NETL

Hybrid PDMS Testing and Techno-economic Model

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Pre-combustion Solvents

NETL CO_2 Capture Conference
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U.S. DEPARTMENT OF ENERGY | National Energy Technology Laboratory

Outline

- Overall goal of project
- Experimental Data on Pre-combustion Solvents
- Discussion of Process Flow Diagram
- Capital & Operating Cost Breakdown of Equipment
- Economic Model / Levelized Cost Estimate
- Future work

High Molecular Weight PDMS - Background

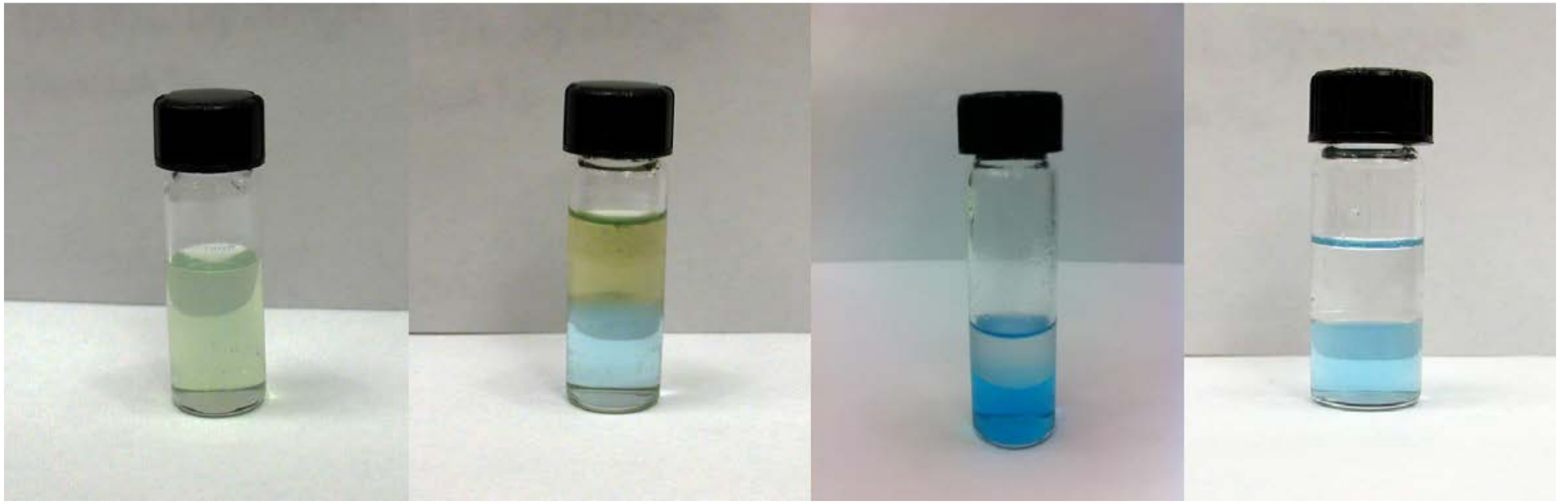
- **Objective:** Lower the cost of capturing CO_2 from syngas
- **Approach:** Develop hydrophobic solvents for separation of CO_2 from warm syngas

PEGDME
fully miscible with water;
Extremely hydrophilic

PPGDME-branched or PPGDME-linear
absorbs ~2wt% water;
separates slowly after shaking; **Hydrophobic**

PDMS-PEGDME hybrid
absorbs <<1wt% water,
Very hydrophobic

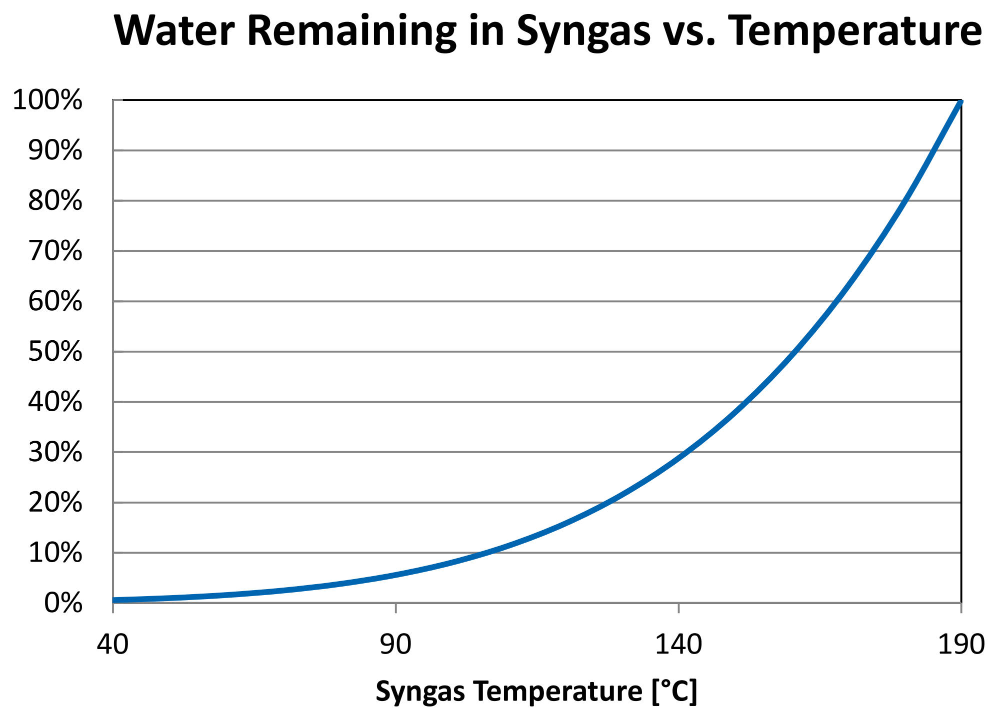
PDMS
immiscible with water, even at 120C and 10000 psi;
separates quickly after shaking;
Extremely hydrophobic



The Solubility of Water in the Solvents

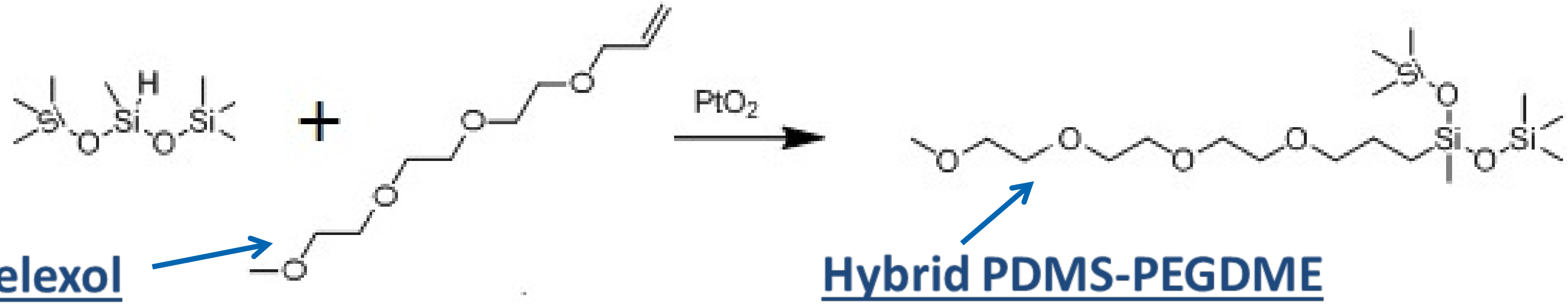
Background: Why Selexol must operate < 40°C

- **Higher CO_2 and H_2S selectivity against H_2 at lower temperature**
- **<u>Constraint</u>: Selexol will absorb any remaining water in syngas**



Experimental Results

Selexol vs. Hybrid @25°C



Selexol

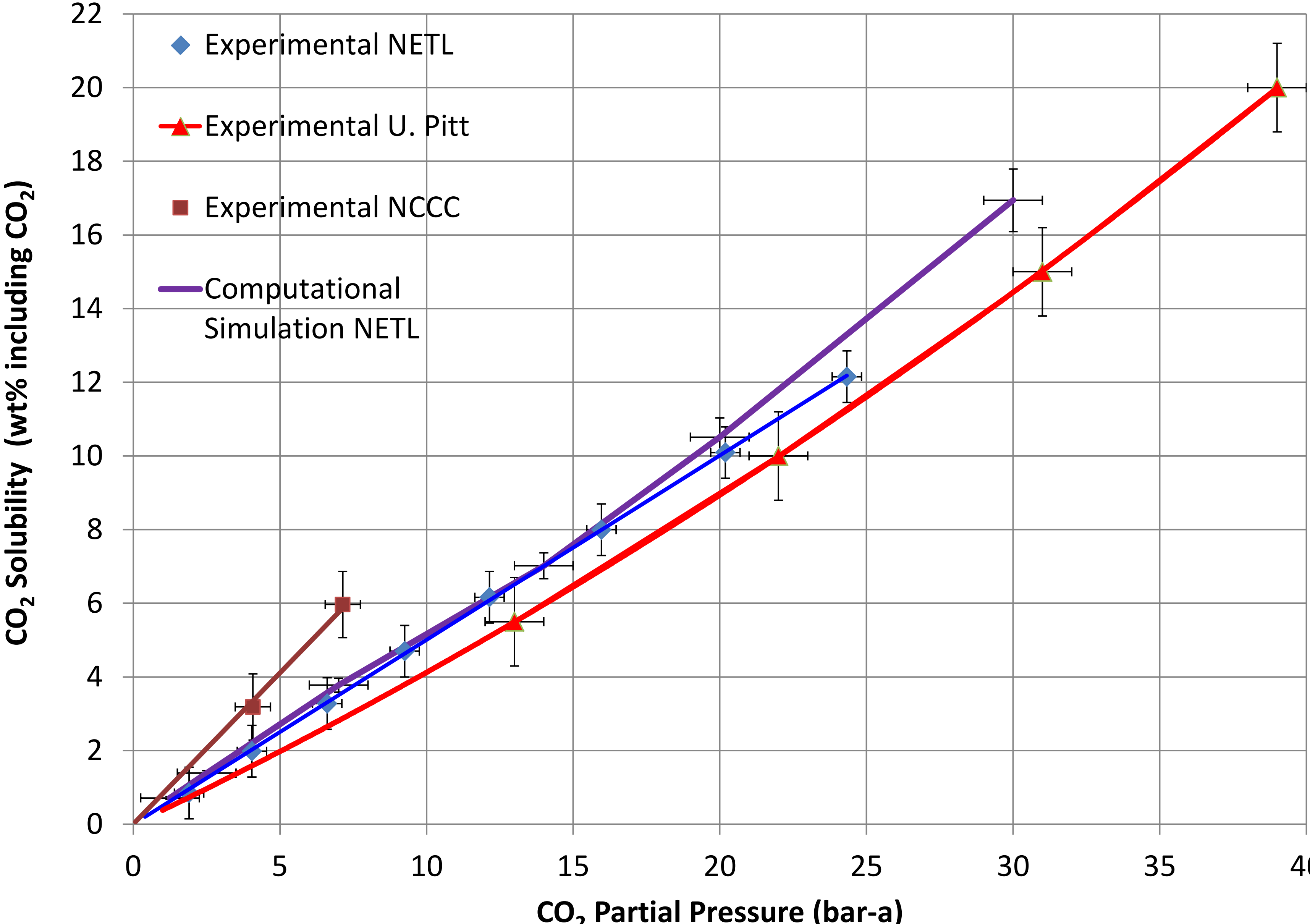
- Hydrophilic
- Viscosity = 5.8 cP
- MW = 280
- Specific heat = 2.06 kJ/kg·K
- Density = 1030 kg/m^3
- Thermal cond = 0.19 W/m·K
- Surface tension ~ 32 mN/m
- Vapor Pressure = 0.0007 mmHg
- CO_2/H_2 selectivity ~ 80

Hybrid PDMS-PEGDME

- Hydrophobic
- Viscosity = 4.8 cP
- MW = 438
- Specific heat = 1.77 kJ/kg·K
- Density ~ 936 kg/m^3
- Thermal cond = TBD*
- Surface tension = 22.1 mN/m
- Vapor Pressure << 0.0007 mmHg
- CO_2/H_2 selectivity ~ 40

*AspenPlus estimates that the thermal conductivity is 0.10 W/m·K

CO_2 Solubility in Hybrid-PDMS 25°C



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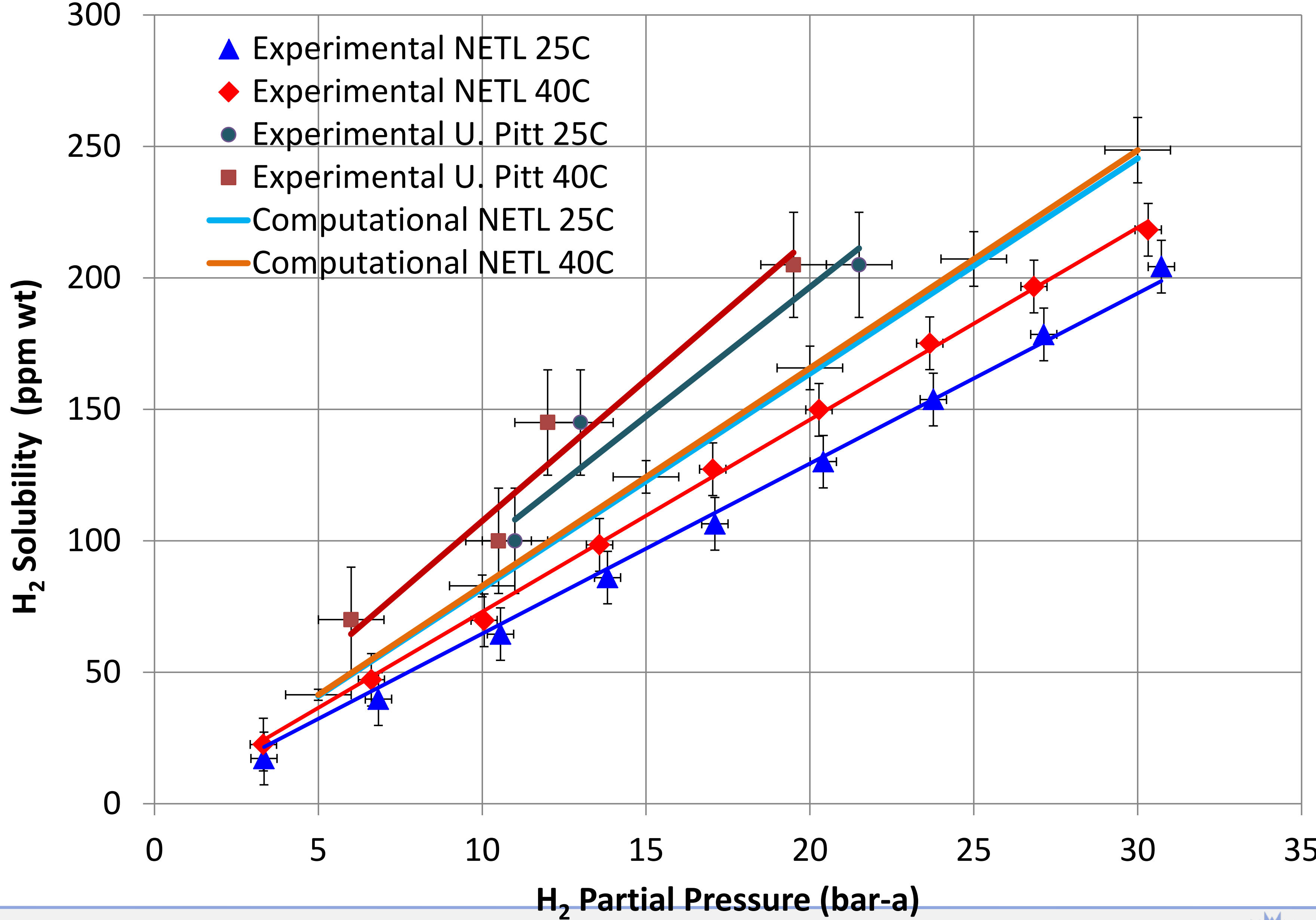
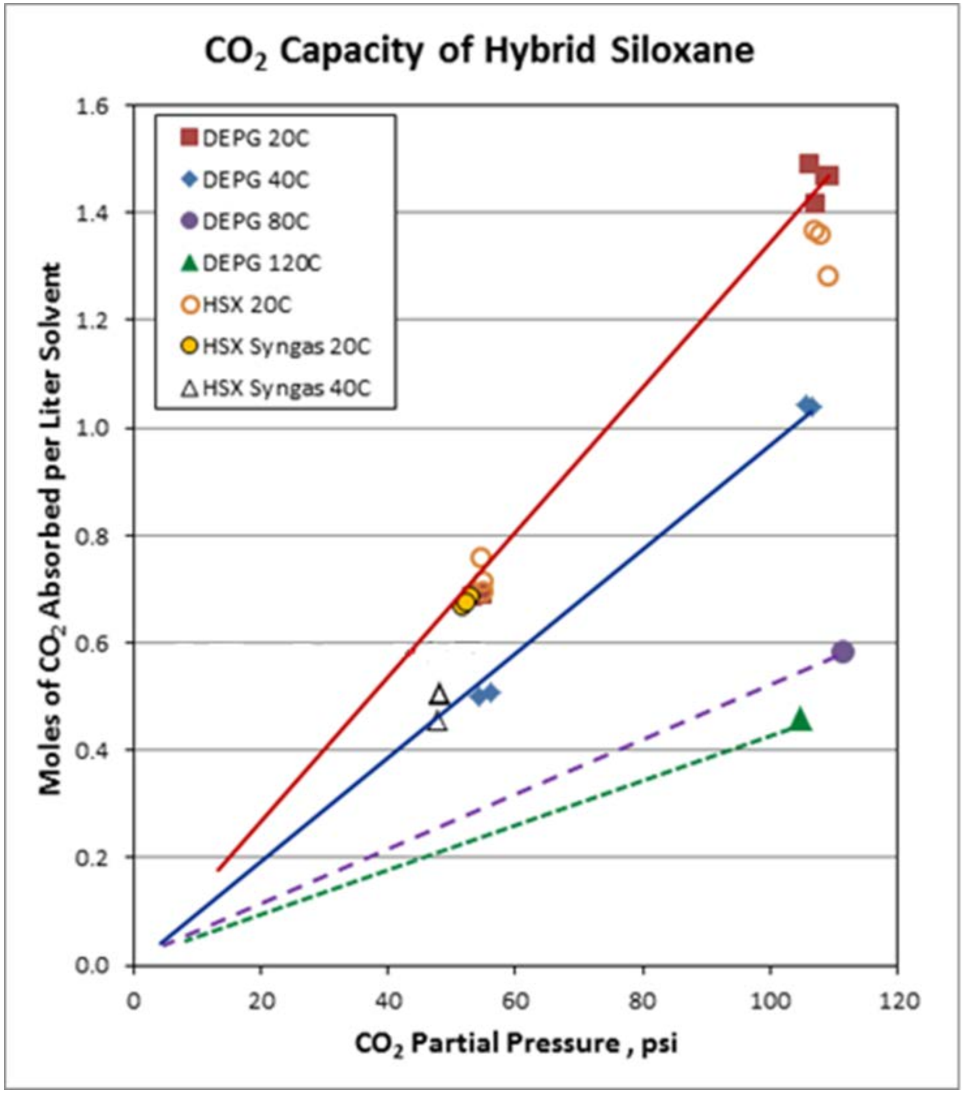
H_2 Solubility in Hybrid-PDMS 25°C and 40°C



PDMS Scale up & NCCC Testing

- **8 L of Hybrid PDMS-PEGDME were synthesized at NETL and shipped to NCCC**
- **Hybrid solvent was tested for CO_2 solubility at 20°C and 40°C**
- **Solvent had tendency to foam and create fine aerosols at higher temperatures**
  - Due to low surface tension, low viscosity, and low density
  - Increases absorber diameter, but can decrease height



Selexol vs. Ionic Liquid @25^oC

Selexol

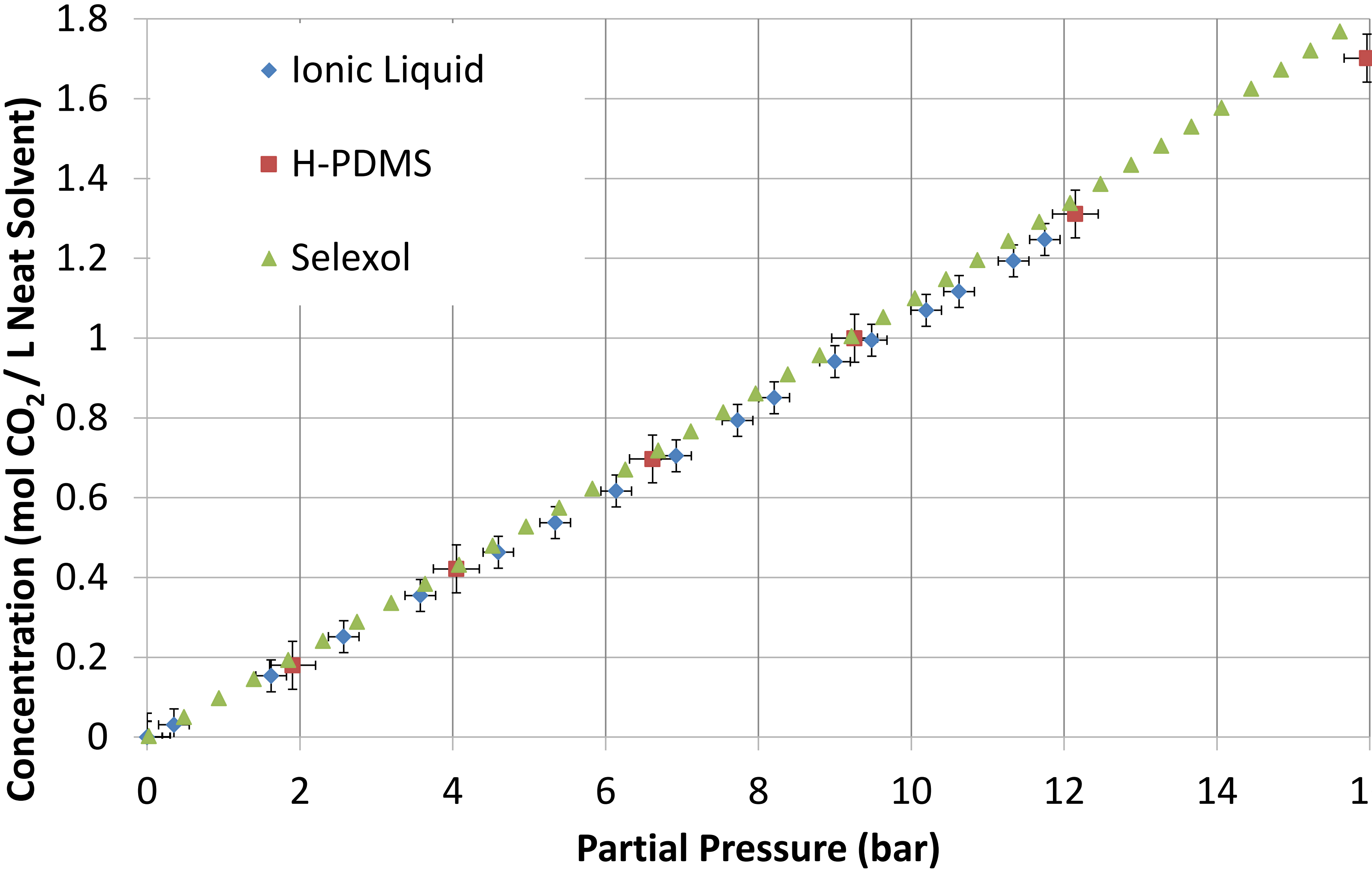
- Hydrophilic
- Viscosity = 5.8 cP
- MW = 280
- Specific heat = 2.06 kJ/kg·K
- Density = 1030 kg/m^3
- Thermal cond = 0.19 W/m·K
- Surface tension ~ 32 mN/m
- Vapor Pressure = 0.0007 mmHg
- CO_2/H_2 selectivity ~ 80

Ionic Liquid

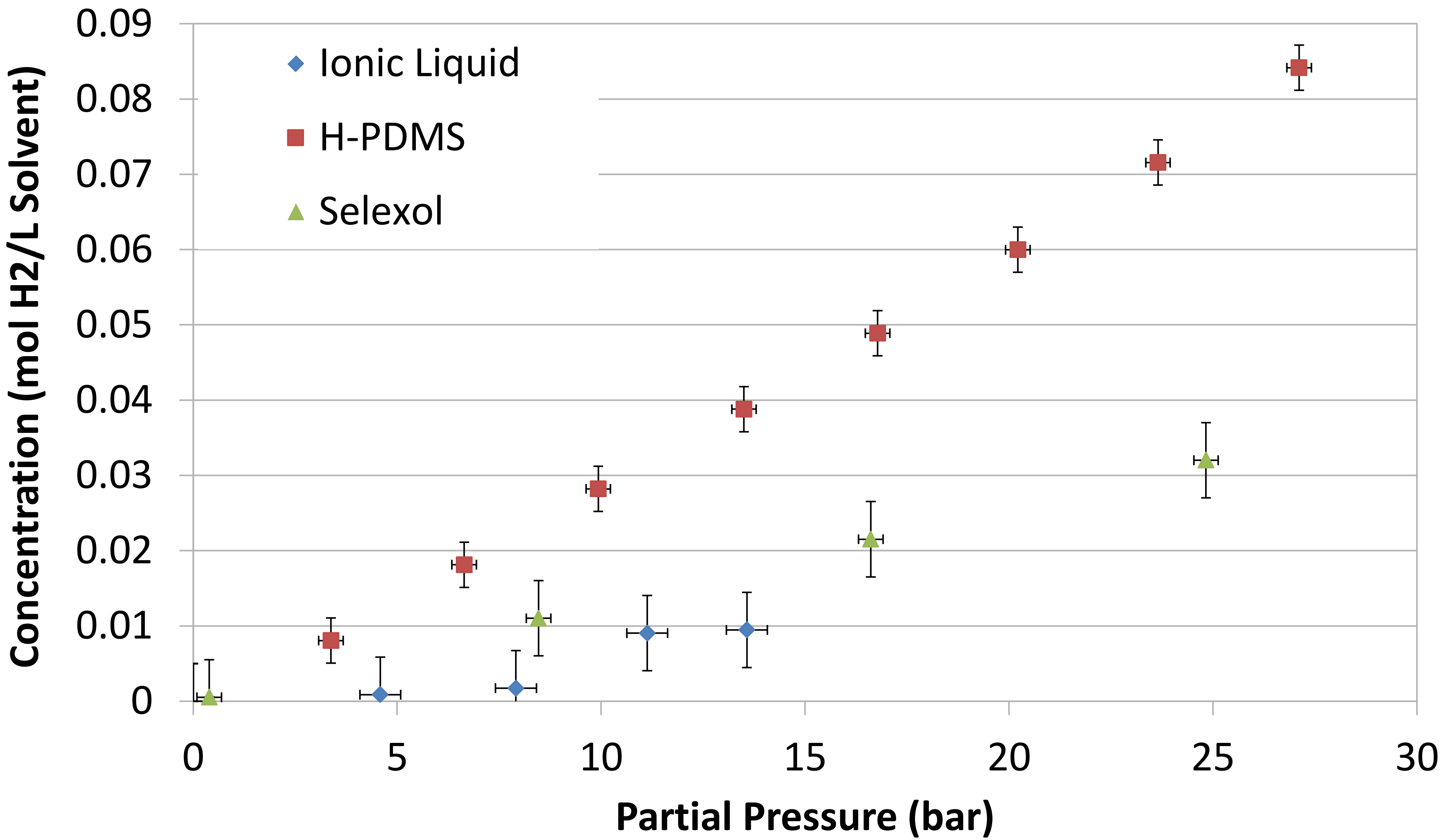
- Hydrophobic (0.23 wt% H_2O)
- Viscosity = 28 cP (wet)
- MW = 399
- Specific heat = 1.11 kJ/kg·K
- Density ~ 1515 kg/m^3
- Thermal cond = TBD*
- Surface tension = TBD*
- Vapor Pressure <<< 0.0007 mmHg
- CO_2/H_2 selectivity ~ 150

*AspenPlus estimates that these values are 0.11 W/m·K and 68 mN/m, respectively

CO_2 Solubility at 25ºC in different Solvents



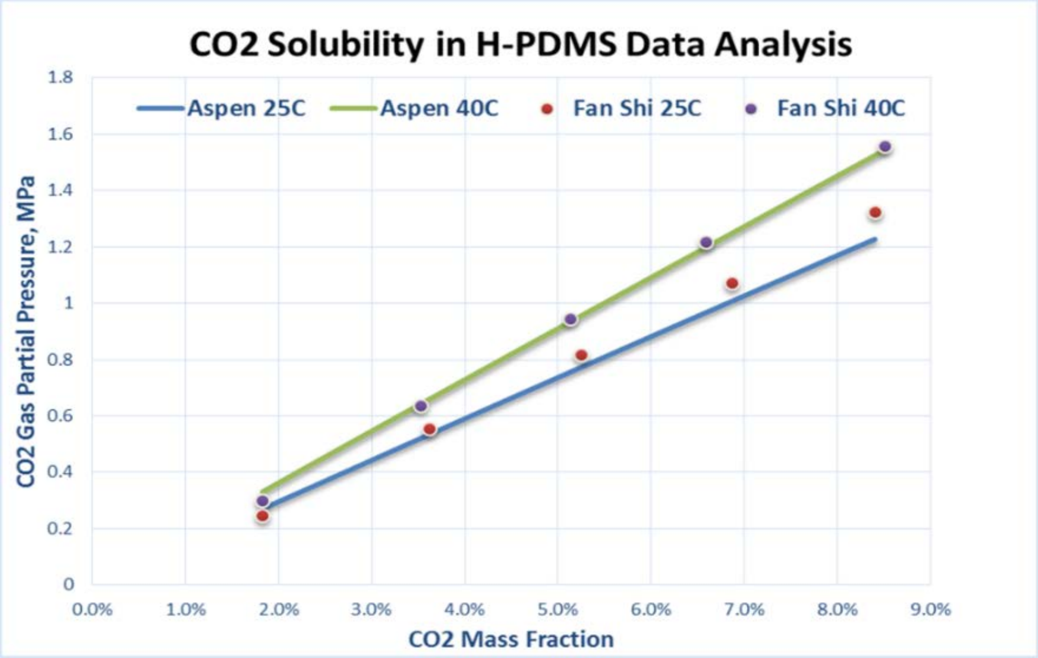
H_2 Solubility at 25°C



System Modeling

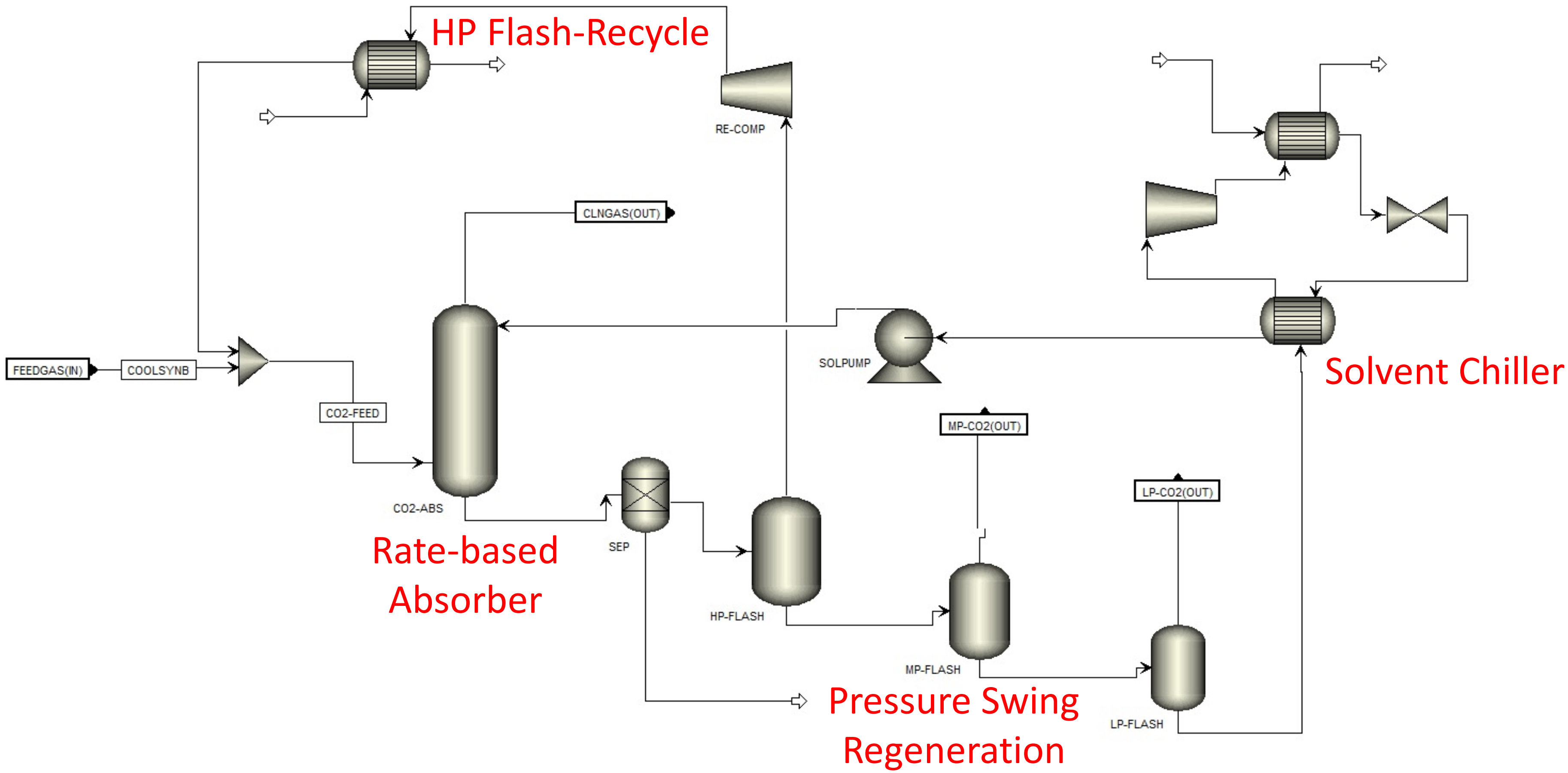
System Modeling: Data Regression in Aspen Plus

- Data Regression to estimate the required pure and binary parameters
- Regression requires input of both thermodynamic & kinetic variable
- PC-SAFT method used for H-PDMS and Selexol
- ENRTL-RK method used for Ionic Liquid



System Modeling:
Aspen Plus Modeling

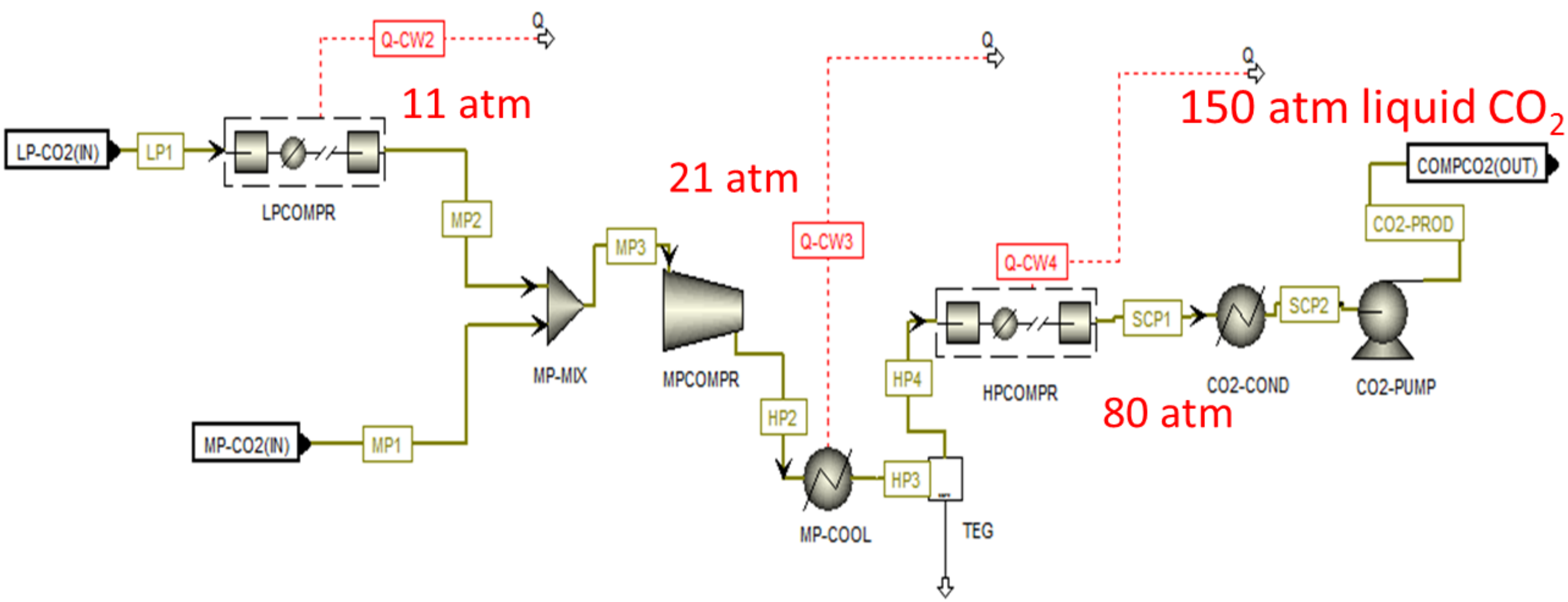
- **Model for Physical Solvent based CO_2 capture using flash regeneration adapted from MIT IGCC-Selexol capture Aspen Model**



Field and Brasington, "Baseline Flowsheet Model for IGCC with Carbon Capture," *Ind. Eng. Chem. Res.*, 2011, 50 (19), p 11306.

System Modeling:
Aspen Plus Modeling

- **Base Model for CO_2 capture using flash regeneration adapted from MIT IGCC-Selexol capture Aspen Model**



Field and Brasington, “Baseline Flowsheet Model for IGCC with Carbon Capture,” *Ind. Eng. Chem. Res.*, 2011, 50 (19), p 11306.

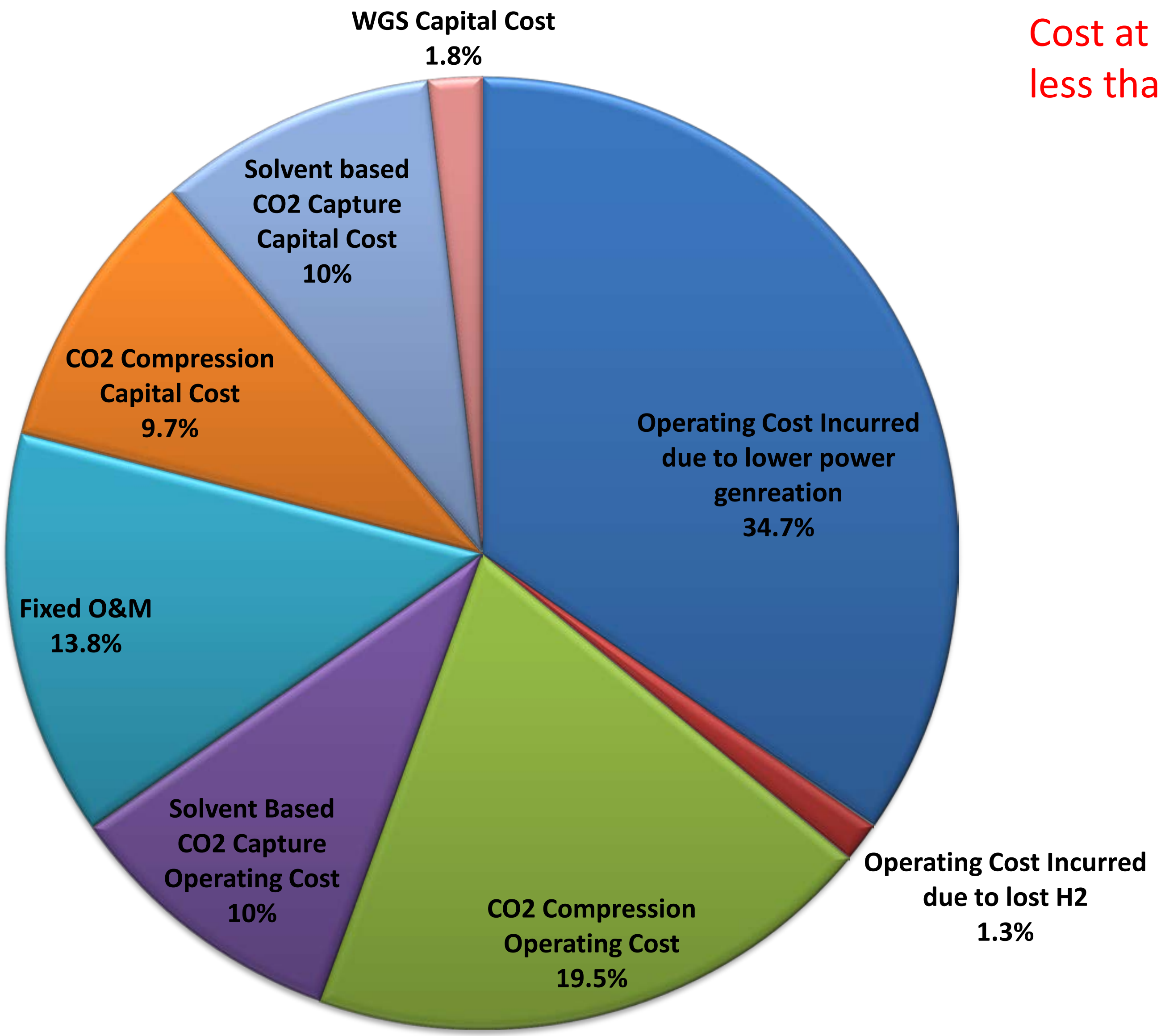
Our Economic Model

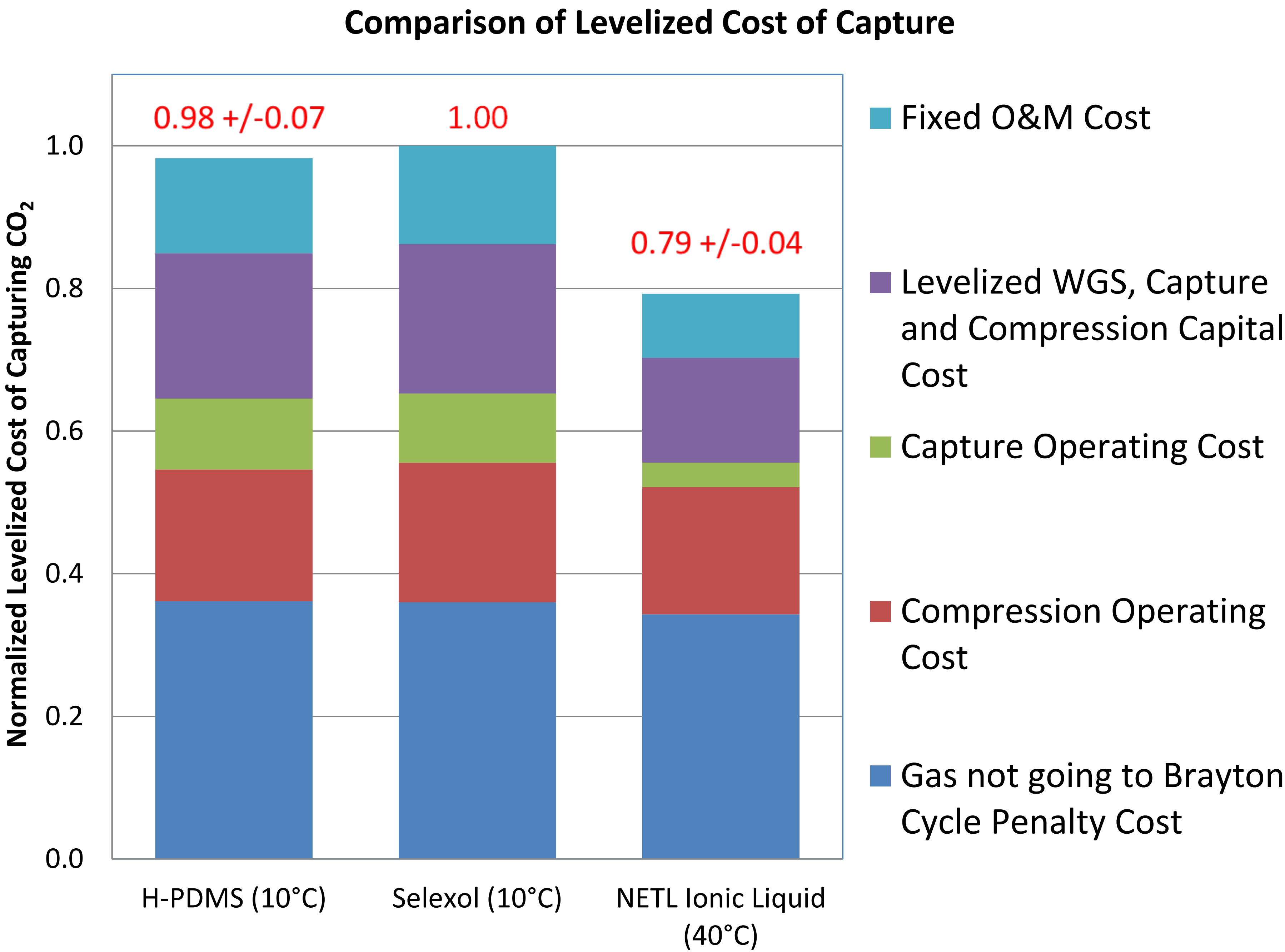
- **Economic Model Assumptions:**
  - There is an existing IGCC Power Plant with H_2S Removal
  - 1 Years for Construction (for CO_2 Capture Equipment)
  - 30 Years of Operations with O&M = 4% of Capital per year
  - 80% Capacity Factor
  - 5% Inflation-Adjusted Interest Rate
  - Plant Cost Ratio = 5 = Total Capital Cost / Bare Equipment Costs
  - Bare Capital Cost estimates calculated from equations taken from various sources (Sieder Textbook, AspenPlus, IECM)
- **Used to calculate the levelized cost of capturing CO_2**
  - Levelized cost = Operating costs plus capital costs levelized per ton of CO_2 captured
  - Values are normalized compared with Selexol

Operating & Levelized Capital Cost Distribution Chart: Selexol

Normalized Value = 1.00 For Levelized Cost per CO_2 Captured

Note: Levelized Cost at 10°C was less than 40°C




Comparison of Levelized Cost of Capture
Normalized Levelized Cost of Capturing CO2
1.0
0.8
0.6
0.4
0.2
0.0
0.98 +/-0.07
1.00
0.79 +/-0.04
H-PDMS (10°C)
Selexol (10°C)
NETL Ionic Liquid (40°C)
Fixed O&M Cost
Levelized WGS, Capture and Compression Capital Cost
Capture Operating Cost
Compression Operating Cost
Gas not going to Brayton Cycle Penalty Cost

Future Work

- **Test Ionic Liquid Solvent at NCCC, and continue testing at NETL**
- **H_2S testing for both H-PDMS and Ionic Liquid**
- **Model both H-PDMS and Ionic Liquid in a full IGCC-CCS system model with two-stage H_2S/CO_2 removal**
- **Include H_2 & H_2O separating membrane upstream of two-stage H_2S/CO_2 removal in order to potentially lower the levelized cost even further**

Thank You

- **Thanks to:** NETL SCC**,** Sweta Agarwal, Hunaid Nulwala, Elliot Roth, Fan Shi, Wei Shi, Regina Woloshun, David Miller, Dave Hopkinson, Bob Enick, John Kitchin, and Dave Luebke

Back-up Slides

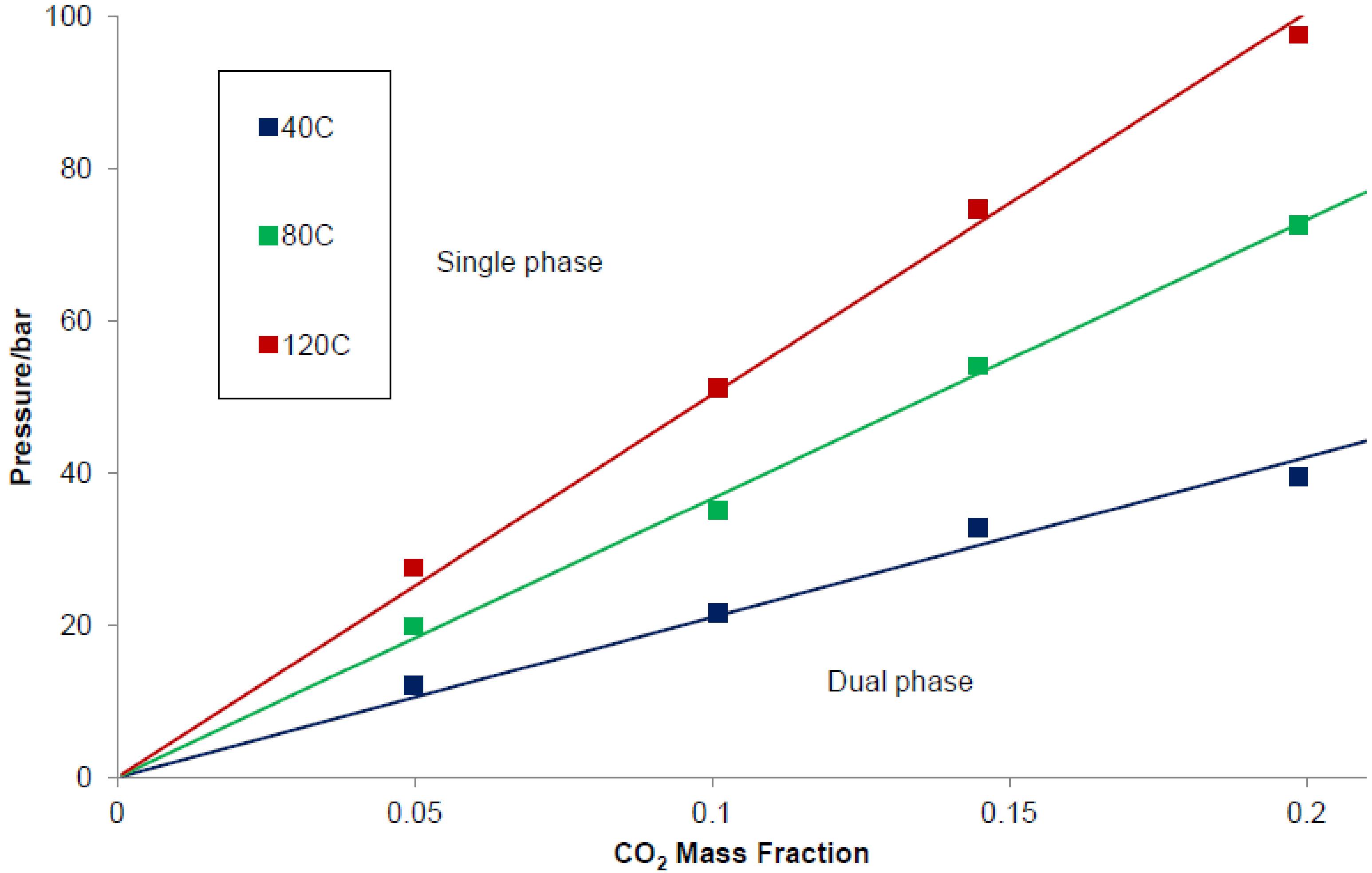
Glossary

PC-SAFT : Perturbed Chain statistical associating fluid theory
NRTL: Non-random two-liquid
ENRTL-RK: Electrolyte NRTL with Redlich Kwong vapor phase properties

System Modeling:
Preliminary Results of Net Power Consumed

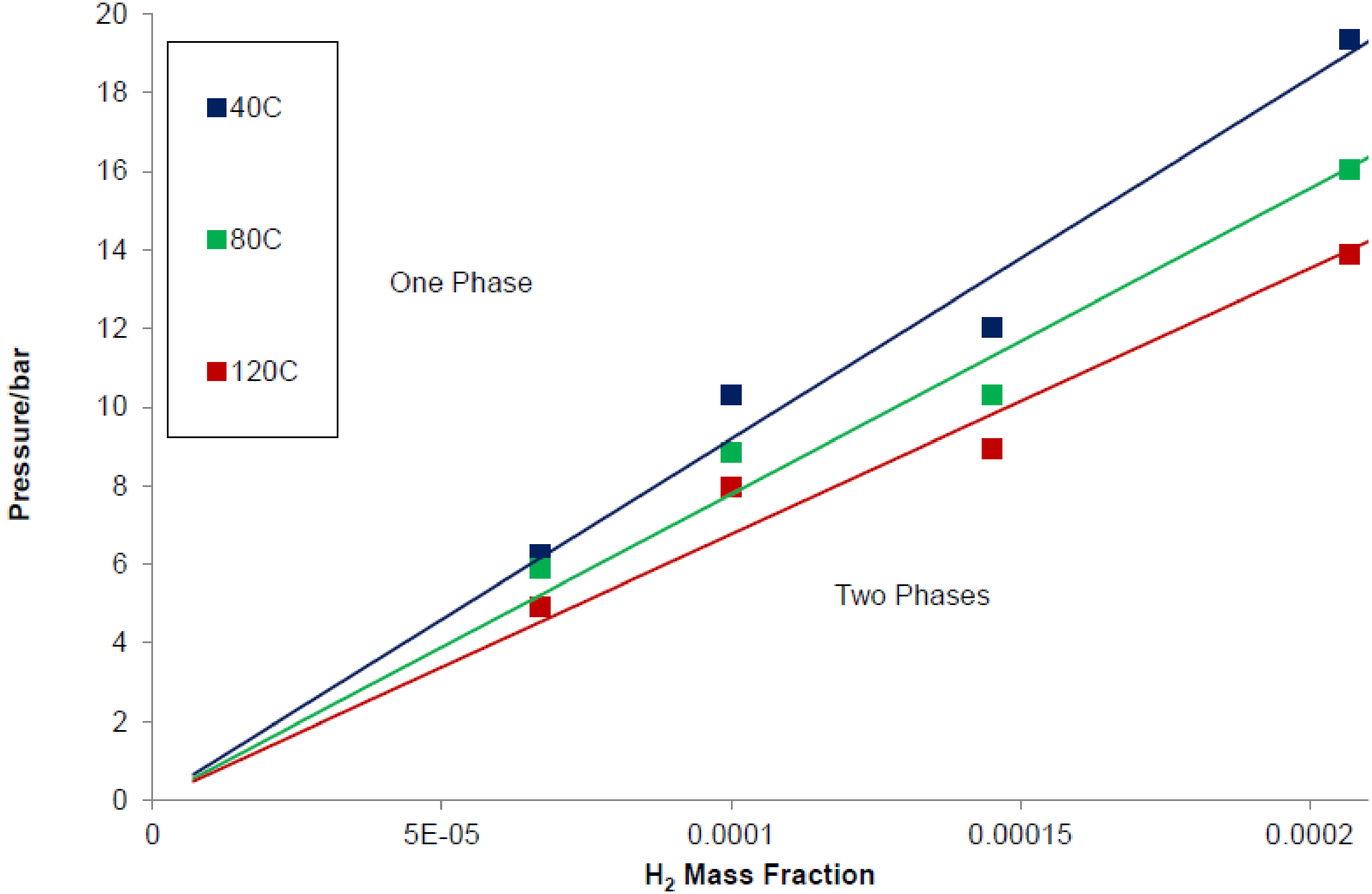
	Case 1	Case 2	Case 3	Case 4
Solvent Used	Selexol	Selexol	H-PDMS	H-PDMS
Model	Optimized	Optimized	Regressed & Optimized	Regressed & Optimized
Absorber Inlet Solvent Temp	10C	40C	10C	40C
Water Volumetric Flow Rate (kL/min)	3.05	2.35	0.08	0.05
Solvent Volumetric Flow Rate (kL/min)	88.20	143.58	101.60	205.45
Power Consumed (kJ/mol)				
CO2 LP Compression and Cooling Work	2.70	2.73	2.22	2.24
CO2 MP, HP Compression, Cooling & Pump Work	8.00	8.08	7.94	8.12
Solvent Pump Work	3.06	5.00	2.44	4.81
Chiller Compression and Cooling Work	1.95	0.33	2.02	0.31
Recycling Compression and Cooling Work	0.30	0.41	1.00	0.28
Energy Penalty due to CO2 exiting	19.00	19.00	19.00	19.00
Energy Penalty due to H2 exiting	0.73	0.34	0.75	1.48
Net Electricity /mol of captured CO2 (kJ/mol)	35.75	35.89	35.38	36.24

Change in CO_2 Bubble Point Pressure with Temperature for PDMS-PEGDME



Enick *et al.*, "Hydrophobic polymeric solvents for the selective absorption of CO_2 from Warm Gas Stream that also contain H_2 and H_2O," CCUS Conference, Pittsburgh, PA, May 15 2013

Change in H_2 Bubble Point Pressure with Temperature for PDMS-PEGDME



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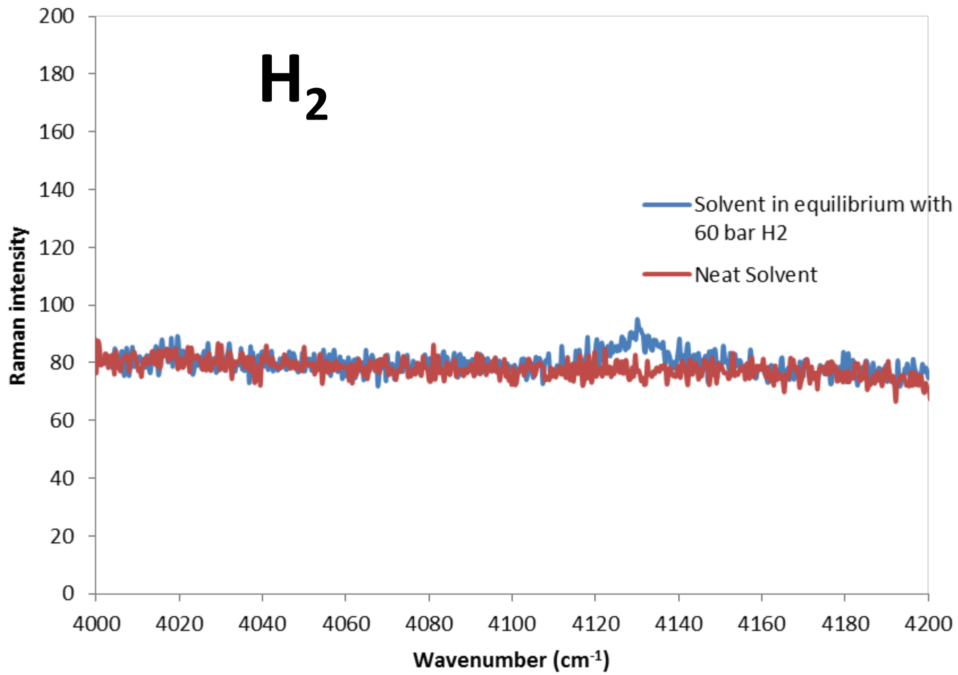
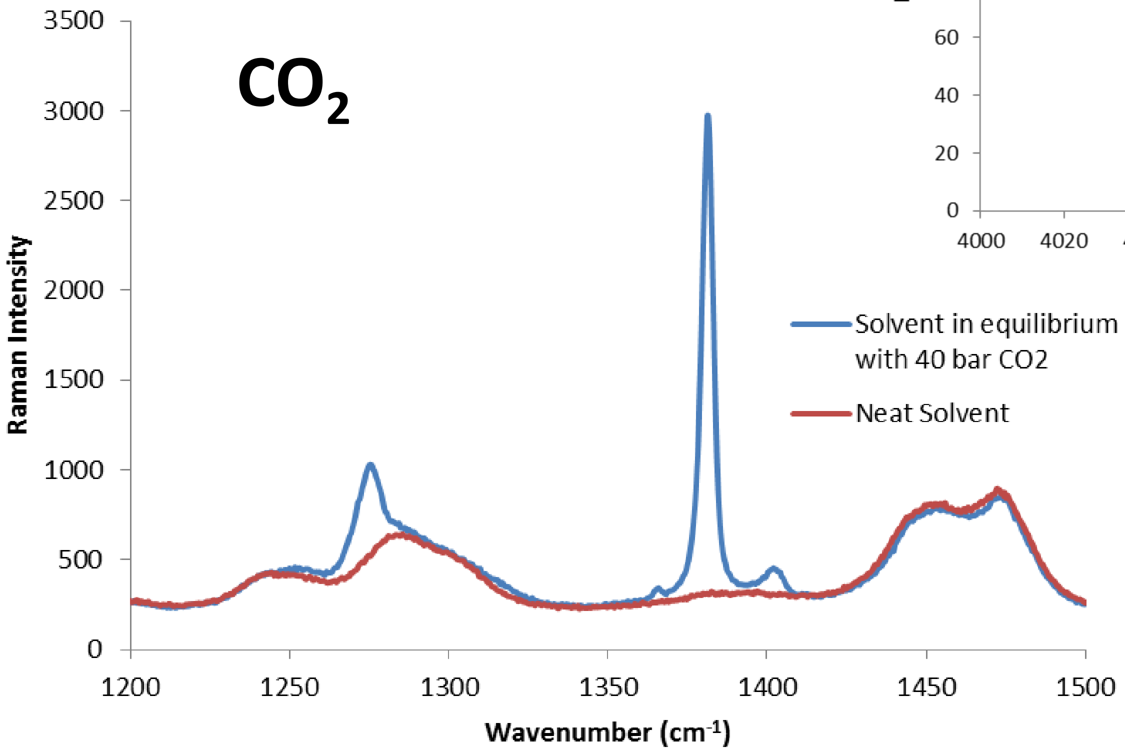
PDMS Solubility using Raman: Dr. Kitchin CMU

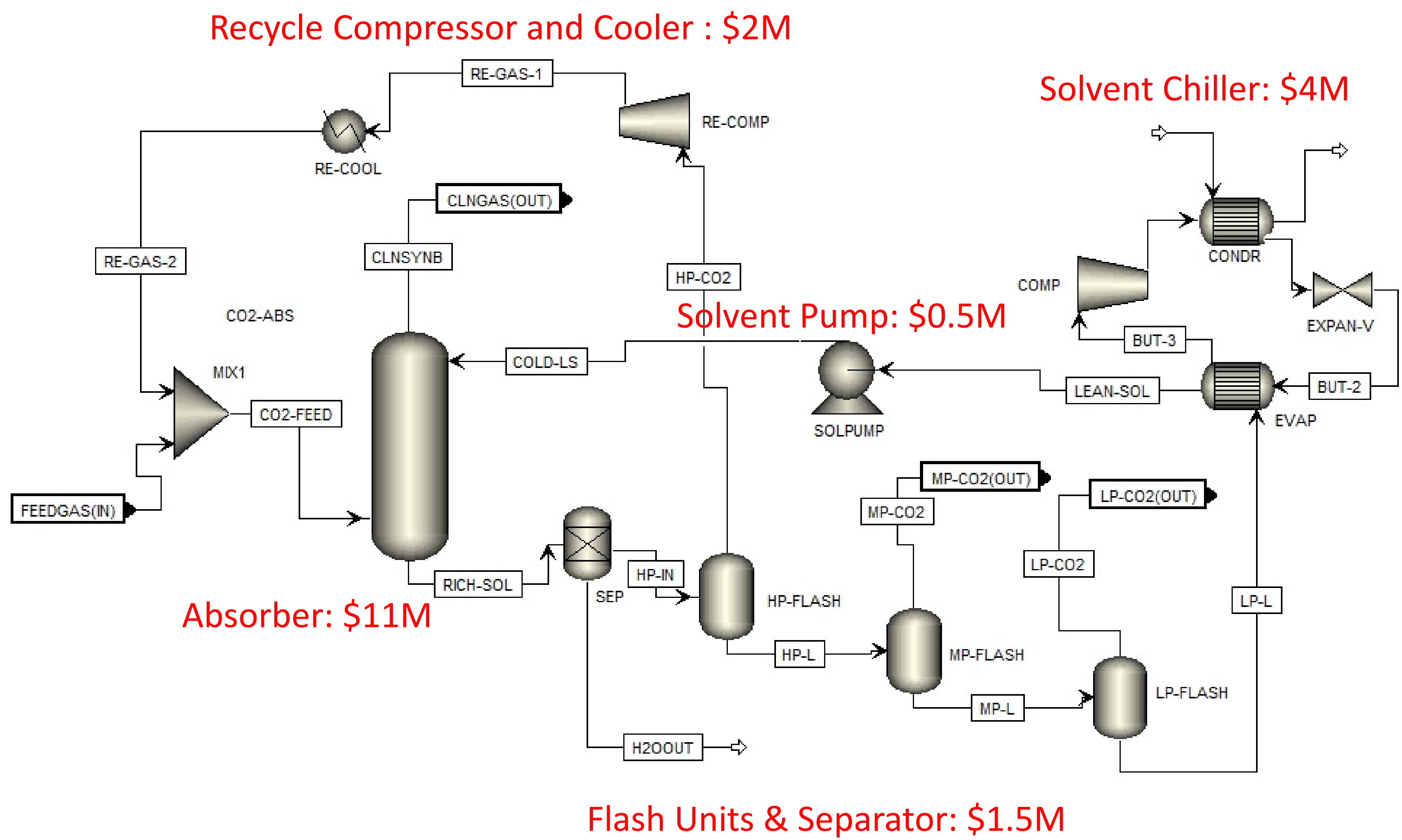
- CO_2 and H_2 Raman spectroscopy can be used to determine solubility





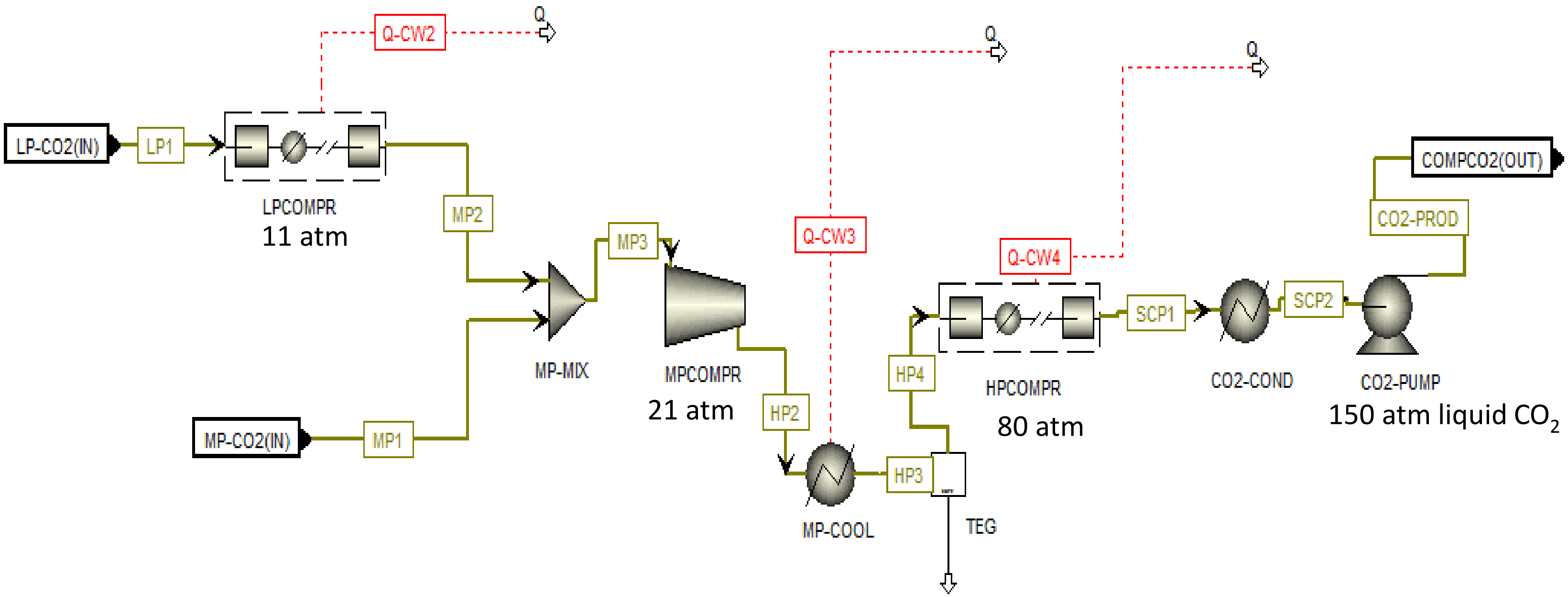
CO_2 and H_2 Raman spectroscopy can be used to determine selectivity

Bare Equipment Costs: H-PDMS



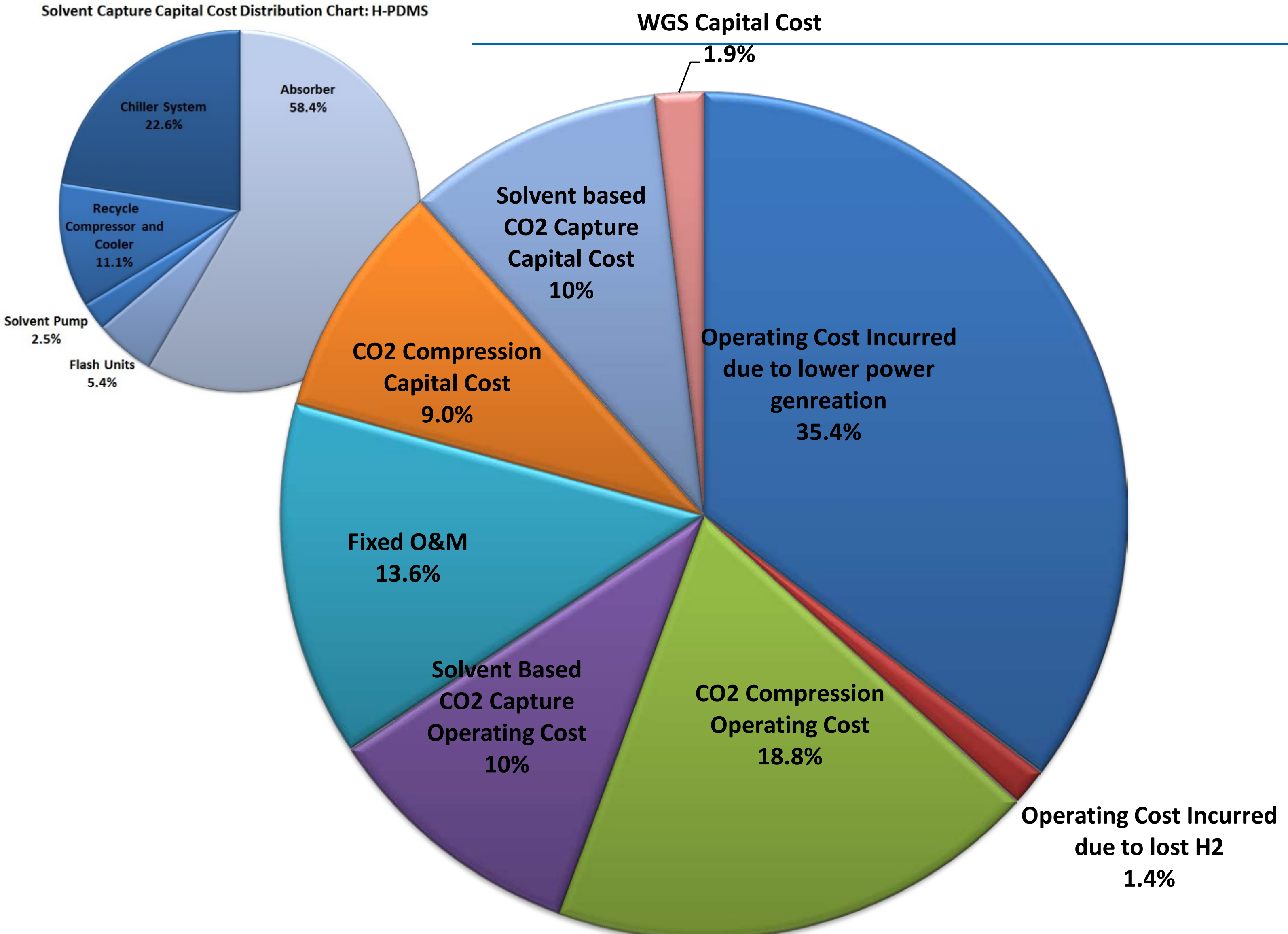
Bare Equipment Costs: CO_2 Compression Cycle

Cost of LP Compressor and Intercooler: $4.5M



Cost of MP, HP Compressors, Intercoolers and Liquid CO2 Pump: $12.7M

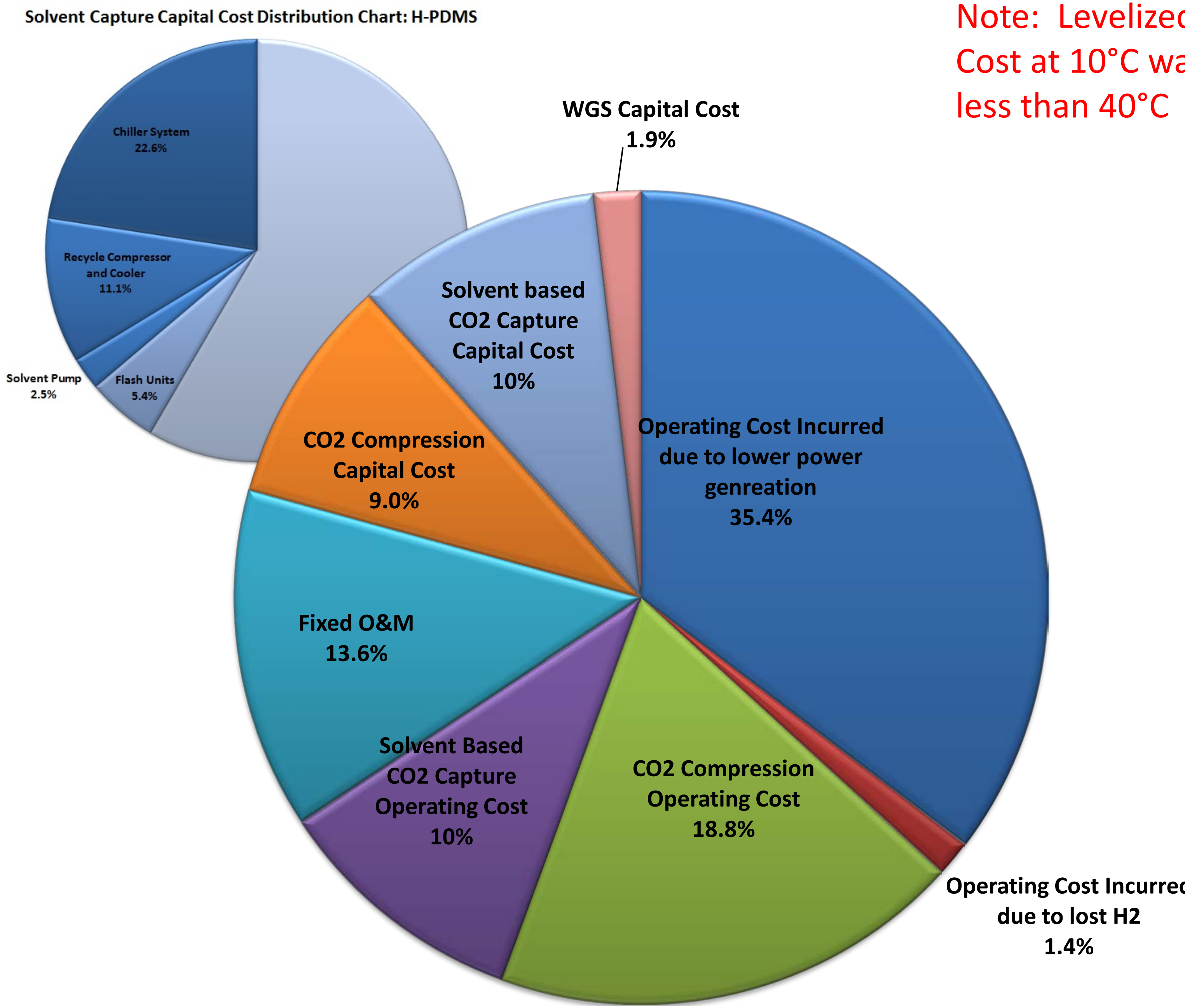
Levelized Cost Distribution Chart: H-PDMS



Levelized Cost Distribution Chart: H-PDMS

Normalized to Selexol, Levelized Cost per CO_2 Captured = 0.98 +/-0.07

Uncertainty reflects uncertainty in CO_2&H_2 Solubility as measured by different researchers

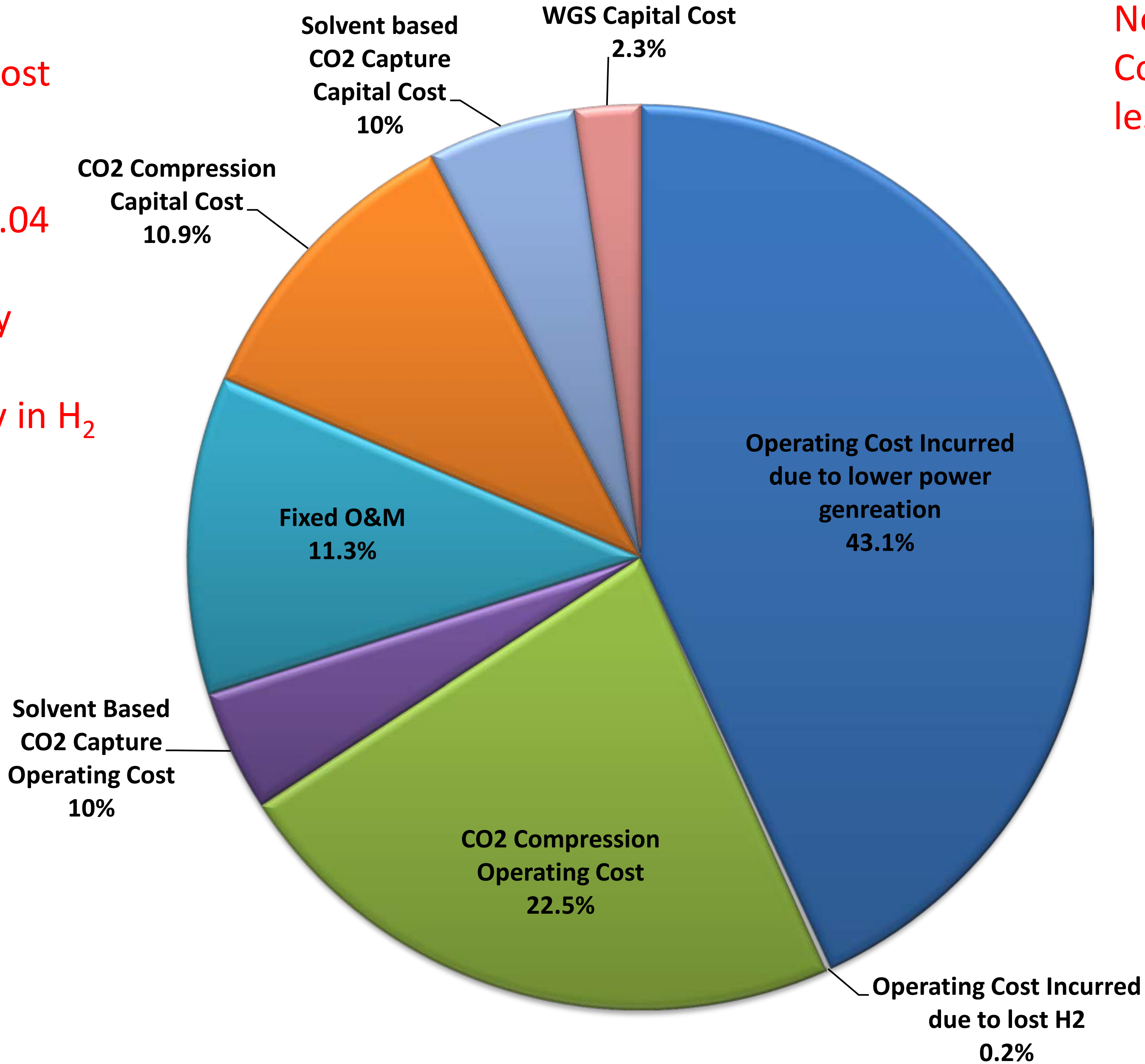


Note: Levelized Cost at 10°C was less than 40°C

Levelized Cost Distribution Chart: NETL Ionic Liquid

Normalized to Selexol, Levelized Cost per CO_2 Captured = 0.79 +/-0.04

Uncertainty reflects uncertainty in H_2 Solubility



Note: Levelized Cost at 40°C was less than 10°C