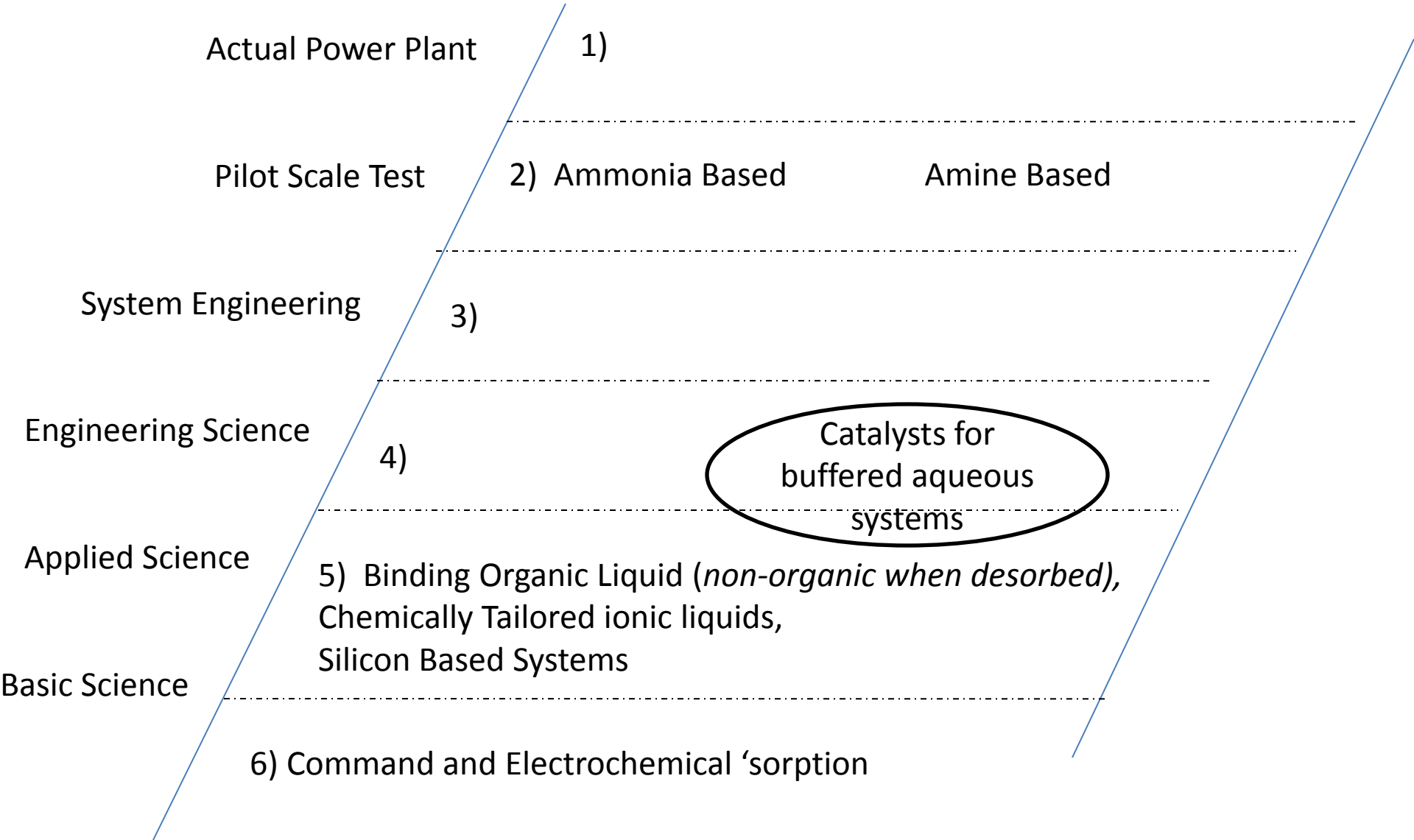
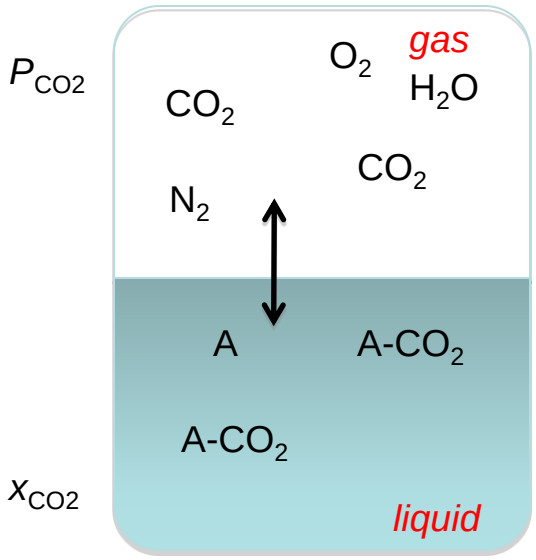
Liquid Adsorbents, Solvents stages of development

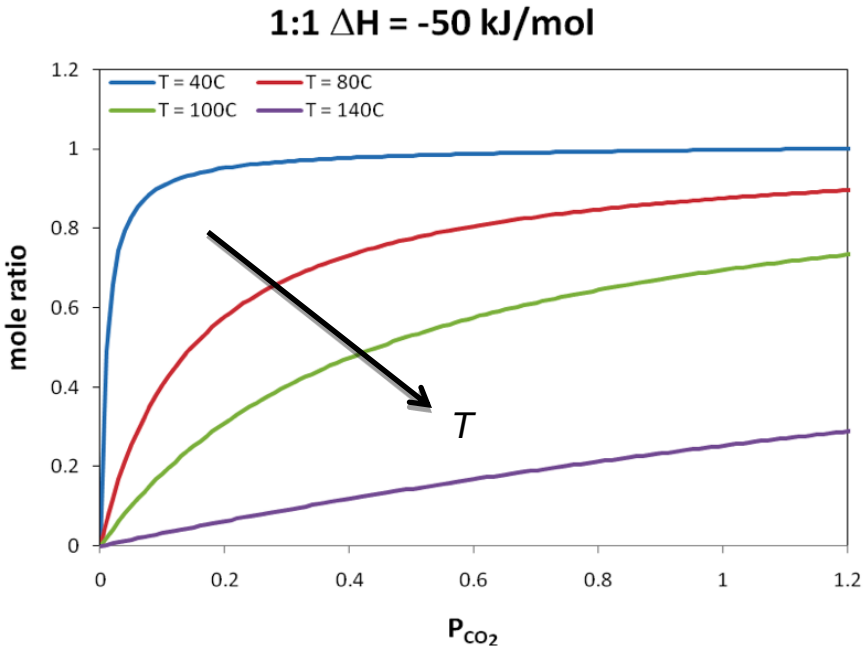


Absorption isotherms

Langmuir (single site) absorption

$$A + CO_2\,(g) \leftrightarrow A{\cdot}CO_2 \qquad K_{eq}(T)$$





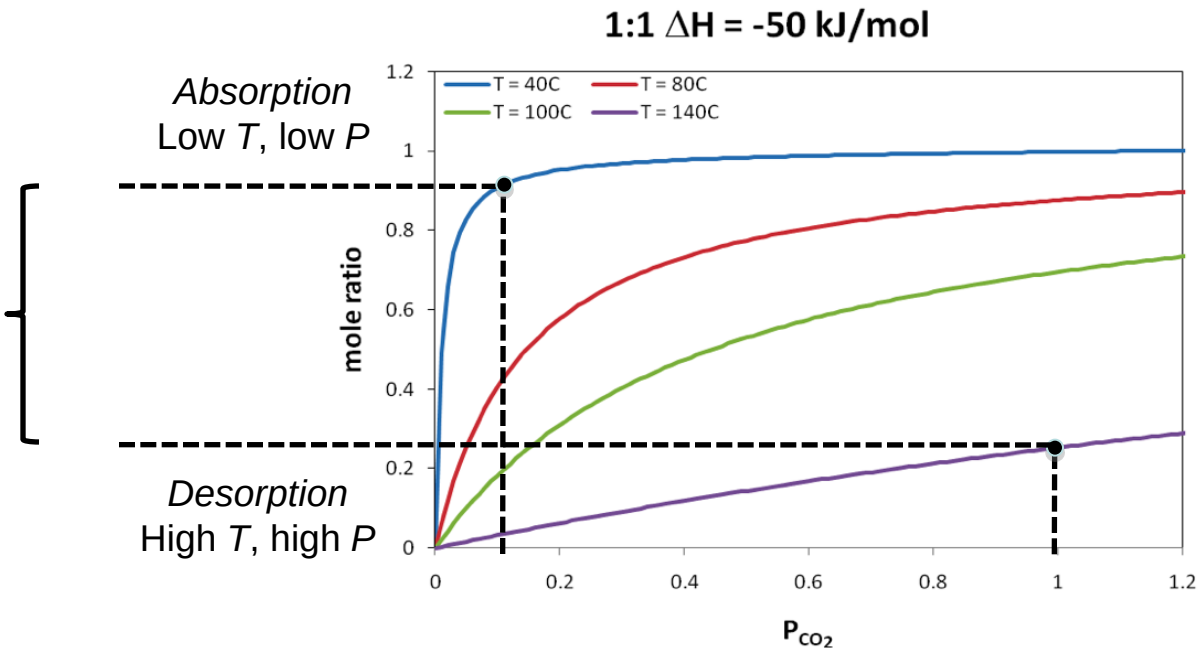
$$x_{CO_2} = \frac{KP_{CO_2}}{1 + KP_{CO_2}}, \; K = e^{-\Delta G^{\circ}/RT}$$

Carrying capacity

Langmuir (single site) absorption

$A + CO_2\ (g) \leftrightarrow A{\cdot}CO_2 \qquad K_{eq}(T)$

Carrying capacity
Mol CO_2/mol absorbent



Ideal Characteristics of an Absorbent (and adsorbent)

- 100% selectivity to Carbon Dioxide
- Low Cp
- Non-toxic
- Fast kinetics
- Fast mass transfer
- Low viscosity
- Low volatility
- Thermal stability
- Chemical Stability
- Cheap or Free

Amine Based Systems

Key Challenges

Challenge	Who?	Level
Determine if theoretical COE for system is good enough to reach DOE goal of < 35% by 2020	FE	Actual Power Plant
Reliable Pilot Scale Data	FE	Actual Power Plant
Chemical Stability of Amines (oxidation)	BES / FE	Actual Power Plant
Determine BOP impacts	FE	Actual Power Plant
Resolve question of toxic byproducts (and environmental fate)	BES	Actual Power Plant
Contactor Design at full-scale	FE	Actual Power Plant
Corrosivity	BES	Actual Power Plant

Ammonia Based Systems

Key Challenges

Challenge	Who?	Level
• Determine Parasitic Load - scale-up	FE	Actual Power Plant
• Determine VLE (vapor liquid equilibrium) at operating conditions - Modeling and actual plant data	FE	Actual Power Plant
Determine BOP (balance of power) impacts, and capture system	FE	Actual Power Plant
Integrating Waste Heat into Power Plant	FE	Actual Power Plant
Examine potential problems with slurries in chilled systems	FE	Actual Power Plant

Silicon Based Systems

Key Challenges

Challenge	Who?	Level
Understand viscosity, chemical stability, corrosion, kinetics to optimally design engineering components	BES / FE	Engineering Science
Understand continuous systems at demo scale to have real flue gas test (contaminants, conductor design)	FE	Engineering Science
Understand impact of large-scale Si usage	FE	Pilot Scale
Integrate system with power plant	FE	Pilot Scale

Chemically Tailored Ionic Liquids

Key Challenges

Challenge	Who?	Level
High quality measurements under process conditions – especially viscosity, thermal stability, mass transfer	BES / FE	Engineering Science
Understand structure property relationships -chemistry -experimental and simulation challenge -optimize selectivity	BES	Applied Science
Analytical models of Isotherms - How to characterize VLE for ionic liquids	BES	Applied Science
Synthesis of materials (inexpensive)	BES	Applied Science
Chemical Stability	BES	Applied Science
Toxicity and environmental fate	BES	Applied Science

Binding Organic Liquids

Key Challenges

Challenge	Who?	Level
Multi-Variate Optimization. Consider viscosity, interaction with water. - Cost may be an issue	BES	Engineering Science
Integration with engineering components (reactor design)	FE	Engineering Science
Many overlapping issues with Silicon Based Systems and Ionic Liquids		

Catalysts for Buffered Aqueous Systems

Key Challenges

Challenge	Who?	Level
Identify catalytic materials with favorable characteristics	BES/ FE	Applied Science
Matching appropriate catalysts to solvent	BES/FE	Applied Science
Understanding thermal and chemical stability	BES	Engineering Science
Understanding limiting equilibrium, and determine how to catalyze	BES	Basic Science
Ability to immobilize (localize) without sacrificing activity	BES/FE	Engineering Science

Command and Electrochemical Sorption

Key Challenges

Challenge	Who?	Level
Understanding of materials with science to trigger adsorption / desorption of CO2	BES	Applied Science
Identify properties that these materials should have -Energy to desorb CO2 with no other thermal or physical energy required -- high mass density to absorb CO2	BES	Applied Science
Understand selectivity, stability, toxicity, and other thermo / physical characteristics	BES/FE	Engineering Science
Integration with plant: electric work instead of steam	FE	Systems Engineering
Scalability, reactor design	FE	Systems Engineering

Crosscutting Themes

- Ability to measure and understand key thermodynamic, chemical, structural characteristics
- Understanding what is limiting equilibrium, and how to catalyze
- Understanding and integrating with continuous system at demo scale (contaminants, corrosion, reactor design)
- Material cost and impact (lifecycle) for scale-up
- Impact on scale-up (degradation)
- Determine impacts on balance of plant and capture system
- Optimization algorithms and methods for complex plants

Opportunity for BES / FE Collaboration

- Going from atoms and molecules to thermodynamic design and functions.