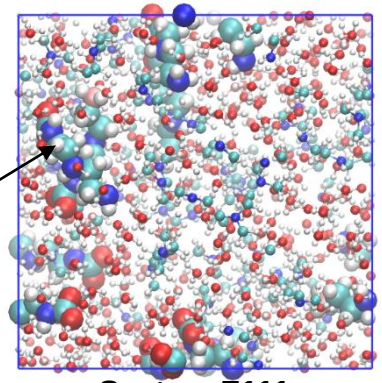




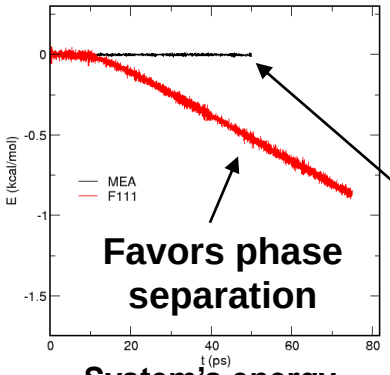
- ΔG < 0: spontaneous reactions; ΔH < 0: exothermic reactions
- Approach is general to screen any stoichiometry & reactions of interest.

- Phase separation efficiency screening is performed via steered molecular dynamics (SMD) simulation

Zwitterions and carbamates "steered" to separate inside the simulation domain



System F111 after SMD run



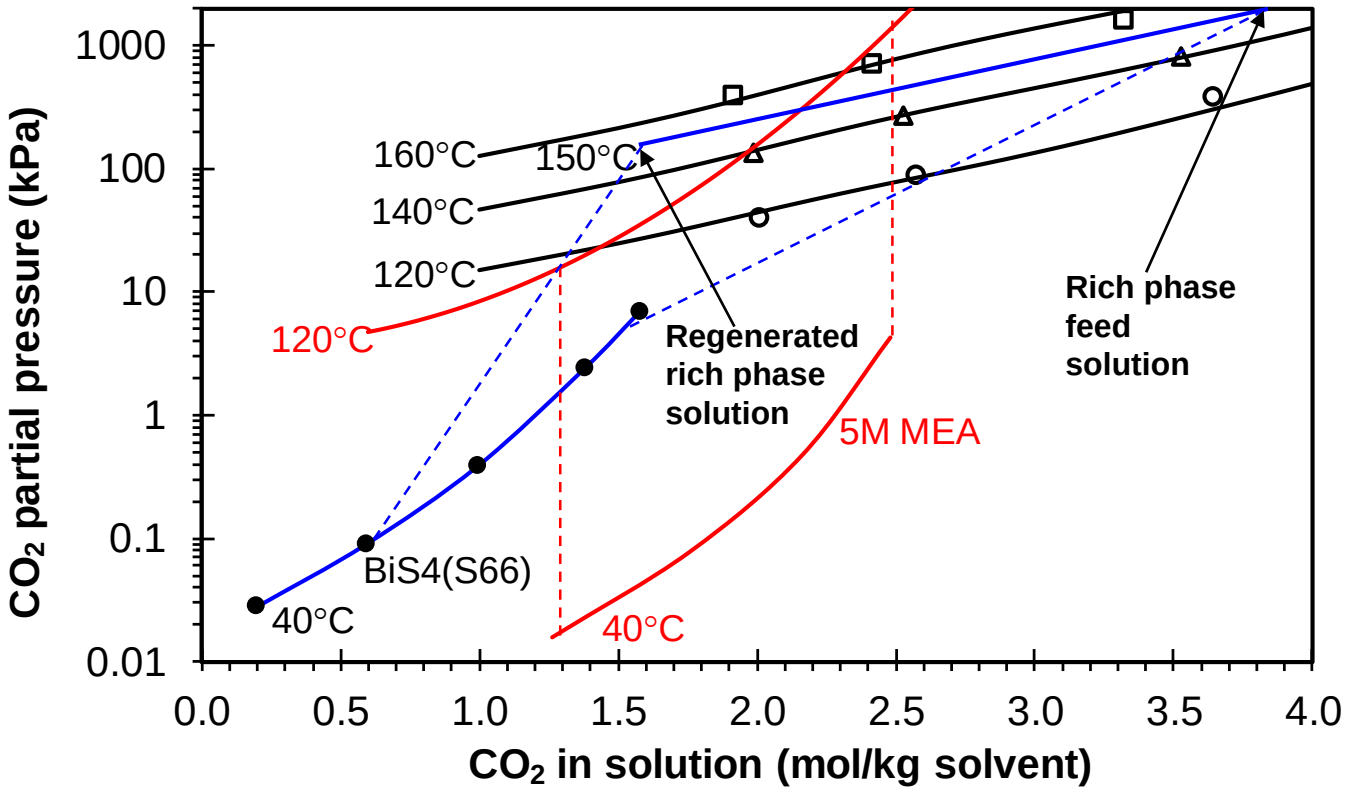
System's energy change during SMD

Phase separation not favored

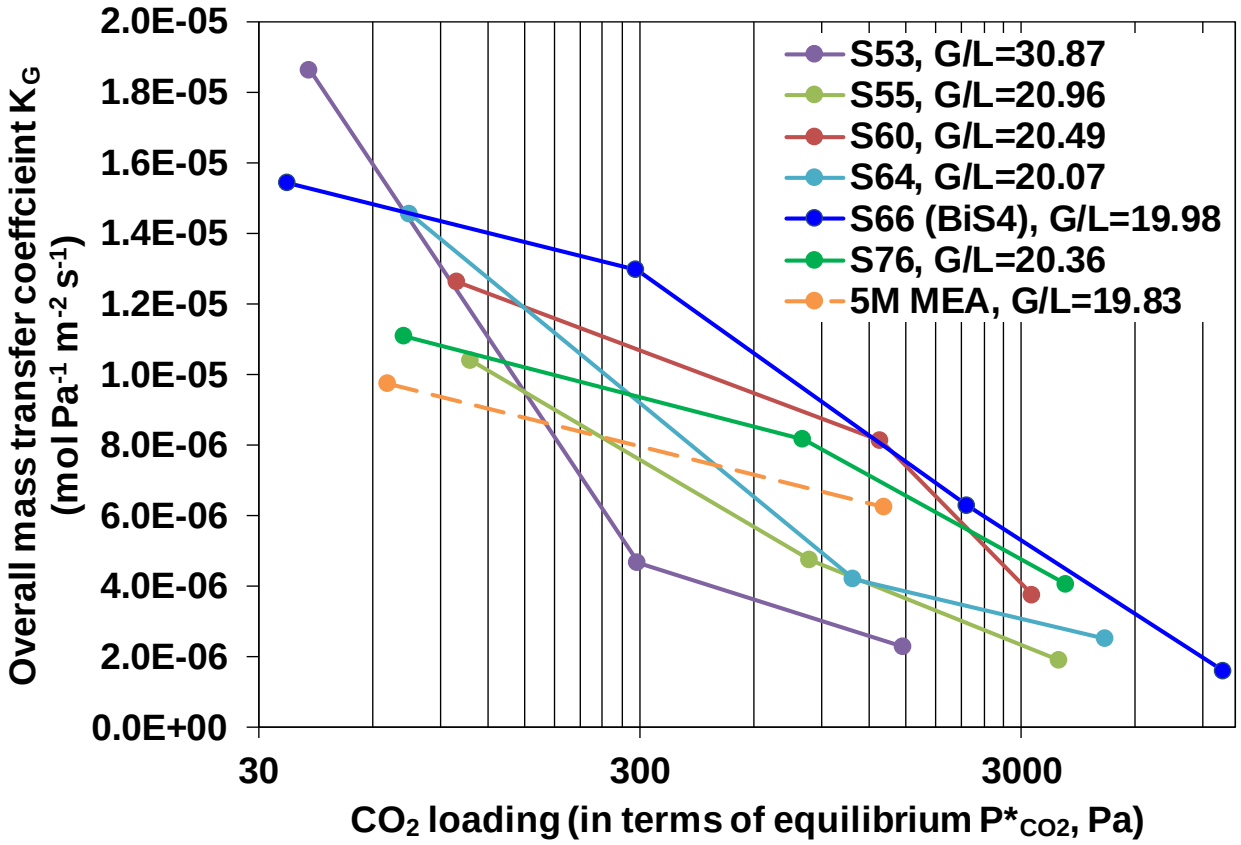
- Work done by the system or constraint is a measure of the driving force behind the phase separation process

Task 3: Phase Equilibria, Absorption Kinetics & Solvent Properties: VLE Measurements

- VLE data for 10 biphasic solvents under absorption conditions (30–50°C)
- VLE data for 6 rich-phase solvents under desorption conditions (100-160°C)

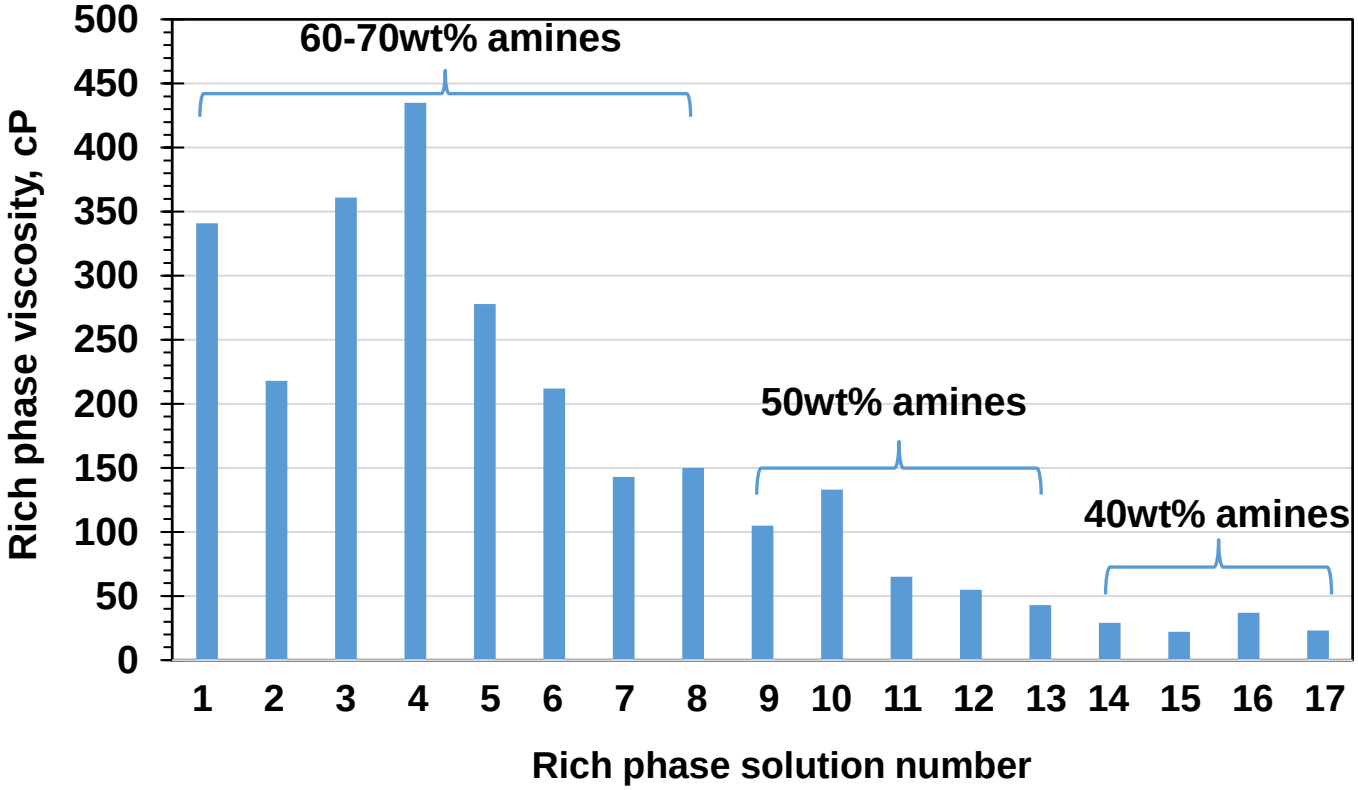


Absorption Rate Measurement with WWC Reactor



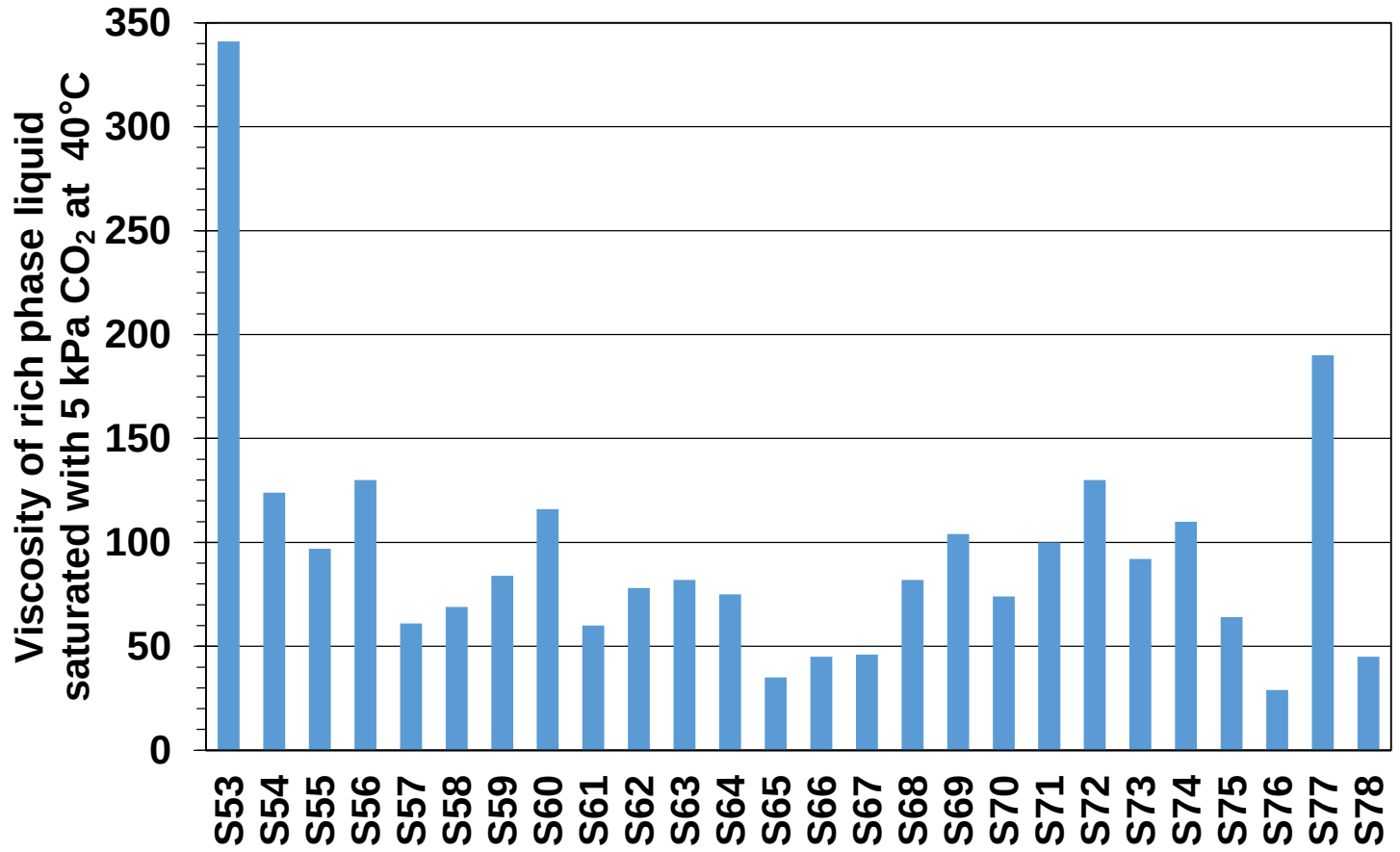
- Absorption kinetics of 6 biphasic solvents measured at 3 CO_2 loadings (equivalent to P^*_{CO2} = ~0.1, 1 & 5 kPa) at 40°C
- Rates comparable (faster at lean loading and slower at rich loading) or slightly faster (at both lean and rich loadings) than 5M MEA

Viscosity Measurement and Optimization



- Lean phase viscosity < 9 cP (data not displayed)
- Rich phase viscosity decreased from ~400 to <50 cP by reducing total solvent concentration or selecting different amine structures

Recent Work on Reducing Viscosity



- Most of recent solvents had viscosity of rich phase solution <100 cP at 40°C (varied from 29 to 341 cP)

Task 5. Thermal & Oxidative Stability of Biphasic Solvents

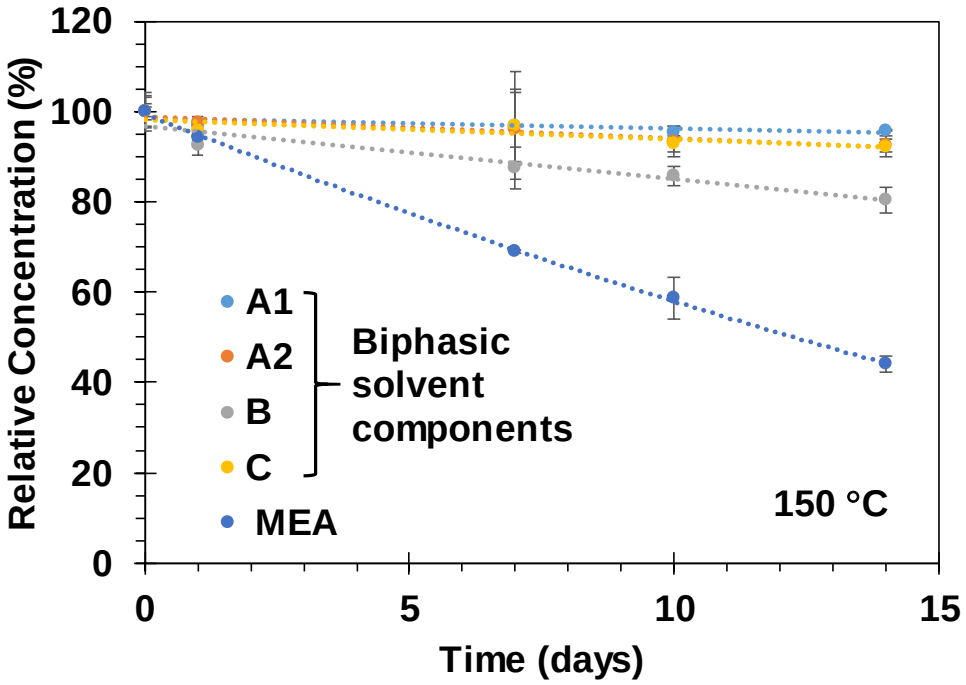
- **Thermal degradation**
  - ≥10 solvents prescreened at 150°C for 1 week;
  - 6 solvents further tested at 150°C for 2 weeks;
  - 3 solvents further tested at 120 and 135°C for 8 weeks

- **Oxidative degradation** in presence of metal catalysts for 10 days at 50°C
  - 7 solvents tested in 95% O_2–4% CO_2 gas (rich loading);
  - 3 solvents tested in 95% O_2–400 ppm CO_2 gas (lean CO_2 loading)

Solvent	Thermal stability			Oxidative stability			Note
	A	B	C	A	B	C	
BiS1 (S56)	√	√	√	×	√	√	Significant A oxidation; Not selected
BiS2 (S70)	√	√	√	√	√	√	Precipitated in rich phase at high temperature; Not selected
BiS3 (S73)	×	√	√	√	√	√	Component A of BiS3 solvent is MEA
BiS4 (S66)	√	√	√	√	√	√	Selected for column testing
BiS5 (S64)	≈	√	√	≈	√	√	To be decided
BiS6 (S65)	√	√	√	√	√	√	Selected for column testing

(√: better, ×: worse, ≈: similar compared with 5 M MEA under comparable conditions)

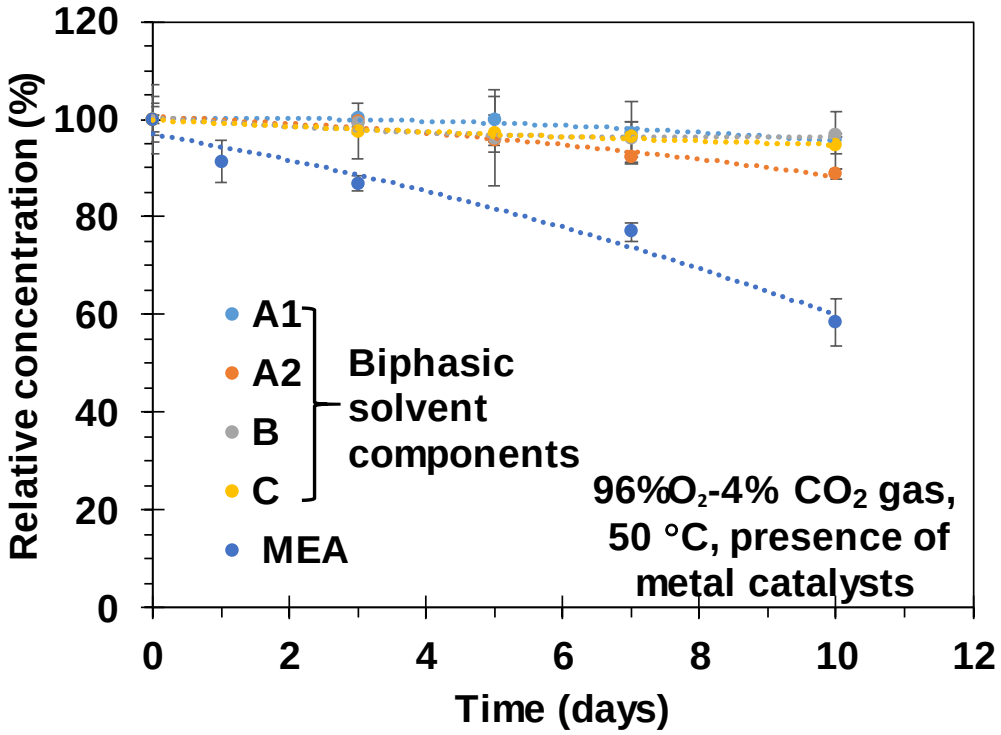
Thermal Stability of Biphasic Solvents



BiS4 solvent (S66, saturated under 5 kPa CO_2) as an example:

- Stability of BiS4 after 2 weeks at 150°C
  - 4-19% of BiS4 components degraded vs. 56% MEA loss at 150 °C
  - Stability of BiS4 at 150°C similar to 5M MEA at 120°C
- Degradation at 120 and 130°C for 8 weeks (not shown in figure) revealed a slower but otherwise similar trend to 150°C

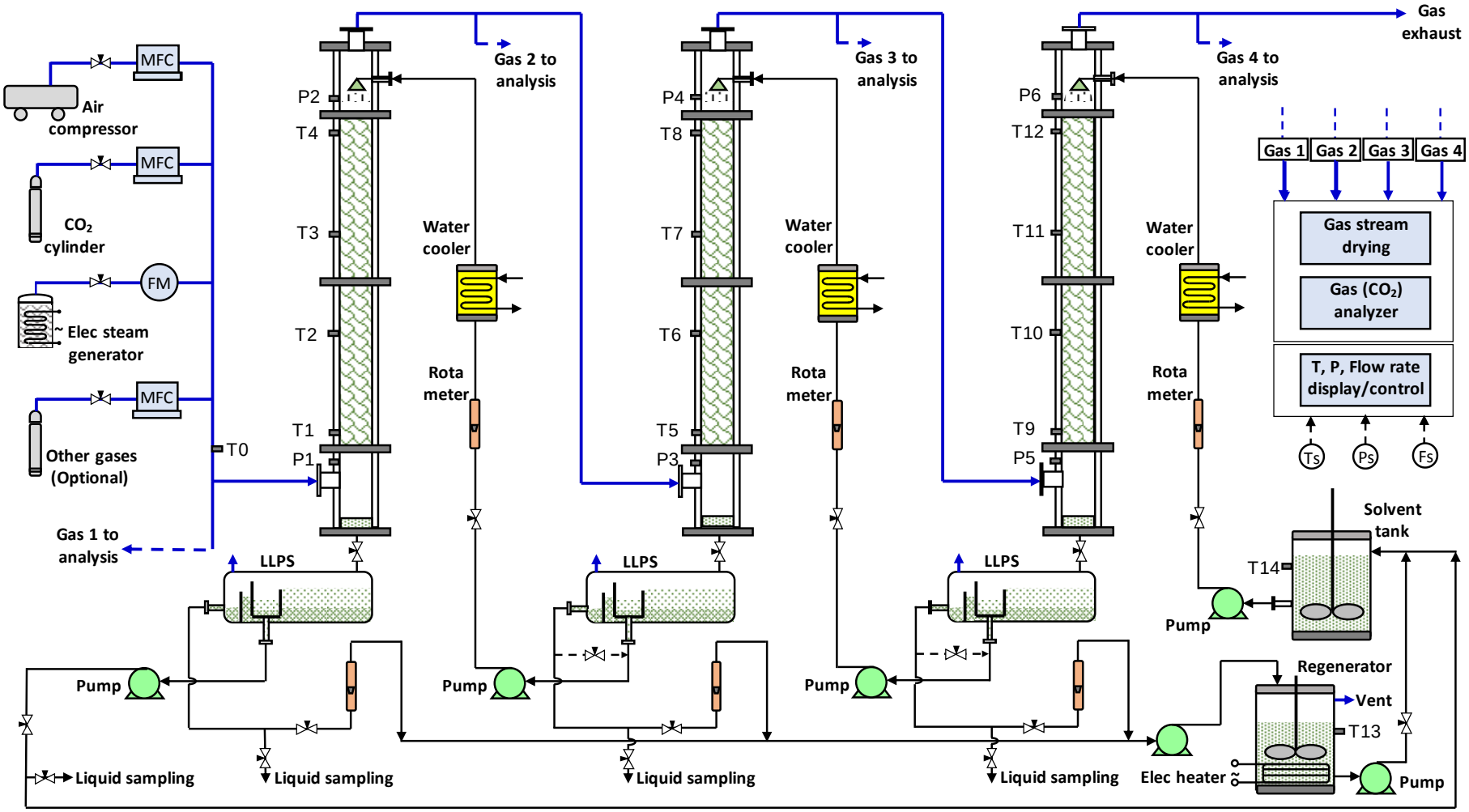
Oxidative Stability of Biphasic Solvents



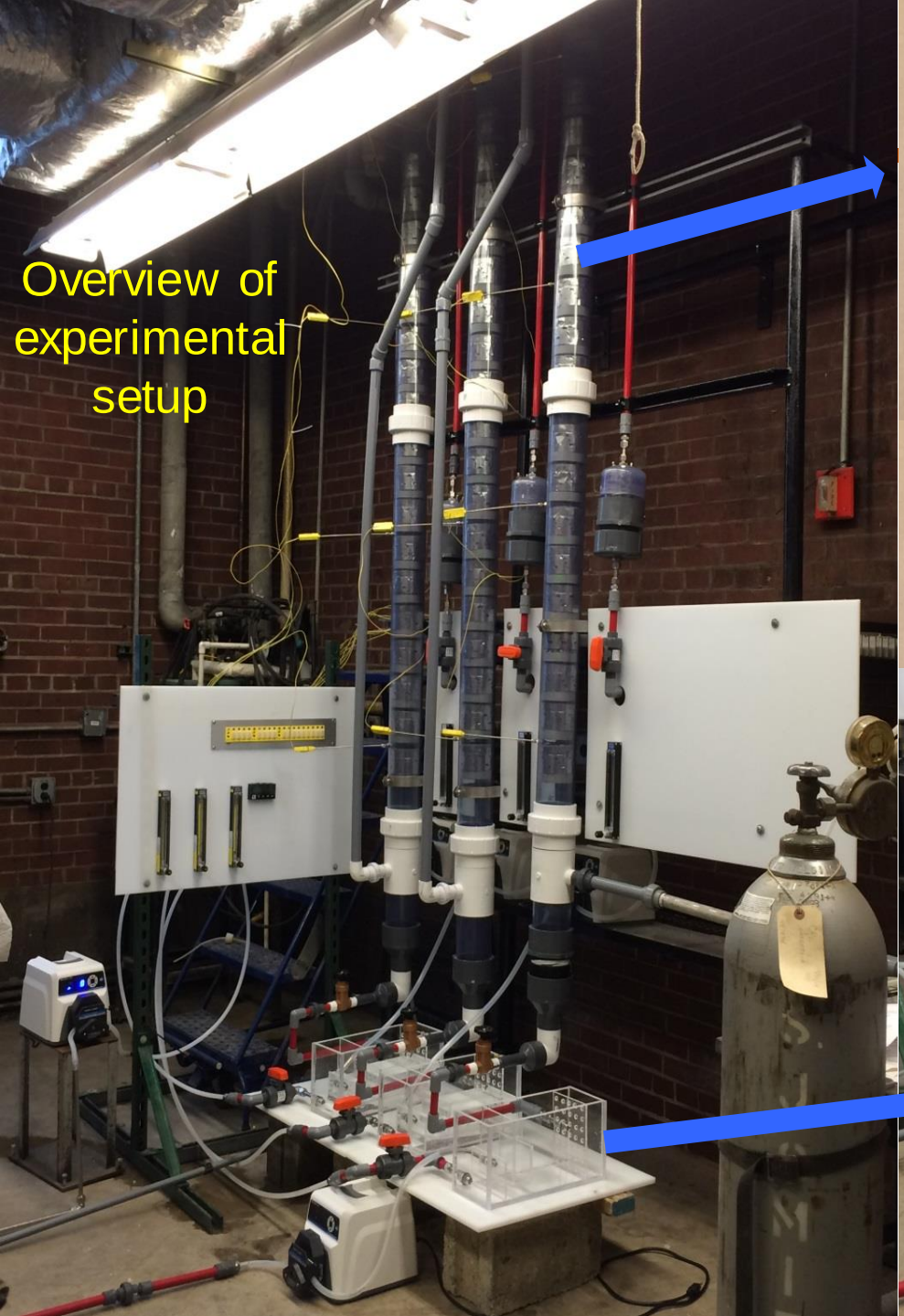
BiS4 solvent (S66) in 96% O_2-4% CO_2 gas mixture as an example:

- <5% A1, B, C and ~11% A2 degraded after 10 days at 50°C vs. 41% MEA loss (Oxidation rate is <27% of MEA)

Task 5. Lab Absorption System with 3-Stages of Packed Beds and LLPS Vessels Fabricated and Tested

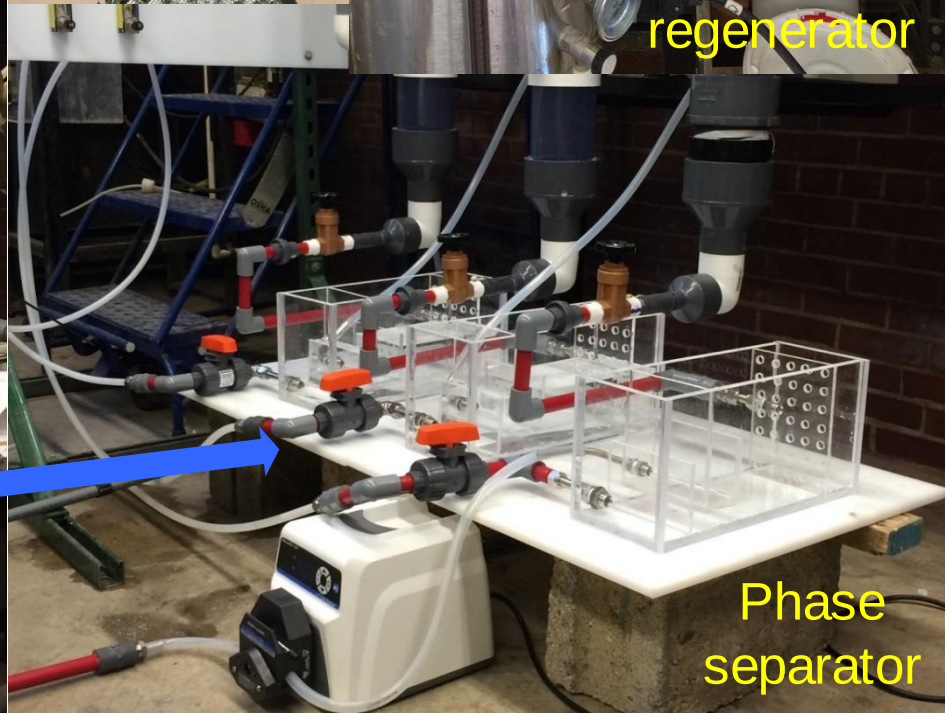


- 3 stages (4-in ID, 7-ft packed-bed for each) arranged side by side to accommodate lab ceiling limit
- 3 stages in one vertical column envisioned for practical use


Overview of experimental setup


Structured packing


Solvent thermal regenerator

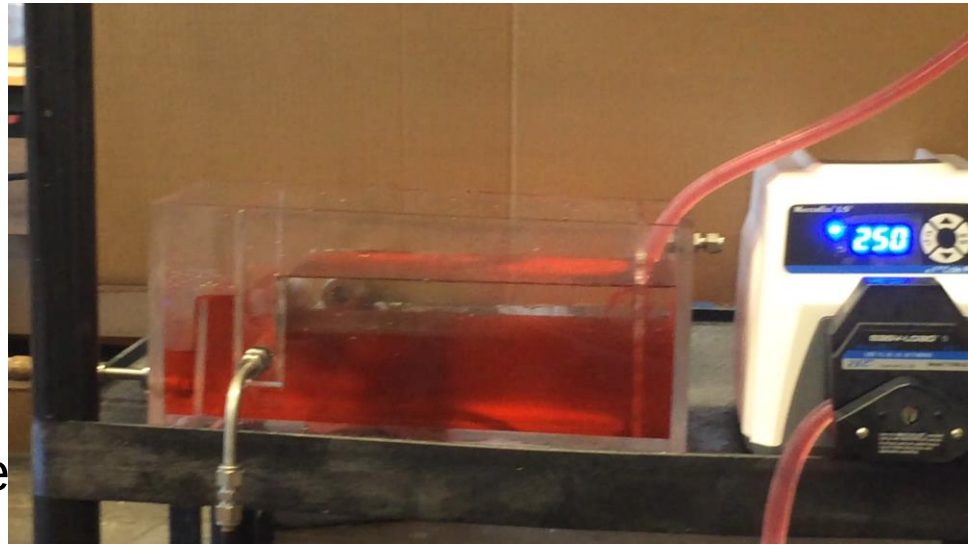

Phase separator

Lab Prototype Phase Separator Achieved Efficient and Stable Separation

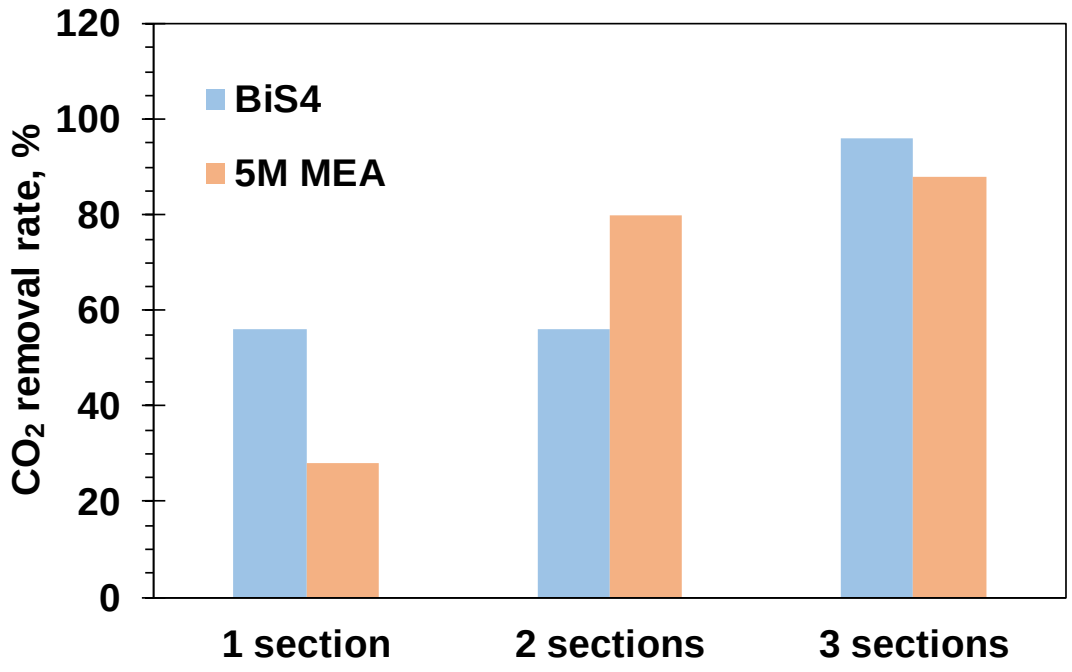
- Phase separator design
  - Based on density difference (lean phase ~0.85 vs. rich phase ~1.1 g/cm^3)
  - Residence time ≤ 5 min (preferred at <1 min)

(Liquid volume of 12 L, total volume of 15 L, liquid flow rate of 2 L/min)

- Actual separation performance
  - Separation efficiency better than the design
  - Able to maintain constant levels of both G-L and L-L interfaces
  - Both interface levels adjustable by adjusting weir heights
  - Very stable operation



Column Testing with BiS4 Biphasic Solvent

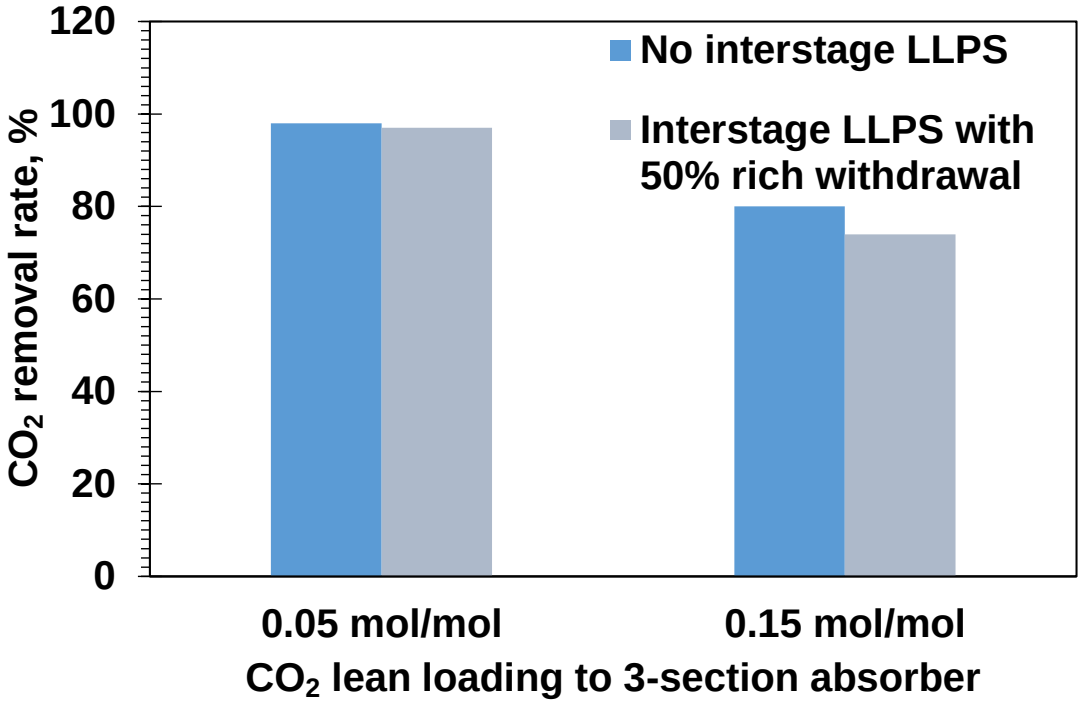


Number of absorber section (with one LLPS for BiS4 solvent testing)

(CO_2 absorption under L/G=4.8 L/m^3, 13 vol.% CO_2 in air, CO_2 lean loadings of 0.05 mol/mol for BiS4 and 0.25 mol/mol for 5M MEA (equiv. to P^*_{CO2}=~20 Pa at 40°C) , 35-40°C)

- Operation steady and reliable for either 1, or 2, or 3 stages of CO_2 absorption and phase separation
- Two phases settled and completely separated in phase separators in <0.5 min

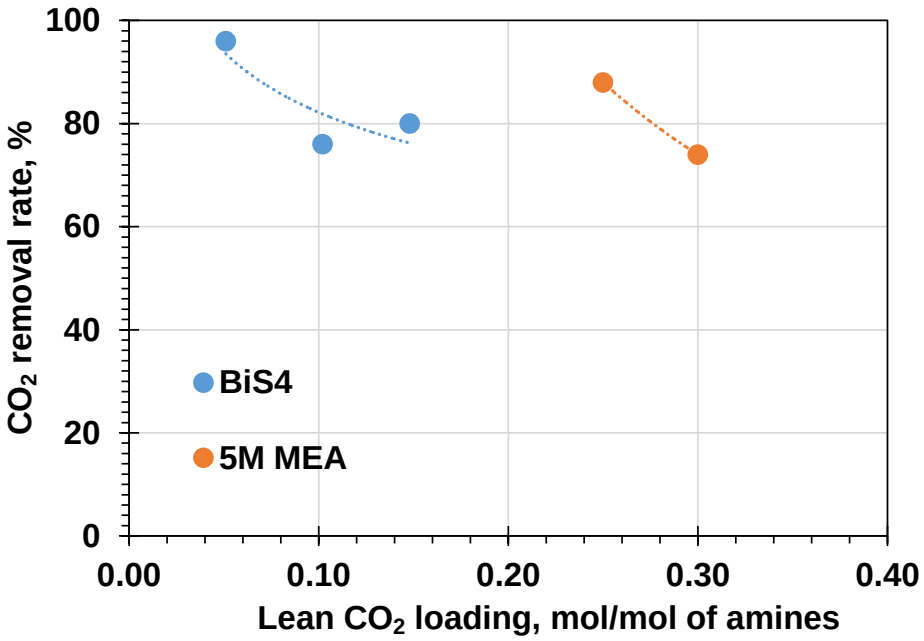
Effect of Inter-Stage Rich Phase Withdrawal (BiS4)

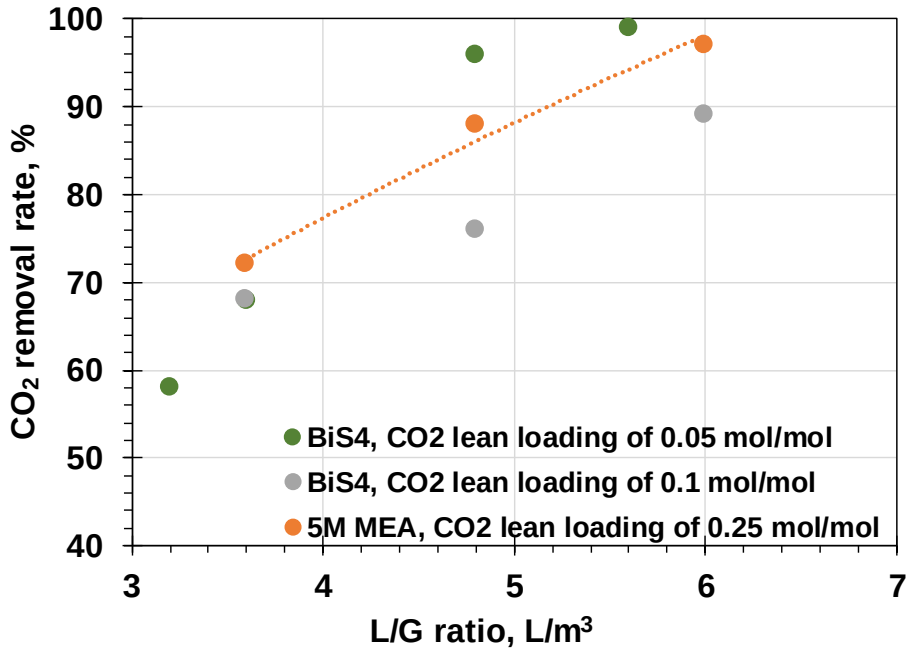


(CO_2 absorption tests under L/G=4.8 L/m^3, 13 vol.% CO_2 in air, and 35-40°C)

- Operation stable at any amount of inter-stage rich phase withdrawal
- Slightly higher CO_2 removal rate achieved without inter-stage rich phase withdrawal for the tested BiS4 solvent
- Inter-stage rich withdrawal could perform better for higher viscosity solvents (e.g., >50 cP); more testing ongoing

Parametric Column Testing (BiS4 Solvent)





(3-stages of CO_2 absorption tests under 13 vol.% CO_2 in air at 35-40°C)

- CO_2 loading capacity and CO_2 removal rate in the absorption step with BiS4 solvent comparable or outperformed 5M MEA under the same L/G and comparable CO_2 lean loading (equivalent to P^*_{CO2}=~20 Pa at 40°C)

Task 6. Preliminary Process Analysis

- Goal: Use preliminary ISGS BiCAP mass and energy balance (MEB) to compare performance and costs to a DOE reference case[1]
  - Perform mass balance and thermodynamic consistency checks on MEB data
    - Compare key process parameters for BiCAP process to reference case (e.g. solvent circulation rate, regeneration process heat input and temperatures, CO_2 compression power)

- Develop Preliminary TEA (continues on next slide)
  - Operating Costs
    - Use preliminary BiCAP MEB to estimate electricity/steam/cooling water requirements
    - Calculate the parasitic load of the BiCAP process and scale the MEB to 550 MW-net

[1] Reference case is Case 12 from DOE Rev. 2a Baseline (DOE/NETL-2010/1397)

Contn'd

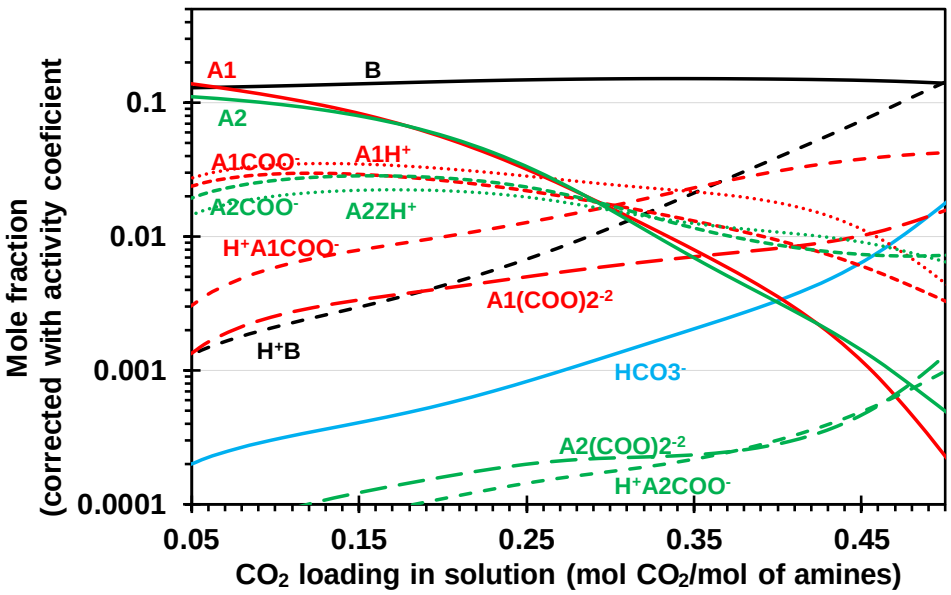
- Operating Costs (continued)
  - Compare the gross power requirement of the BiCAP process to the reference case
  - Compare BiCAP solvent degradation to MEA based on ISGS thermal and oxidative stability tests and estimate solvent losses and associated makeup costs

- Capital Costs
  - Use a previous Trimeric MEA TEA[2] to estimate component (e.g. absorber, stripper, lean-rich exchanger) costs for the reference case
  - Develop key sizing criteria for common components in BiCAP flowsheet, size equipment, and use scaling methods to estimate purchased equipment cost (PEC)
  - Perform bottom-up sizing and costing for novel BiCAP equipment (e.g. liquid-liquid phase separator)
  - Compare total plant cost (TPC) for the BiCAP and reference case processes based on the estimated PEC

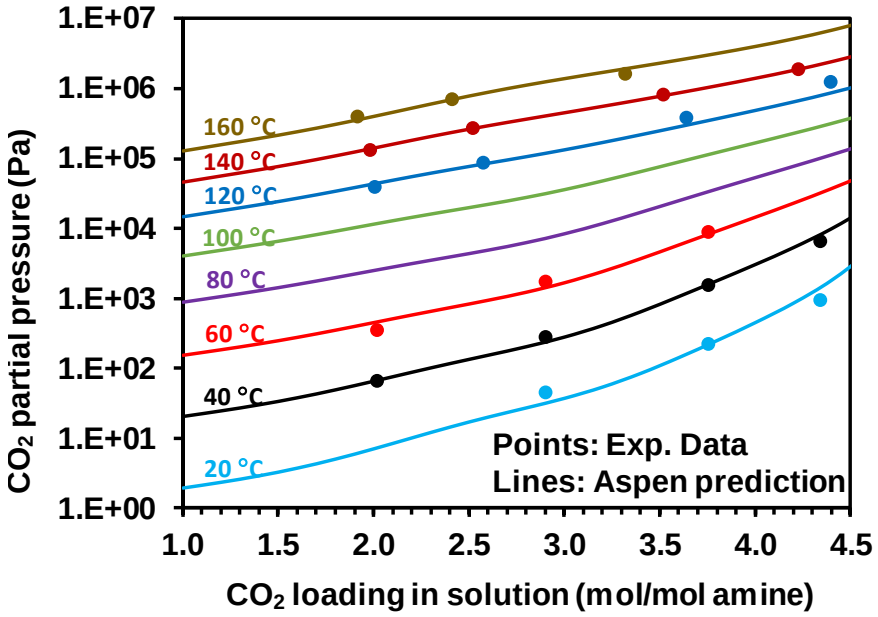
[2] "Advanced Amine Solvent Formulations and Process Integration for Near-Term CO_2 Capture Success". DE-FG02-06ER84625

Simulation of BiCAP Process

- A rigorous thermodynamic model based on electrolyte-Nonrandom Two-Liquid (eNRTL) activity coefficient approach developed with Aspen Plus
- Model used for process simulation to generate MEB data for preliminary TEA



Speciation distribution of BiS4 solvent at 40°C predicted by the model



Comparison of Aspen Plus predictions and experimental data for BiS4 solvent

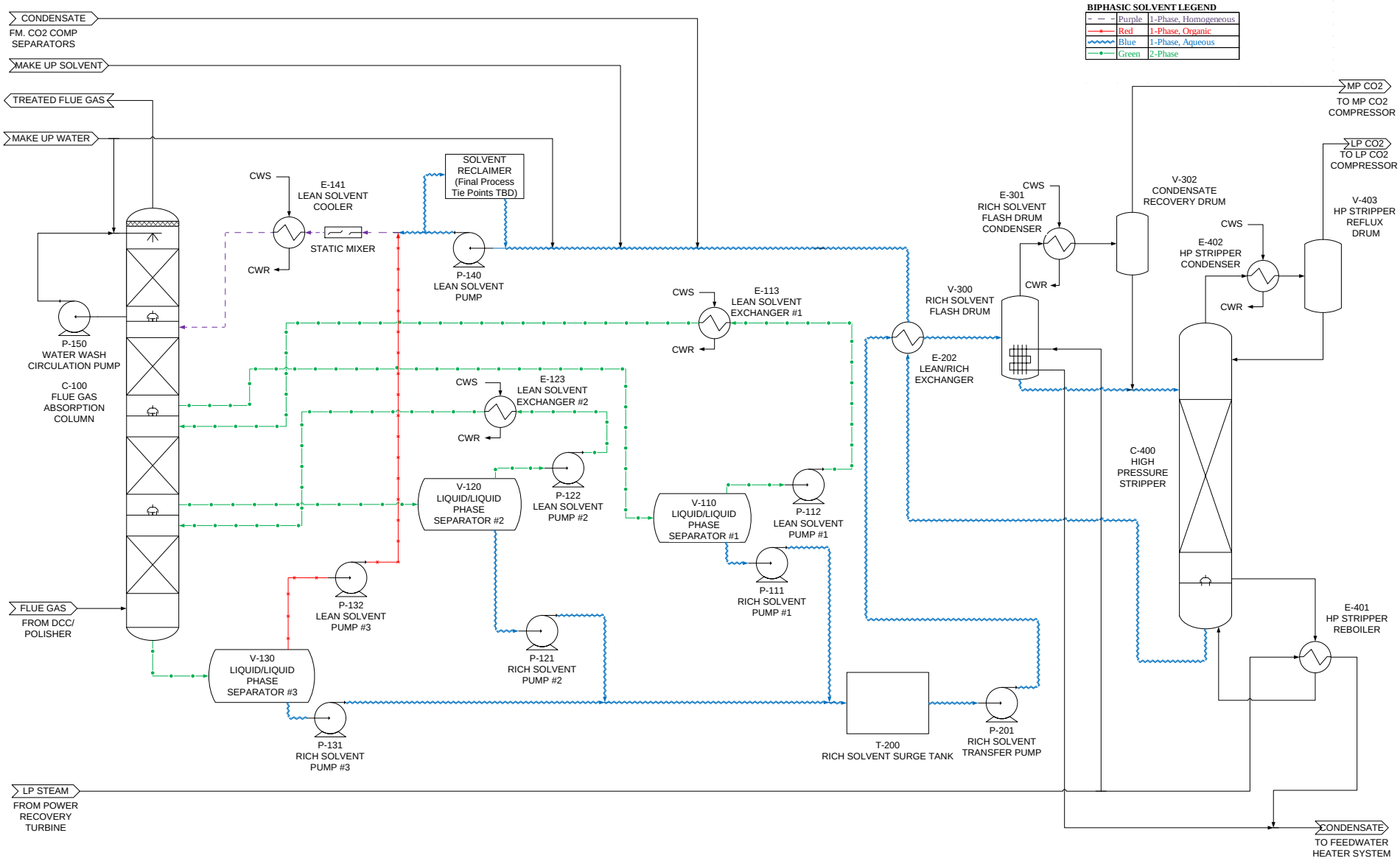
Initial, Preliminary Process Comparisons

Parameter	BiCAP	Baseline	Comments
Lean Solvent Circulation Rate	13,591,000 kg/hr (Only 5,643,000 kg/hr to Regen)	9,029,000 kg/hr	From IECM
Regeneration Heat Input	409 MW th @ 160 °C	542 MW th @ 152 °C	Baseline p. 313[1]
Regeneration Temperature	Flash: 137 °C Stripper: 150 °C	120 °C	Reference Estimated from Previous Project[2]
Regeneration Pressure	Flash: 10.0 bar Stripper: 5.1 bar	Stripper: 1.6 bar	Baseline p. 412[1]
CO_2 Compression Power	27.5 MW	44.9 MW	Baseline p. 413[1]

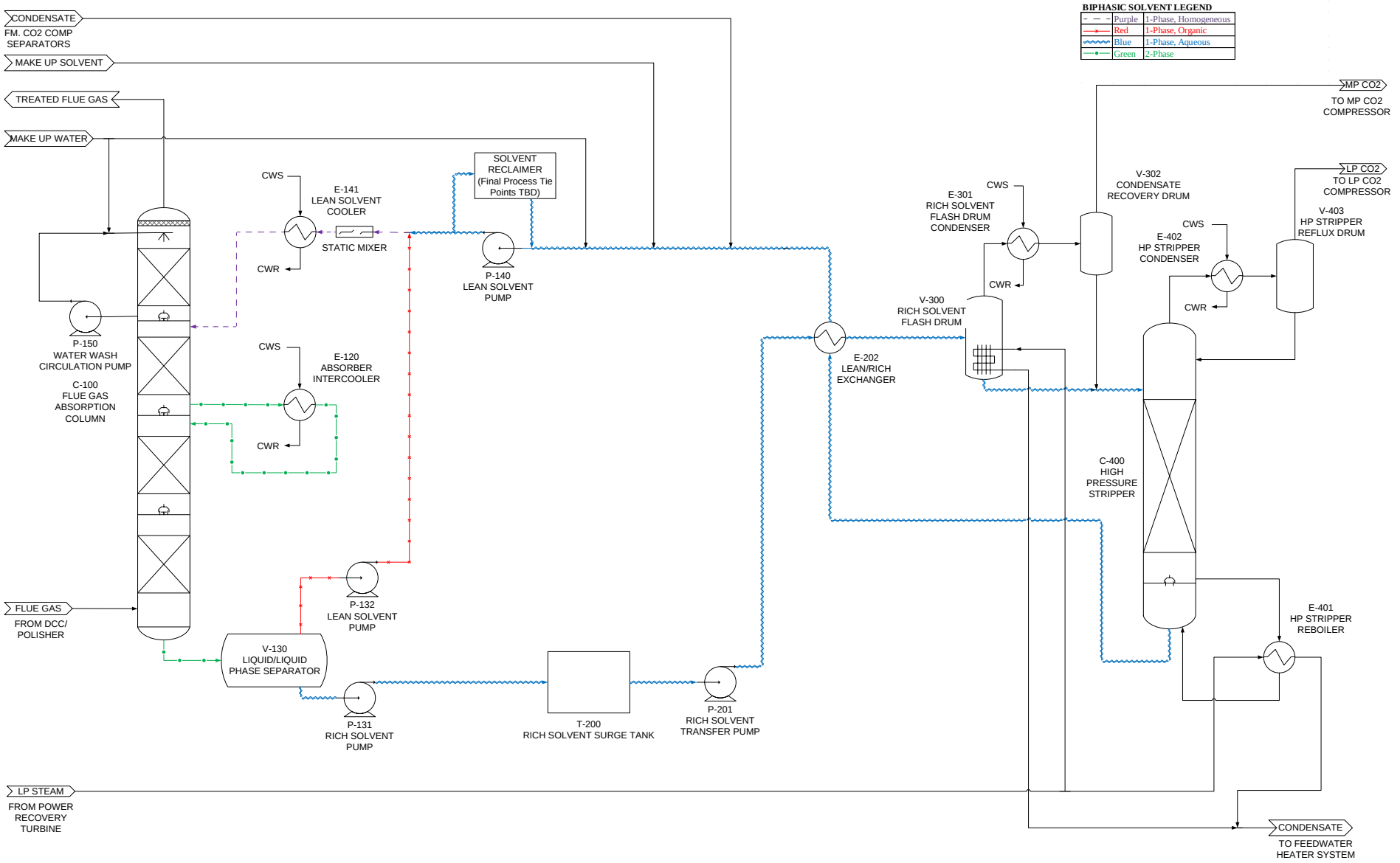
[1] Reference case is Case 12 from DOE Rev. 2a Baseline (DOE/NETL-2010/1397)

[2] "Advanced Amine Solvent Formulations and Process Integration for Near-Term CO_2 Capture Success". DE-FG02-06ER84625

BiCAP Process Flow Diagram (3 LLPS)



BiCAP Process Flow Diagram (1 LLPS)



Presentation outline:

- Project Overview
- Technical Background
- BP1 Work and Budget Status
- BP1 Technical Activities and Major Findings
- BP2 Work and Budget Plan

Major Work Activities Planned in BP2

- **Task 7. Testing CO_2 desorption in a high pressure flash & stripping column**
  - Fabrication of a flash and stripper system
  - Parametric testing of CO_2 flash and stripping
  - Modeling of CO_2 flash and stripping

- **Task 8. Assessing the impact of solvent on the equipment corrosion**
  - Carbon steel corrosion by 2-3 selected solvents
  - Stainless steel corrosion by 2-3 selected solvents

- **Task 9. Final techno-economic analysis**
  - Updated process simulation and mass & energy balance calculations
  - High-level cost and sensitivity analysis

- **Additional work when necessary**
  - Solvent improvement & characterization based on Task 7-9 results
  - Process configuration optimization to achieve a parasitic power loss of 0.22 kWh/kg CO_2.

No Budget Change Requested for BP2

- Estimated cost by 6/30/17 is close to the BP1 budget plan
- No change requested for either federal budget or cost share in BP2

	BP1 Budget Plan (US$)	BP2 Budget Plan (US$)
DOE share	1,079.663	920,333
Recipient cost share	269,920	231,132
Total	1,349,583	1,151,465

Other Potential Work

Extended work if additional funding is available

- Extended MD simulation studies to improve solvent analysis
  - Multiscale computational MD methodology developed in BP1;
  - Model further used for an extended solvent screening & predictions
- Rigorous process modeling and optimization to enhance performance
  - Aspen Plus model established in BP1
  - Model further developed to include rate (with G-L-L mass transfers) and LLPS modules
- Extended solvent characterization for selected biphasic solvents
  - Solvent volatility
  - Amine aerosol emissions

Next stage scale-up work

- Close-loop bench or small pilot testing (0.1-0.5 MW) with a simulated or actual flue gas (vs. separate absorption & desorption tests in current project
- Analysis of technical risks & mitigation for scale-up

Acknowledgements

- Funding Support by USDOE/NETL through Cooperative Agreement No. DE-FE0026434

- DOE/NETL Project Manager: Andrew Jones