Information for New Graduate Students
Fall 2012

# *Engineering and Chemistry for Sustainable Technology*

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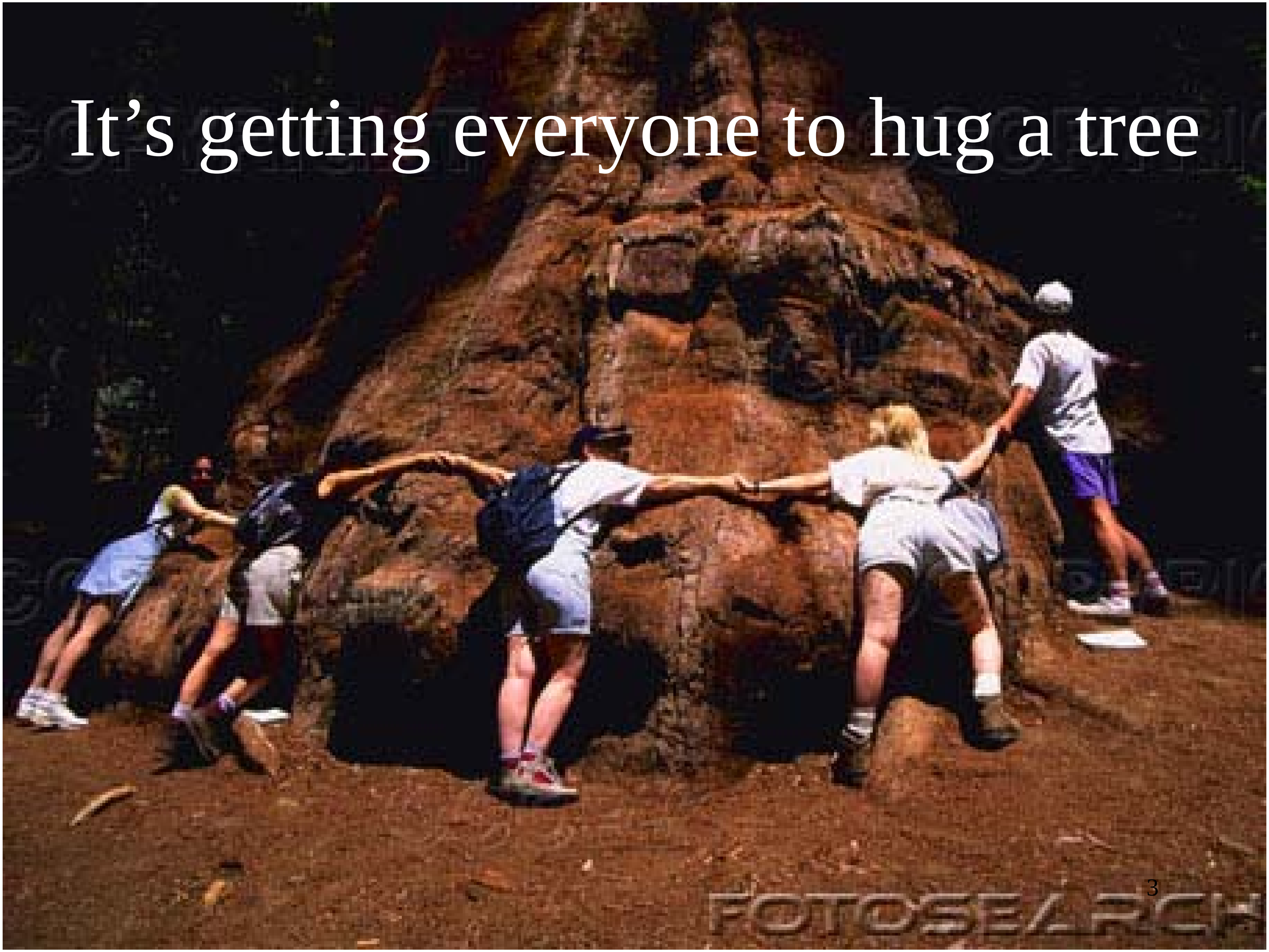
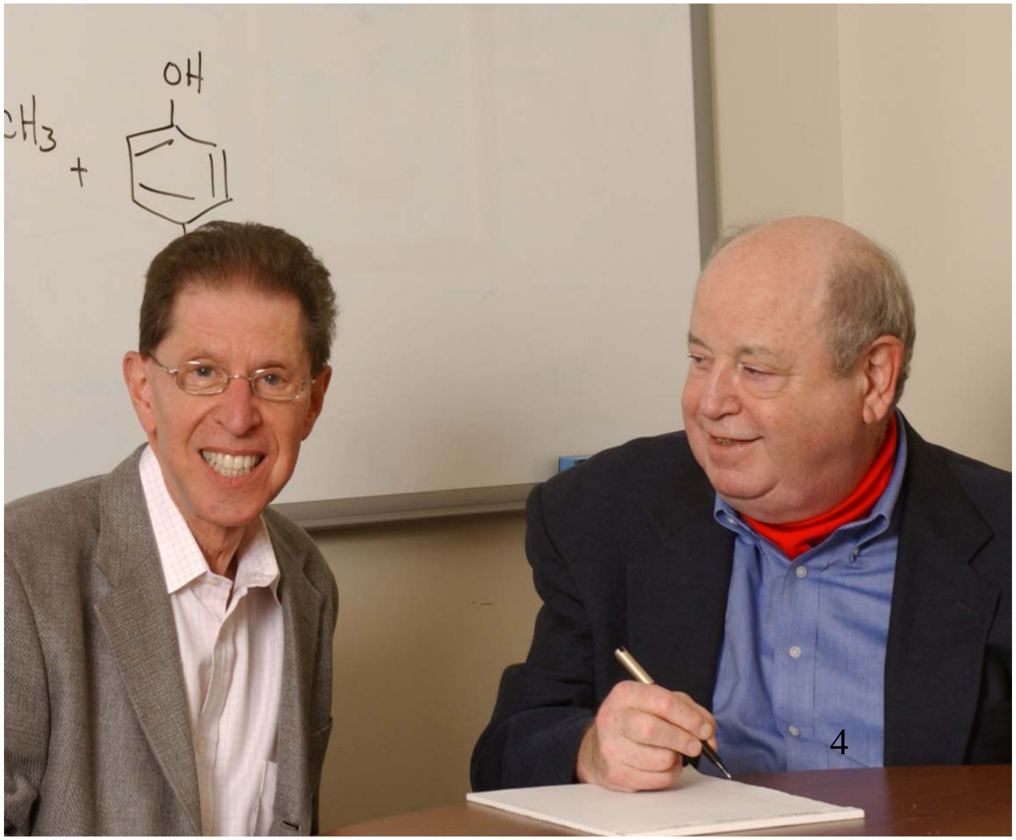
"Sustainable" is not just hugging a tree…

# It’s getting everyone to hug a tree



# *Chemical Engineering and Chemistry 23-Year Collaboration*

- Jointly Directed PhD Students
  - ✓50 Completed
  - ✓12 In Progress
- ~50 Joint Research Grants
- ~250 Publications and Presentations
- 2004 Presidential Green Chemistry Challenge Award



# *Current Group – ChEs and Chemists*

- Students – All Co-Advised
  - ✓ PhD Candidates: Emily Nixon, Kyle Flack, Will Heaner, Mike Mojica, Amy Rohan, Jackson Switzer, Wilmarie Medina, Chris Butch, Amber Rumple, Imani Jones, Mark Conley, Wes Woodham.
  - ✓ Undergraduates (8 at present)
- Staff
  - ✓ Senior Scientists and Postdoctorals – Pamela Pollet, Beth Cope, Rani Jha, Elizabeth Biddinger, Steve Saunders, Andrea Song
  - ✓ Coordinator, Deborah Babykin
- Other Collaborators
  - ✓ Other GT Students and Faculty
  - ✓ Students and Faculty at Other Universities
  - ✓ Industry Partners

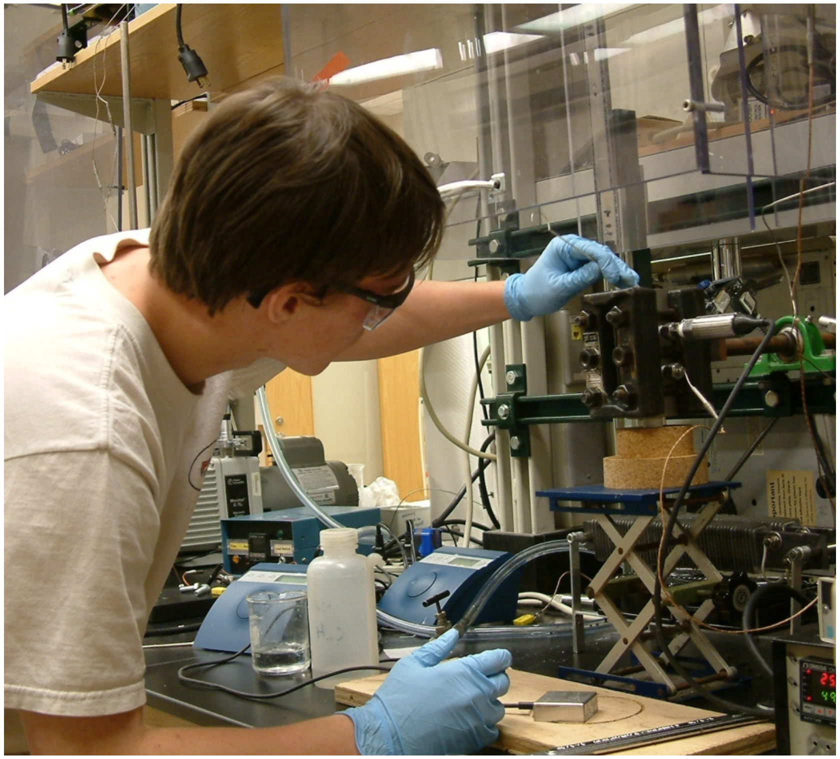
# *We Work Together*

- Each Problem Has a Team
  - ✓Multilevel, Multidisciplinary
- Each Person Is on Multiple Teams
- Advantages
  - ✓Not All Problems Are Four Years
  - ✓Facilitates Communications
  - ✓Able to Do High Risk, High Return Research

Michelle Kassner, PhD ChBE, 2008, Chevron; Tori Blausucci, PhD ChBE. 2009. ExxonMobil

# *What Do We Do – and Why?*

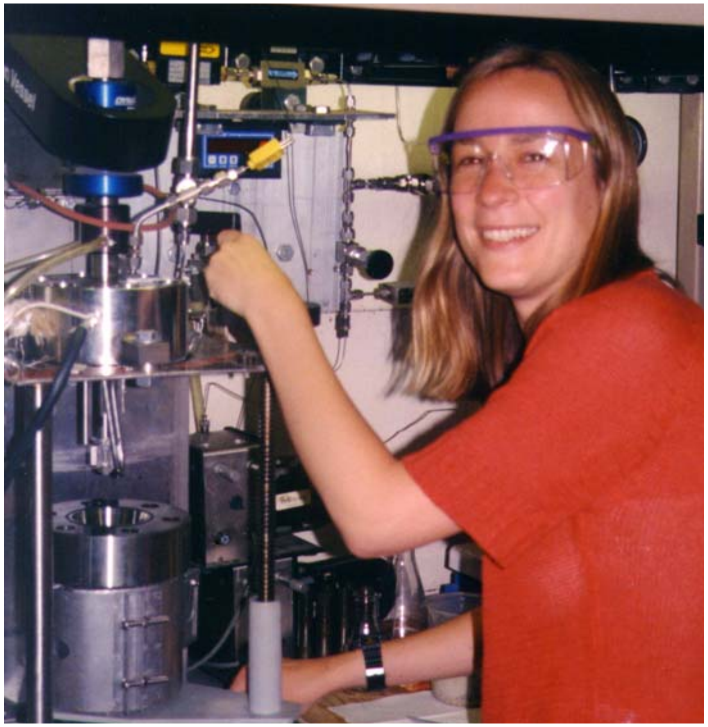
- Tunable Solvents
  - ✓Supercritcal Fluids
  - ✓Nearcritical Fluids
  - ✓Gas Expanded Fluids
- Smart Solvents
- Advantages
  - ✓Benign
  - ✓Better Transport Properties
  - ✓Faclile Downstream Processing



Ryan Hart, PhD, ChBE, 2010, Exponent

# *Examples of Sustainable Technology*

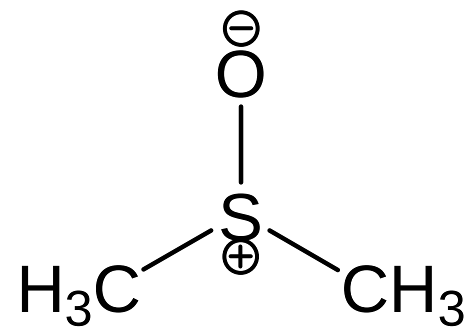
- Goals
  - ✓Environmentally Benign
  - ✓Cost-Effective
- Energy Applications
  - ✓$CO_2$ Recovery from Flue Gas
  - ✓Benign Harvesting of Sands and Oil Shale
- Green Pharmaceuticals
  - ✓Continuous Reactions for Pharma
  - ✓Benign Reactions in Nearcritical Water
  - ✓Coupling Reaction + Separations
    - ❖Homogeneous Catalyst Recycle



Heather Patrick, PhD ChBE, 2000, Emory University

# *Example: Smart Solvent Replacement for Supersolvent -- DMSO*

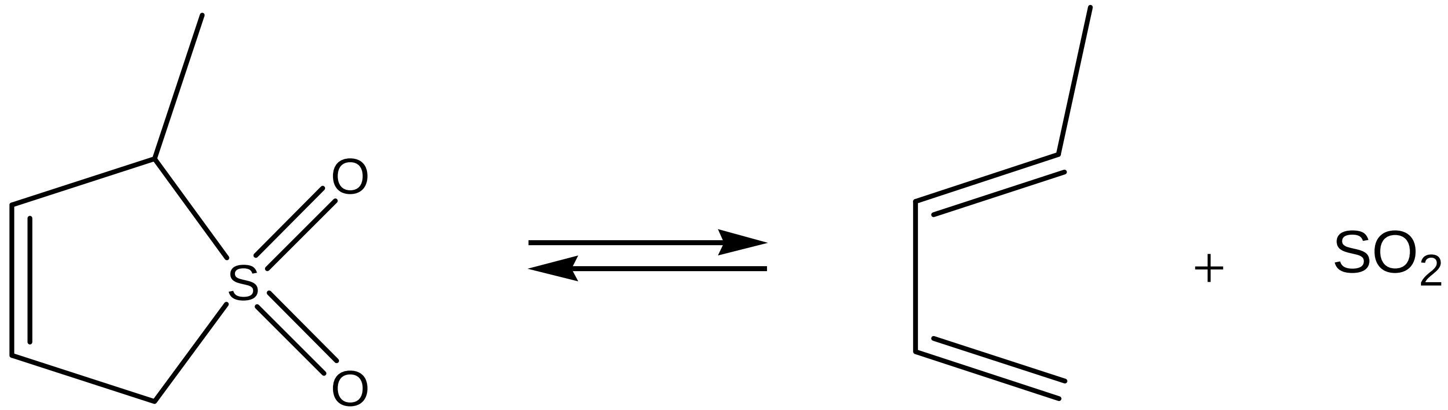
- Product Isolation from DMSO
  - ✓ Add water, precipitate
  - ✓ Extract with another organic
- Problems with DMSO Removal
  - ✓ Isolation is product dependent.
  - ✓ Contaminated aqueous waste
  - ✓ No solvent recycling
- Smart Solvent – Changes Properties on Command
  - ✓ As good as DMSO
  - ✓ Decomposes into Volatile Fragments on Command
  - ✓ Easy to Remove
  - ✓ Can be Reformed and Recycled Later




***Dimethyl sulfoxide***

# *DMSO-like Solvent Has “Built-In” Recycle*

## *Pipyrlene Sulfone*

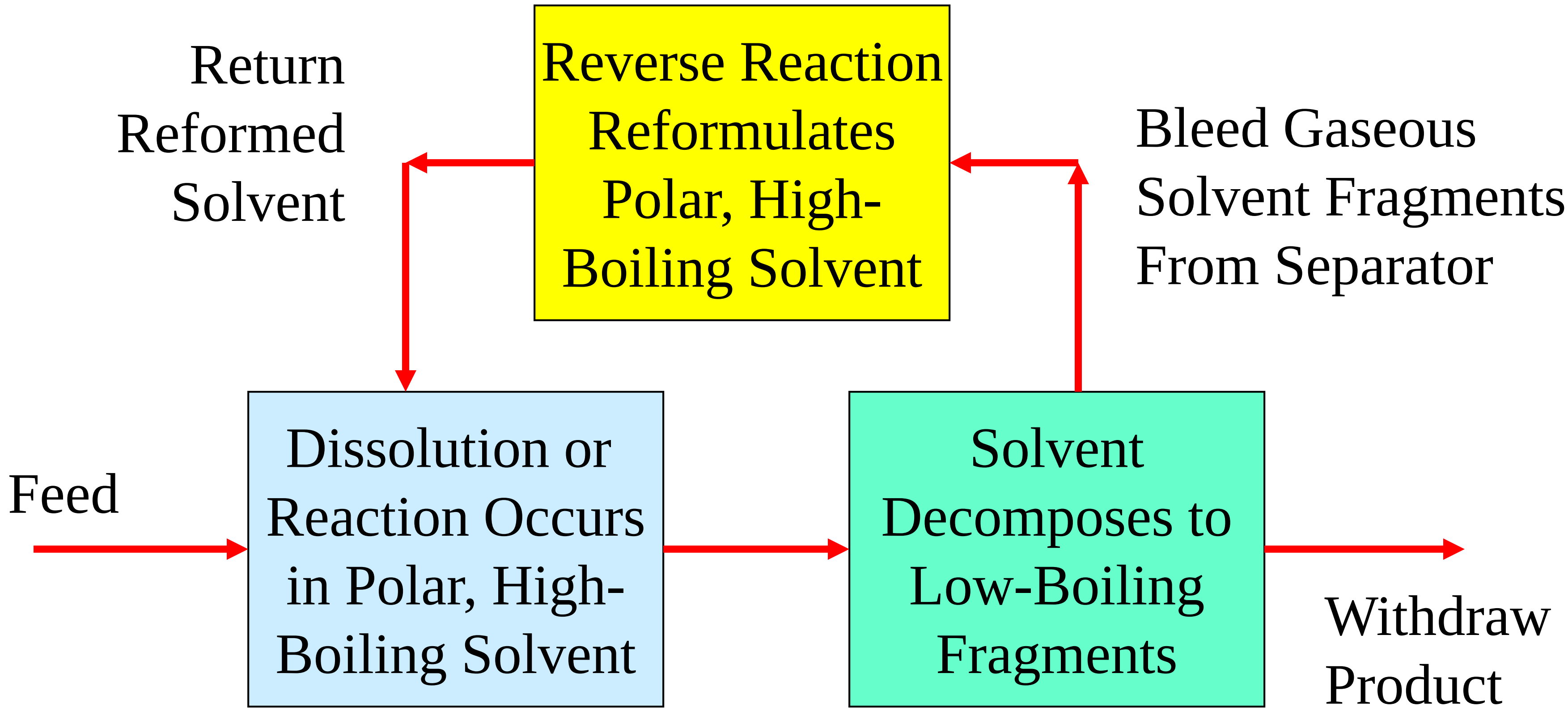



m.p. = –12 °C

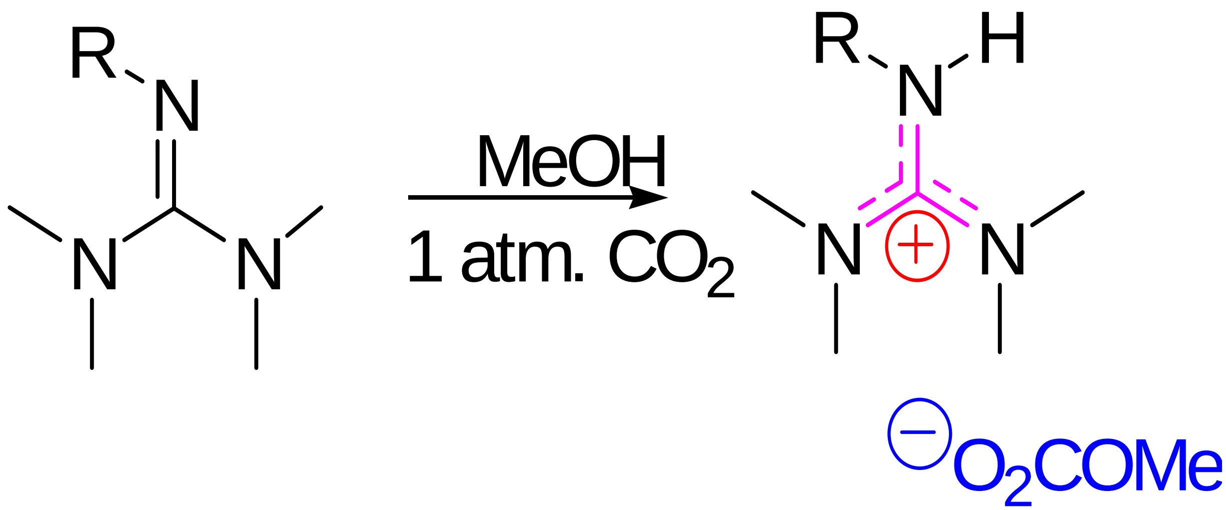
b.p. = 42 °C -10 °C

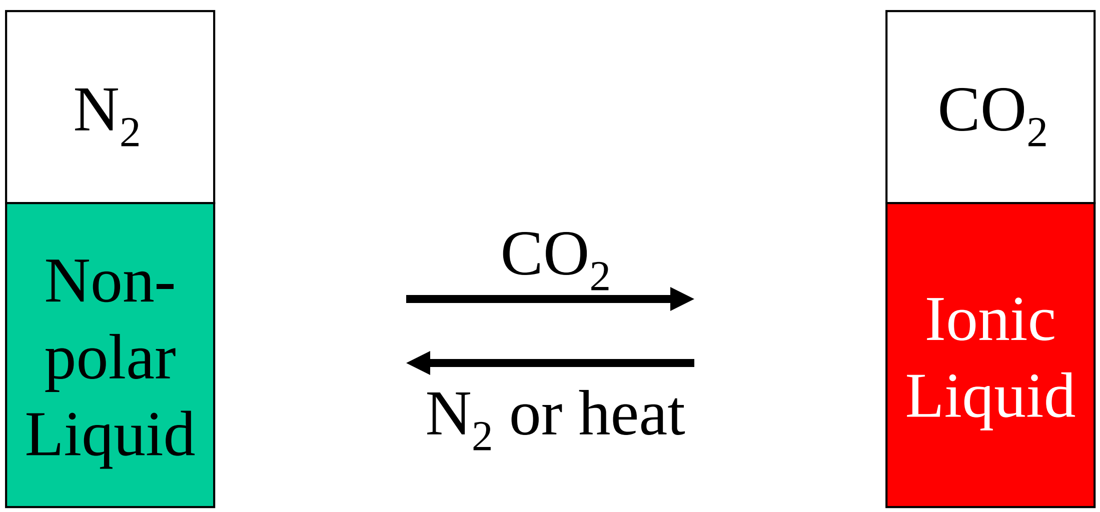
- Solvent Properties Comparable to DMSO
- T-Based Switch, Decomposition ~110°C
- Reaction is Reversible
- Equilibrium and Rates Are Good

# *Potential Process Cycle*
# *Extraction or Reaction with Smart Solvent*

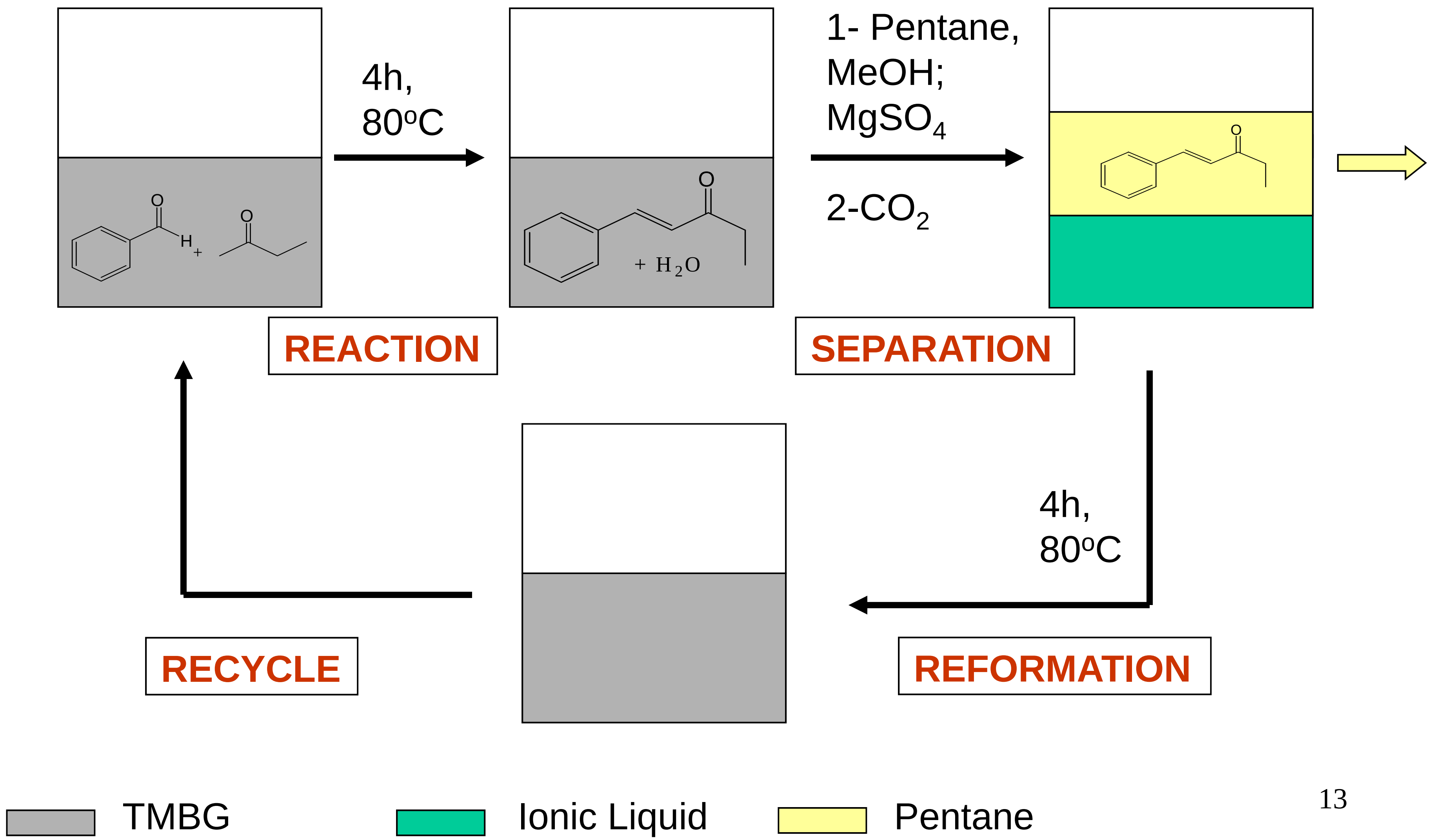


# *Example: Reversible Ionic Liquids*
# *$CO_2$ Switch, Reverse by Heat*

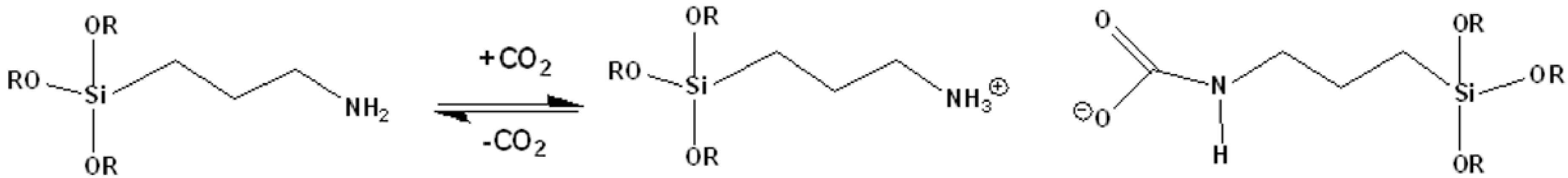


# *Process: Claisen-Schmidt Reaction and Separation Using Reversible Ionic Liquid*



# *$CO_2$ Recovery from Power Plants Using Single-Component Silyl RevILs*

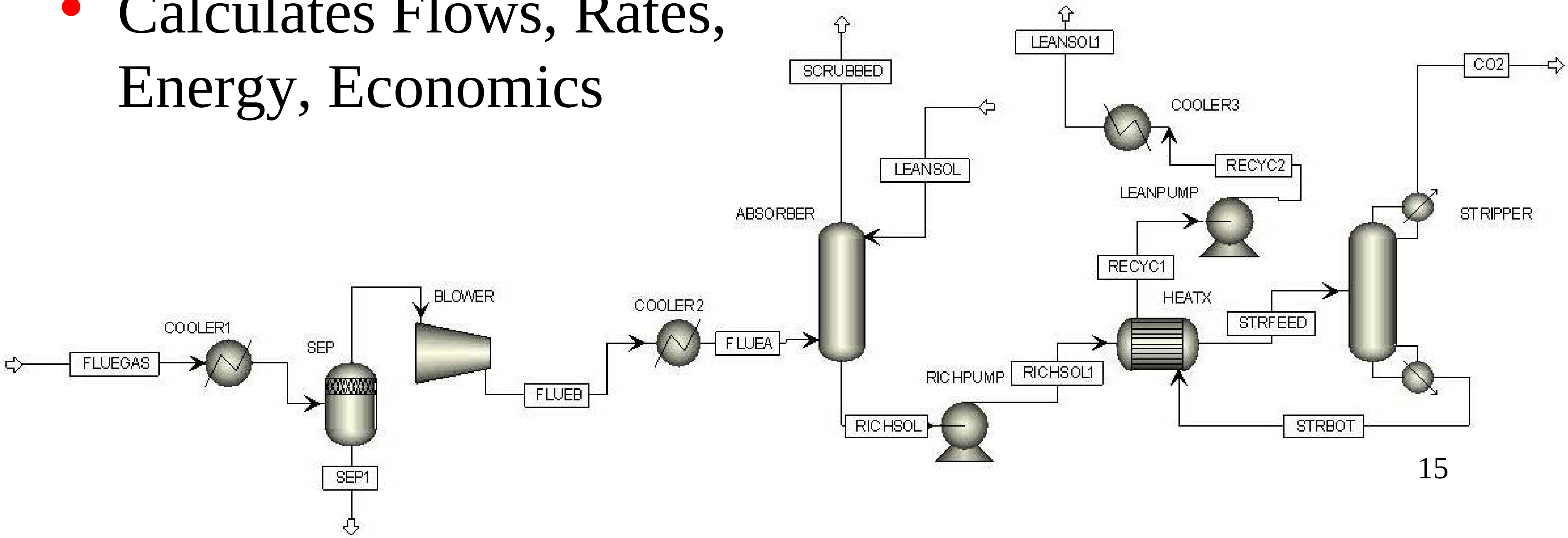



- Dual Mechanism Solvent Absorption
  - ✓Chemical Absorption
    - ❖By Reaction of $CO_2$ with RevILs
  - ✓Physical Absorption
    - ❖By Dissolution of $CO_2$ in RevILs
- Increases Capacity
  - ✓Better Separation with Less Energy Penalty

# *ASPEN Flow Sheet*

- Industry Standard Design Software
- Permits Process Alternatives, Optimization
- Calculates Flows, Rates, Energy, Economics

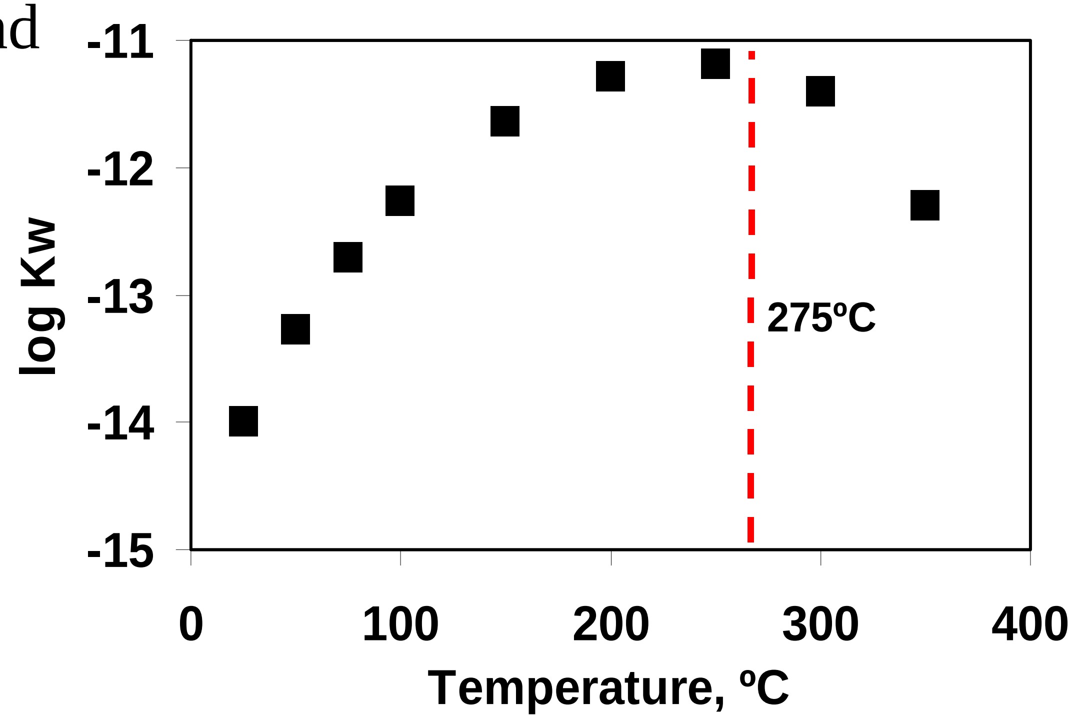
| | **Simulation Results** $ per ton of $CO_2$ removed |
|---|---|
| Fixed Costs | 4.50 |
| Regeneration Energy (Steam) | 3.61 |
| Electricity | 4.06 |
| Cooling Water | 0.87 |
| Materials | 2.16 |
| **Total** | 15.20 |



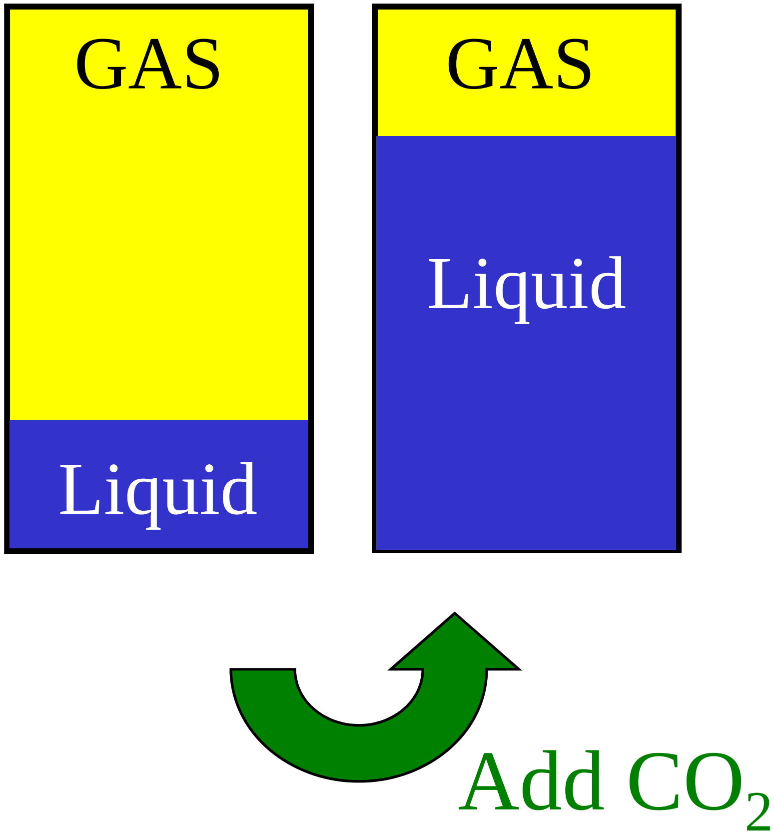
# *Nearcritical Water: A Benign Solvent*

- Research Partner: Lilly
- Water at 250-350º C
  - ✓ Like Acetone
  - ✓ Dissolves both Salts and Organics
- Natural Acid (Base)
  - ✓ Catalyzes Reactions
  - ✓ Eliminates Waste
- Facile Processing
  - ✓ Homogeneous Reactions
  - ✓ Separation by Cooling

$$H_2O \xleftrightarrow{K_W} H^+ + OH^-$$



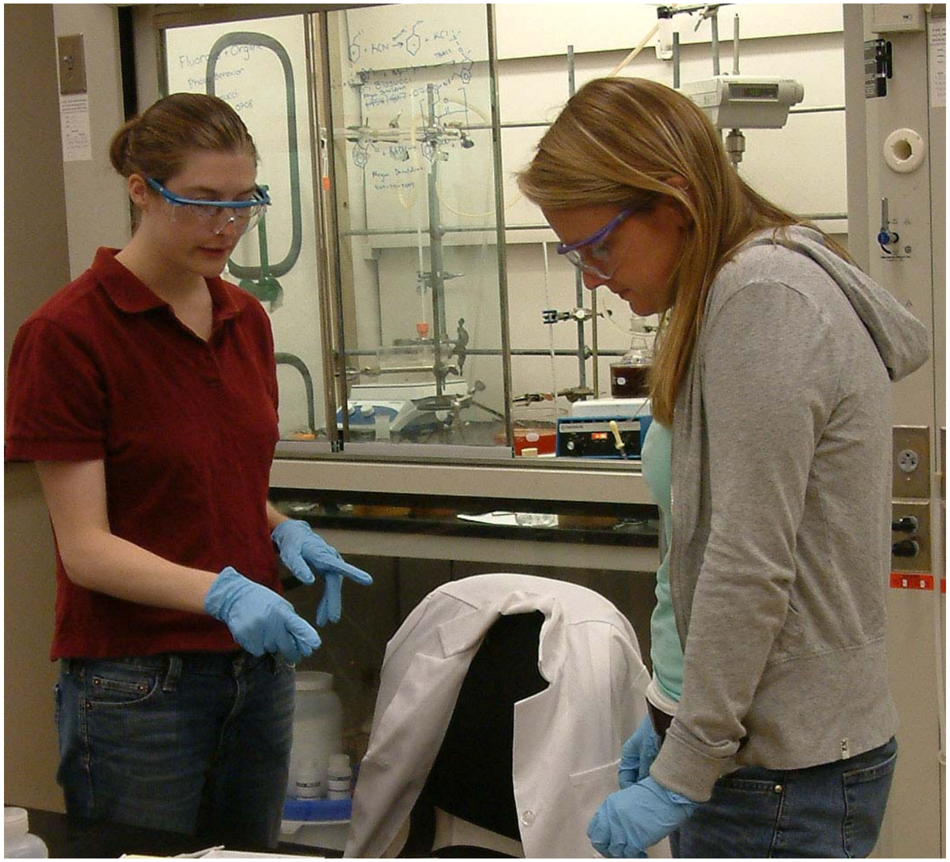
# *Gas-Expanded Liquids (GXLs)* *Tunable Organic-$CO_2$ Mixtures*




- Good Organic Solvents Miscible with $CO_2$
- Solubility is Pressure Tunable
- Solvent properties are pressure tunable
- Separation by Depressurization

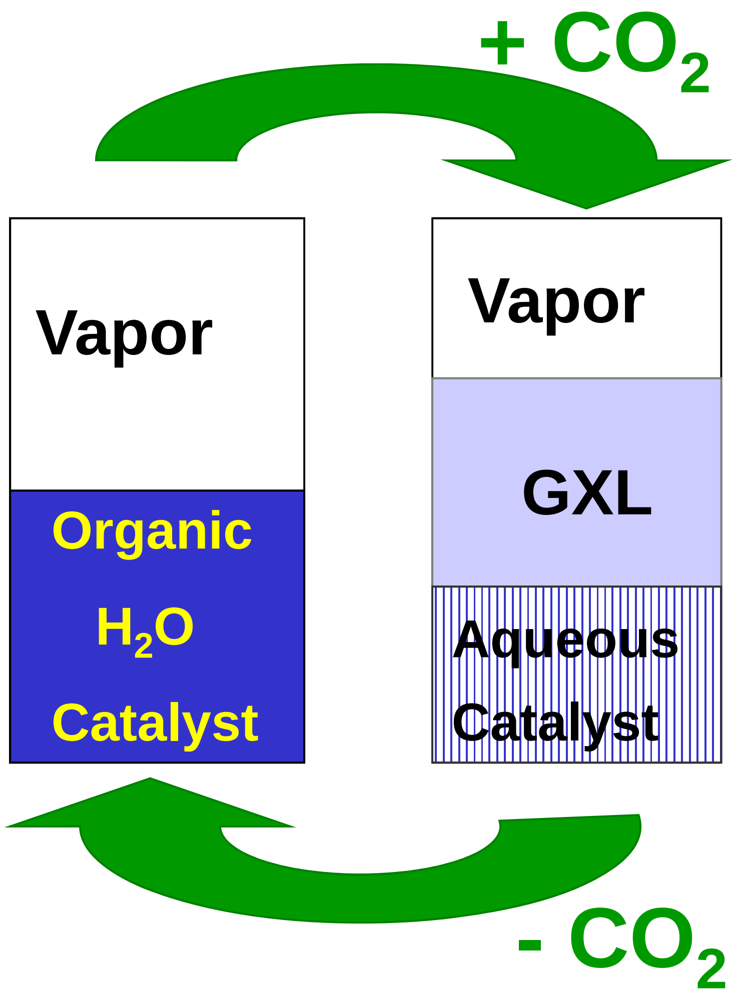
# *Homogeneous Catalyst Recycle with GXLs*

- Homogeneous Catalysts
  - ✓ Selectivity, Rates
  - ✓ Asymmetric Synthesis
  - ✓ Difficult to Reuse
- Paradigm
  - ✓ Homogeneous Reaction
  - ✓ Change Phase Behavior for Separation
- “Designer” Solvents
- “Designer” Catalysts



Megan Donaldson, PhD ChBE 2008, Dow;
Nicole Hess, BS ChBE 2008, Berkeley

# *$CO_2$ Induced Immiscibility:*
## *Organic Aqueous Tunable Solvents (OATS)*




- Homogeneous Reaction
  - ✓Organic/Aqueous Solution
  - ✓Ambient Pressure
- $CO_2$ Induces Phase Split
- GXL Poor Solvent for
  - ✓Ionic Catalysts
  - ✓Enzymes
- Decant, Depressurize
  - ✓Catalyst Recycle
  - ✓Product Purification

# *OATS for Biocatalytic Synthesis and Purification of Hydrophobic Drugs*

- Enantioselective Biocatalysis
  - ✓ Water Insoluble Substrates
  - ✓ Facile Product Isolation and Catalyst Recycle
- OATS Mixture
  - ✓ Benign Alternative for Organics
  - ✓ Higher Enantioselectivity
  - ✓ Higher Efficiency
  - ✓ Higher Stability of Enzymes
  - ✓ Facile Purification of Pharmaceuticals

James Brown, PhD, ChBE, 2000, ExxonMobil; Jason Hallett, PhD, ChBE, 2002, Imperial College, London

# *Typical Projects: Recent Grants*

- NSF, Application of Reversible Ionic Liquids
  - ✓ Coupling Reactions and Separations
- AMPAC, Many Topics
  - ✓ Novel Routes to Pharma
  - ✓ Specialty Chemicals
  - ✓ Flow Reactors
  - ✓ Heterogeneous Catalysis
- NSF, Corning
  - ✓ Flow Reactors for Pharma
- Lilly, Applications to Pharmaceuticals
  - ✓ DMSO Substitute
  - ✓ Reactions in NCW
- DOE and ConocoPhillips, $CO_2$ Capture
  - ✓ Single-Component Reversible Ionic Liquids
  - ✓ Silylation
  - ✓ Molecular Design
- PRF, Smart Solvents for Nanoparticles
- Dow, Polymers
  - ✓ PVC Reactions
- Dow, Smart Solvents
  - ✓ Gas-Expanded Liquids for Pharma
  - ✓ Catalyst Recovery and Recycle
  - ✓ Recylable DMSO Replacement
  - ✓ Phase Transfer Catalysis

# *Finishing the Degree*

- Interviewing -- A full-time job
- Connections and Recommendations
- Average time for PhD = 4.3 years
- Typical Pattern
  - ✓ ~1/3 Academic Employment
  - ✓ ~2/3 Industrial Employment


Greg Marus, PhD ChBE 2011, Albemarle

# *Recent PhDs from Research Group*

## *In Chemistry and Chemical Engineering*

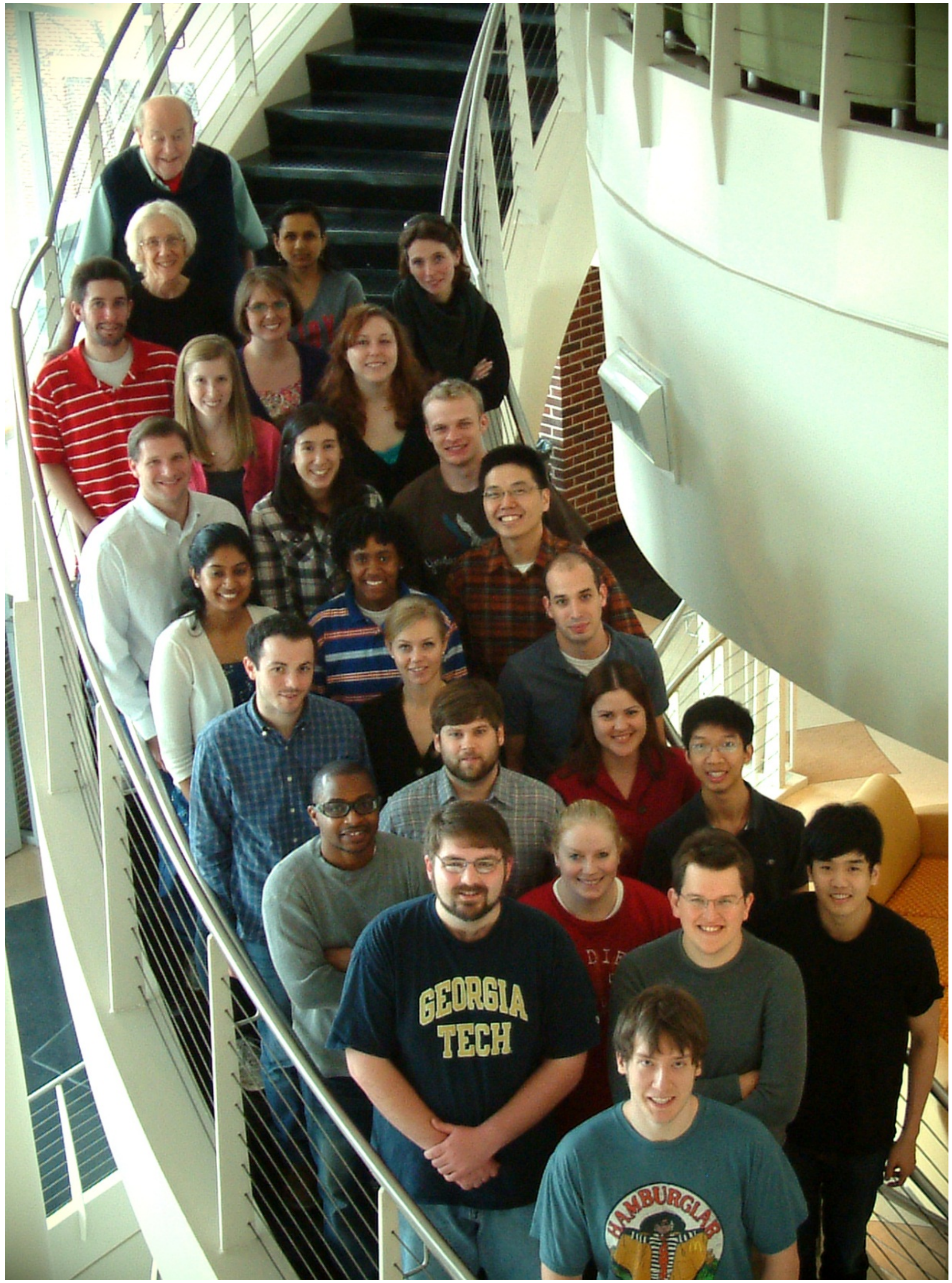
- 2007
  - ✓ Charu Panday, SW Research
  - ✓ Susanta Samanta, Milliken
  - ✓ Liz Hill, Rohm & Haas
  - ✓ Laura Draucker, EPA
  - ✓ Ejae John, U. Trinidad
  - ✓ Jack Ford, U. Kansas
- 2008
  - ✓ John Gohres – Evonik
  - ✓ Megan Donaldson – Dow
  - ✓ Reagan Charney – Law Firm
  - ✓ Michelle Kassner – Chevron
- 2009
  - ✓ Tori Blasucci – ExxonMobil
  - ✓ Kristin Kitagawa – BASF
- 2010
  - ✓ Hillary Huttenhower – Pratt and Whitney
  - ✓ Ryan Hart -- Exponent
  - ✓ Ali Fadhel – GE
- 2011
  - ✓ Greg Marus -- Albemarle

# *Decision Process – Pick a Group*

- Research Goals
  - ✓Education
  - ✓Satisfaction
  - ✓Personal Growth
- You Should Seek
  - ✓Enthusiasm
  - ✓Motivation
  - ✓Creativity
- We Seek
  - ✓Molecular Viewpoint
    - ❖Heavy on Chemistry
  - ✓Teamwork
    - ❖Multidisciplinary Approach
  - ✓PhD degree
  - ✓Experiment + Modeling
  - ✓Enthusiasm, Motivation, and Creativity

# *If You Might Be Interested in Joining Us*

- Talk to the Professors
  - ✓Chuck Eckert, 2206 ES&T, 4-7070
    - ❖Coordinator, Deborah Babykin, 2301 ES&T, 4-3690
  - ✓Charlie Liotta, 2201B MS&E, 5-3111
    - ❖Coordinator, Michele Yeager, 2201C MS&E , 4-8222
- Talk to the Students
  - ✓All in the NW Wing, Level 2, ES&T
  - ✓Go in any office and ask for a tour
- Come to our Group Meetings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