# WORKSHOP RESULTS

## Introduction

The following pages are a transcription of the brainstorming sessions that took place during the "Barriers to Ionic Liquid Commercialization" workshop. The workshop began with an effort to capture the personal objectives (below) of all the participants, so that workshop planners could determine how well those objectives were met. The pages thereafter reflect the results of each breakout session; two process sessions: separations and catalysis, and three product sessions: bulk chemicals, fuel production, and polymers. As a result of the nature of the breakout sessions, the ideas captured here may not be in complete sentences or may not always be clear outside the context of the discussion that took place within the session itself. The ideas here are also repetitive, showing the crosscutting nature of many of the barriers to ionic liquid commercialization and the need for integrated approaches in addressing these barriers.

### Objectives of Workshop Participants

- Meet contacts with similar interests for joint development of new projects
- Determine new direction of field
- To define which industrial processes we are trying to replace and why, e.g., formation of isooctane – the industry would like to get away from HF as the catalyst
- Development of task specific ionic liquids
- Missing information about availability of products for different applications
- Discussion about price of ionic liquids for a new technology – without discussion about advantages!
- Get a better feeling about the commercial interest in ionic liquids in the USA industry
- To understand the "true" barriers for commercialization
- Industry identified technology development based on the "expert" research groups
- Define and prioritize research topics to enhance value and expand the knowledge of the science of ionic liquids to accelerate commercial implementation
- Identify potential business partners to collaborate on commercialization of ionic liquid process or technology
- Industrial collaboration/input to help move discoveries to commercialization
- I want to know what industries need that ionic liquids can do – better yet, how I can contribute within the context of my specialty (making new ionic liquids).
- Prioritize R&D activity for ionic liquid research related to commercialization
- Contacts for further development (collaborative) of ionic liquids in industrial applications
- Get to know some of the people active in the field of ionic liquids
- Share knowledge and expertise
- List of key barriers and list of key players to overcome the barriers
- I would like to learn how serious different companies are about developing ionic liquids and the associated technologies. What role can academics play, and will there be financial support?
- Strategies for new material development

- To learn more from industrial partners about their concerns and needs in relation to room temperature ionic liquids
- Definition/ID of path forward for lifetime evaluation of ionic liquids, i.e. will they survive repeated regenerations?
- I want to know and discuss what the barriers to commercialization are
- Improve my familiarity with some of the companies and people associated with ionic liquids at the commercial (industrial) level
- To bring together diverse views/experience on ionic liquids and identify opportunities to move forward
- Define the parameters limiting the use of ionic liquids in the future
- Obtain a sufficient level of education in the ionic liquids field to go back to my corporate headquarters with recommendations/action items
- Contribute industrial perspective to break out sessions
- I would like to have an idea of the highest potential areas for collaborative research in ionic liquids
- Find out where the ionic liquid areas of opportunities are and see how far away we are from a real application

## Separations Barriers

What are the Barriers to the Commercial Use of Ionic Liquids in Separation Processes?
(The number of votes is shown in ())

Process Design (1)
- Process design for ionic liquid separations has not been designed, optimized or demonstrated under industrial conditions

Lifetime Recycle (9)
- Long-term stability unknown (1000's of cycles?)
- Worry about how many times I can reuse ionic liquids
- Lack of process engineering info on long-term performance with recycle, reuse
- Insufficient chemical stability under long-term real-life conditions

Real Process Feed (1)
- Sensitivity to trace impurities unknown (e.g.: SOx, NOx,)
- Lack of data on "real" feeds under "real" process conditions

Health, Safety, & Environment (4)
- Toxicity of ionic liquids and potential breakdown products are not well understood
- Lack of information on toxicity and environmental impact of ionic liquids
- Toxicity issues/residuals
- Recycle
- Unknown toxicity data
- Environmental issues (2)
- Toxicity data not available

Cost (5)
- Cost (1)
- Cost
- Lack of economic analyses by process engineering groups for industrial decision making: capital costs, operating costs, feedstock reduction costs (1)
- Cost
- Precursor cost/availability (intrinsic)
- Precursors (inputs) to ionic liquids are too expensive to be solvents, therefore ionic liquids will be too expensive
- Timeframe to scale is a barrier
- Costs too high
- Engineering evaluations missing
- Cost of IL: risk of $ loss (working capital too high)
- Supplier Perspective - Sufficient ROI (return on investment?) not probable
- Toxic Substances Control Act (TSCA) registration cost = risk

Know How (2)
- Technology outside current group experience

- Need better information on which ionic liquids to try – no time for hit/miss
- Technology (ionic liquids) has no commercial track record – mid-size companies will avoid the risks associated with ionic liquid use
- Basic Knowledge
    - "Limited knowledge" – we don't know the phase behavior of the compounds of interest with ionic liquids (gas solubilities, Liquid Liquid Equilibrium, distribution coefficient, carrying capacity) or how that is controlled by choice of cation, anion, substituents ($10^{18}$ …) to design or choose the best ionic liquid for the application (2)
    - Not well understood physical properties (pure and mixtures) (5)
- Uncertainty: need information on properties, lifetime/loss, impact on processes
- Non-existing material, non-existing production procedures

Competitive Technology (1)
- Lack of comparison to existing technology, i.e. side-by-sides
- Specific performance
- Alternative technology available that is commercially demonstrated

Tradition (6)
- Current R&D climate: difficult to try something new (also relates to cost)
- Unfamiliarity (also relates to cost)
- (Know how) ionic liquids are not cheap/readily available (in lab R&D environment)
- Cultural barrier to transfer ionic liquids to scale-up plants
- Timeframe to scale (difficult sell to business/financial decision makers)
- Advantageous v. existing/known process? (Given the uncertainties IL will have to be obviously much better in process performance)
- Multiple suppliers not available – "not invented here" (1)

Relationship Building (5)
- I want to use ionic liquid – not make them. Who am I going to get them from in quantities needed? (supply issue)
- Need for "deep" collaboration between ionic liquid producer and user (also culture is a barrier)
- A designed material – need cooperation with each company
- Intellectual property: Can I use ionic liquid if I want to?

Compatibility/Retrofits with Existing Equipment (2)
- My equipment is designed for use with molecular solvents. Can I use ionic liquid in it?
- Ability to retrofit existing equipment vs. new equipment

Specific Input Availability
- Availability (beyond R&D samples)
- Raw materials for scaling up

## **Separations Strategies**

What are the Strategies Needed to Overcome the Barriers to the Use of Ionic Liquids in Separation Systems?

Lifetime/Recycle

- Performance/recyclability
- Suppliers responsible for clean-up and recycle
- Robust performance, i.e. works in the presence of contaminants
- Development of task specific ionic liquids for concrete application (should know which)
- Identify "key model" systems to perform engineering-scale studies to obtain lifetime recycle data
- Basic data: government funding programs, - some supply component, - involve manufacturer/producer and user, - lifetime modeling component
- Basic data: ID (problem) systems of interest, then use combination modeling/experimental studies to predict and measure 1) solubility, 2) viscosity, 3) etc., etc., etc., for individual species and mixture

Basic data

- Collaborate with separation experts to gain data
- University collaboration
- Measure chemical and physical properties needed for process simulation/design for specific separation: pure compounds/mixtures, Vapor Liquid Equilibrium, Liquid Liquid Equilibrium, density, viscosity, interfacial tension …
- Engineering demonstrations of processes: - lifetime, recycle, - "generic" systems
- Understanding fundamentals: which ionic liquids or class of ionic liquids can we use for a specific separation problem?
- Develop collaborative organization to prioritize and obtain physical properties data through a combination of government and private sector funding
- Database project (International Union of Pure and Applied Chemistry)
- Use toxicity and thermal/chemical (viscosity?) stability to eliminate "classes" of ionic liquids
- Residuals in precipitated polymers with/without rinsing
- Identify process of interest ➔ identify possible ionic liquid types ➔ $$ mechanism for evaluation of physical properties of these ➔ $$ evaluate in process (determine high opportunity applications to help focus R&D direction)
- Focus on hard separations, something that is energy intensive or simply very hard to do – a small scale niche market? - As opposed to bulk product separations
    - purifications in the ppm/ppb range,
    - areas where intellectual property is not totally filled up, i.e. no room to develop conventional solution
- Application (patents) screening: design basic experiments to obtain technical "gate 1" feasibility ➔ drive 1st techno-economic evaluations/process design models

Relationship building

- Strategic alliance
- Form strategic alliance with ionic liquid supplier/experts

- Companies share applications targets with academics to focus efforts to understand what factors control phase behavior and physical properties (also Basic Data)
- Build up a relationships, - exact information about process, - exchange of data, - simulation of process
- Find partners in sectors with need for replacement of current technology/solvent
- Strategic alliance: university-company and/or company-company
- Call up the researchers! Let them come to your company and tell you about what they (and others) are doing in separations?
- Partner under Non-Disclosure Agreements, - discuss likelihood/opportunities, - discuss capabilities, - define role for each participant, i.e. value chain/business models/manufacturing, production
- Research center along model of NSF industry/university centers – allows multiple parties to participate in research while protecting intellectual property, similar to University of Texas Separations Research Program, Colorado University Membrane Center

Tradition
- You have to prove real benefit with ionic liquid separation
- Longer term: Get ionic liquid into basic unit operations/separations courses, so student carry to industry
- Show superior advantage, have internal champion
- Identify "key model" systems to obtain process engineering data for equipment design and retrofit capability (sensitivity analysis to clarify direction)
- After performing process engineering studies to get data on select "model" systems, have industrial groups do economic analyses
- Look at what's already out there commercially!!
- Aim at applications that are new or emerging so that the existing solvent choices are either non-existent or clearly not optimal

Cost
- Minimize volume of ionic liquid in process
- Use existing/known process and see if ionic liquids can be substituted. Compare economics! (MP DMF as proxy)
- Focus concentration on to low-priced, readily available ionic liquids, starting from precursors as cheap as possible
- Reduce inventory (high capacity), efficient contact/separation
- Total novelty (no competition)
- Scaling up some of ionic liquid for concrete application (should know to what)
- Economy of scale
- Find ionic liquid based on cheap cation (no pyridine, no imidardine) and anions (no F)
- Consider ionic liquid as capital investment vs. reagent (solvent) as an expense

Summary

Key demonstration projects with partnerships of

Industry (specific projects, business issues)
National lab
University (know how)

1) Can be generic to facilitate widespread dissemination,
2) Can make use of expertise in each area,
3) Decide on key systems

<u>Potential Partners</u>

Merck KGaA Germany
Solvent Innovation
Notre Dame/Joan: gas separations
J. Davis: ionic liquid production    put in proper names for all
U. South AL: Spec. prop. of IL
W. Arlt/Technical University of Berlin: extractive distillation
U. AL: liquid IL
QUILL
Chevron
Air Force: long term stability

## Catalysis Barriers

What are the Barriers to the Commercial Use of Ionic Liquids in Catalytic Systems?
(The number of votes is shown in ())

Risk Benefit (10)
- Lack of previous successful process experience w/IL in similar process work
- Risk to change, uncertain long-term effects
- Advantages of current process! Why change? (4)
- Cost-performance benefits – Not well defined
- New product (market) and new process is a double barrier

Properties and Selection (6)
- Know how about ionic liquid properties
- What kind of different ILs could fit my problem?
- Unknown HS&E (health, safety, & environment) related issues
- Long-term effects
- Why not use an IL? I don't know much (anything) about the physical properties of the liquid, or chemical kinetics
- Toxicity characterized? Toxicity? Safe to use? (1)
- Viscosity possibly too high
- Lack of adequate engineering knowledge on the material
- Clear understanding of mechanisms, "comfort"
- Lifetime of ionic system and cradle to grave to cradle process

Economics and Availability (4)
- Availability of ionic liquids
- Cost? Economics? (1)
- Impurities in commercial grade RTIL?

Process Engineering (6)
- Lack of basic process engineering limits opportunities. Type of reactor is key to maximize benefits from ILs and deliver maximum performance. Little information outside of a few industrial developers and "Quill" members
- Nothing, except the knowledge that the ionic liquid concept is not the right solution to this specific problem
- No clear assurance that ionic liquids will perform in a continuous high volume catalytic chemical process. (No known commercial process, lack of pilot plant demonstration facilities)
- Difficult to separate products

Knowledge Management & Communication (5)
- Complexity; Misleading information (1)

Catalysis Strategies

What are the Strategies Needed to Overcome the Barriers to the Use of Ionic Liquids in Catalytic Systems?

Risk Benefit

- Strategy to include: 1) Identify industrial problems/opportunity (realize dream reactions); 2) discuss with a real expert; 3) do a risk/potential analysis of the research effort; 4) research effort ➔ networking
- Choose appropriate IL, based on cost analysis, to replace a current process with proven market
- Process evaluation, market evaluation, market accessibility, process risk, competitive advantage
- Do a direct comparison to the old process and show how the new ionic liquid process works better; example – develop a catalytic process vs. stoichiometric process for acylation
- R&D – demo ➔ rate/solubility/system; collaborate ➔ cost/performance; bench mart ➔ current process; collect data- additional: life, recycle, disposal, HS&E (health, safety, & environment)
- Identify ionic liquid features that may solve major existing process deficiencies: activity, selectivity, stability, product separation, environmental, etc.
- Focus on problems in current process (can ionic liquids help)
- Prioritize existing processes needing improvement
- Look for applications in high value processes; - specialty chemicals, -pharmaceuticals; commodity chemicals have too low of capital/R&D investment for initial applications-----?????cards
- Learn from previous work and studies
- "Early" flow sheeting linked to "appraise" ideas – cost benefit per unit operation if retrofit
- Know where the intellectual property resides

Quill (all)
Engineering University (all)
Chemical University (all)
National Laboratories (all)
Rogers (Alabama) (all)
Wasserscheid (Germany) (all)

Properties and Selection

- Form a consortium of academia, companies and national labs to measure properties and develop process models and form a database (like DIPPR) (efforts at NIST already underway), must address intellectual property rights
- Thorough literature review followed by specific experimentation to fill in need data points
- Properties database
- Create databases for properties

R&D Players

Notre Dame

Economics and Availability

- Talk to vendors on availability and cost
- Bring engineers together to assess economic benefits
- Get a ballpark cost estimate for four commonly used ILs
- Total cost price levels related to different application
- Potential to reduce production costs of expensive ILs
- Intellectual property - what and who

R&D Players

Specialized companies in Ionic Liquids: Solvent Innovation, Merck KGaA

Process Engineering

- Ensure adequate screening procedures and early reactor design selection; “define process early”; “need multidisciplinary team – engineers and chemists”
- Overcome the viscosity of ILs by development of new ILs (non-halide)
- Overcome the separation issues related to the ILs process based on product selection
- Define stability window; Temperature, $H_2O$, corrosion, environmental for four ionic liquids
- Water, separation rate/clean, corrosion

R&D Players

IFP

Knowledge Management and Communication

- Create and communicate a roadmap. That’s why we are here.
- Read literature!
- Increase availability of ionic liquid databases
- Example and case studies (advantages)
- Take the top 50 chemicals, identify the most needed process improvement for each of the top chemicals
- Intellectual Property
- Shared database on toxicology

R&D Players

Chemical Press

## **Bulk Chemicals Barriers**

What are the Barriers to the Commercial Use of Ionic Liquids in Bulk Chemical Production?
(The number of votes is shown in ())

Retrofit or Replace (6)
- Cannot fit into existing equipment, - return on investment must be short timeframe, - ROA grading system
- Expensive replacement costs to go to new technology
- Scale concerns? Bulk = big. More interested in ILs for specialty applications/niche applications
- Currently have something which works/making money, - not increasing base business right now, -consolidation, considering minor improvements only
- Physical and chemical data specific to own process
- Companies not investing in new bulk chemical plants these days – would only be considered if simple retrofit

Process Definition (5)
- Why use a solvent? Process contamination
- Test ionic liquid technology only if your problem fits the concept! Save time and money: try to understand first! Discuss with a real expert!
- Scale concerns
- Cost: the volume of "bulk" chemicals is very large. Even a small usage/loss would require a large amount of IL inventory
- Long-term stability
- Need to know what kind of ionic liquids the industry needs or can commercially apply

IL Cost (3)
- "The usual" cost, toxicity, supply
- Too high priced
- Potential for loss of expensive ILs in large volumes, i.e. little data to date in process design for losses. Bulk chemicals means large volumes and low cost margins
- Too expensive to use large (bulk) quantities of ILs

Product Quality (1)
- Risk
- Product sells on "specification" and "price" – must be cheaper and contain no unknown byproducts that could interfere with downstream customer applications
- Plant write-down costs
- The risk of using unproven technology in billion lb per year application is unacceptable

Communication (1)
- Communication
- Mix of misinformation/good information
- Misinformation
- Specific ionic liquid information (not grouped as a whole)

Health, Safety, & Environment (3)

- Environmental safety is issue when using large volumes of ILs
- No registration present

Business Strategies (5)

- Command and control
- Supply of raw materials? Many partners? Loss of independence/dilute value chain

<u>Bulk Chemicals Strategies</u>

<u>What are the Strategies Needed to Overcome the Use of Ionic Liquids in Bulk Chemical Production?</u>

Retrofit and Replace

- Basic data on materials compatibility (equipment special needs)
- Invest and be clever ("creative") process engineer
- Evaluate retrofit chances by mini pilot study. Can it be done? Try in existing pilot plant
- Publishable process design/process engineering study for using ILs in retrofitted equipment

Business Strategies

- 1) Identify the problem, 2) communicate problem to expert ➔ discussion, 3) start research, ➔ ionic liquid as additive//support, ➔ process retrofit
- Seek partner with complementary knowledge
- Work small scale (niche application) to deal with regulatory/registration early (can seriously hold up commercialization)

Process Definition

- Think of ILs as: - liquid catalyst support, modifier, catalyst, …etc., not as bulk solvent
- Attack smaller side streams first (waste recovery), main stream second or target expansions over shutdown
- Process engineering studies to determine life of ionic liquid in real systems

Environmental Health and Safety

- IL lifetime
- Involve regulators early
- IL = mixture of two already registered products (use combination)

IL Cost

- What is the cheapest ionic liquid that solves the problem? What ionic liquid quantity can be accepted? Quality ←→ Price
- Focus design of new ILs for low costs, low toxicity, and ability to handle contaminants to increase IL lifetime
- Process engineering IL lifetime

Product Quality

- Retrofit ionic liquid to product (design/select IL to fit)
- Process engineering
- Need pilot plant.  Role for government funding

Communication

- Local seminars on IL (industry, research, government)
- Present to industry business leaders – A.C.C., IRI
- PR (success story): public news, not tech journals
- BASIL™

R&D Players

National Lab → Oak Ridge NL
Universities → University of Alabama, University of Notre Dame

## Fuel Production Barriers

What are the Barriers to the Commercial Use of Ionic Liquids in Fuel Production?
(The number of votes is shown in ())

IL Characteristics and Compatibility to Fuel Production (Measures) (3)

- Essential properties of ionic liquids for fuel production
- Analyze how/why ionic liquid would be more advantageous than current processes (lack of expertise, general knowledge)
- Few homogenous catalytic processes
- Catalytic requirements poorly match capabilities

Possibilities and Effects of Contamination (2)

- Sensitivity to contaminants
- Potential for contamination of gas stream unknown
- Burnability, how significant are impurities contributed by the IL process

Capital Costs (1)

- High throughput processes, - investment, - cost of IL/lifetime/loss
- Very large processes (high capital)
- Resistance in industry to build new capital
- No new construction

Risk (2)

- Resistance to change a well developed process, e.g. formation of octanes from butene/butane (HF now), reluctant to change
- Can the health, safety, & environment issues be addressed/overcome?

Demonstration

- Develop and demonstrate a continuous operation for months/years (including expected process upsets)
- Uncertainty about longevity in harsh environment
- Lack of published process data on real systems (1)

Communication

- Communication: how might we help? Need information from gas industry
- Low vapor pressure value (this is more of a strategy/solution of IL)
- Education? Role of education, knowledge-sharing, time to evaluate, "properties"
- What performance and/or economic benefits do ILs have in any fuel production? (6)

Broader Fuel Applications (4)

- Fuel, traditional areas, look at opportunities in Hydrogen, in broad fuel market and nuclear! In new fuel areas! (1)
- Use of RTILs in nuclear industry
- Hydrogen (alternative fuels) creation, processing, generation, storage
- Solar, working thermal fluids

- Biomass application, scale of application.
- Coal gasification, oil shale; are there ionic liquid applications?

Operating Costs (4)
- Losses in liquid-liquid systems, IL, dissolved agents, cost, environment (1)
- Cost of change – market is such that margins are on the order of pennies
- Low margins between raw materials and product (2)
- No waste or low value by-products

Fuel Production Strategies

What are the Strategies Needed to Overcome the Barriers to the Use of Ionic Liquids in Fuel Production?

Operating Costs
- Focus on critical problematic processes
- Identify stages of processing (downstream?) where ionic liquids are possibly cost effective
- Measure true "cost" of operations – water, energy, etc. Ionic liquids may have an advantage over traditional processes on a true or "total" cost basis

Communication
- What are the needs, e.g. do we need better sulfur removal. Which specific regulations (benzene extraction, sulfur regulations, SOx, NOx) need to be addressed?
- Put together existing ionic liquid literature in fuels area, how far are IL processes away?
- Industry-led group identify classes of processes where ionic liquid introduction is feasible, communicate → R&D
- Identify opportunities to significantly improve existing processes using ILs – determine if there is enough potential to continue development (e.g., in alkylation, isomerization, separations, others)
- Don't be shy about talking to people already working in ILs
- Need bridges between/among ionic liquid researchers, corporate technology officers, and engineers, to establish common knowledge base: what are fuel-related processes? What are relevant ionic liquid properties?
- Develop small "teaching" modules on ionic liquids for undergraduate chemistry and chemical engineering classes
- Ionic liquid champion with deep pockets

IL Compatibility to Fuel Production
- Identify ionic liquid where contaminants are tolerant of structure/property/reactivity patterns of process chemicals
- Identify low-cost, low-impact (toxicity, etc.) ILs targeted for applications: gas separation, extractive distillation
- Increase solvency of biomass starting materials/product in IL, radiation stabilities (relates to compatibility, re: broader fuels)
- Develop new catalysts which operate at lower temperatures

Broader Fuel Applications

- Research directed at learning more about use/compatibility of ILs for alternative fuel production, and/or purification
- Define current state-of-the-art and where it needs to be! (Solar cells)
- Synopsis of state-of-the-art in ionic liquid by means of 3-4 very recent review articles. Connect with recent summaries of R&D needs in energy fields (web-based reports)
- Create government-funded initiative to alternative energy technical issues
- Network of research group for "new fuel applications" (labs, energy companies, engineering schools; will need NDAs and CDAs in place at onset)
- Little market driver for broader applications. Government funding of focused R&D, demonstration
- Identify areas in nuclear industry where ILs could play a role, - processing, reprocessing, separations
- Investigate new technologies, hydrogen production (low-T process?), storage, and use, -fuel cells, etc.
- Cellulosic processing for fuel production using IL
- Increase interaction with alternative fuels community

Possibilities and Effects of Contamination

- Develop quantitative/semi-quantitative information (data) concerning tolerable level of contaminants for specific processes
- Identify specific contamination problems, company-specific proprietary issues
- What are the key contaminants and temperature levels and corrosion issues (proprietary)

Demonstration

- Develop catalytic/separation process which allow compliance with environmental regulations
- Are there any good examples where ILs have helped in fuel production? (oil shale)
- Partnerships, $
- Engineering demonstration of potential processes, - real streams, -lifetime, - economics
- Demonstrate non-contamination of ionic liquid in final fuel product → after identifying process where ionic liquid is viable
- Test and demo: -benzene removal (at small scale), -sulfur removal. Demos should be driven by environmental regulations, that is the key driver
- Treatment of produced water, removal of assorted ions and/or organics
- Cleaning up natural gas, acid gases, water
- Find the "right" application that you can demo to break out of the mold and get everyone on board

Risk

- Collaborate to reduce development/demonstration costs
- Develop process with novel capability
- What is the most likely path of ionic liquid discharge in the process?
- Health, safety, & environment specific: develop common method of quantifying potential problems and comparing with those related to common solvent, e.g. structure-activity relationships

- Lifecycle testing, long-term performance (ppm ionic liquid in fuels)

Capital Costs

- New/novel catalysts and processes (new ideas to revolutionize capital cost reduction; hard to displace distillation, which is cheap and entrenched)
- High throughput experiments (try different catalysts in plant trials, work with teams of suppliers, capital providers)
- Process intensification: - micro-technology, reduce liquid requirements, reduce capital equipment requirements

<u>Collaborative Partners</u>

- Refining industry (bp, Exxon-Mobil, UOP)
- National labs (especially NREL for outside of petroleum)
- Ionic liquid manufacturers
- Integrated plan for demonstrations
- Industry
- Universities
- Labs
- Design/engineering companies

## Polymers Barriers

What are the Barriers to the Commercial Use of Ionic Liquids in Polymer Production?
(The number of votes is shown in ())

Data/Properties (6)
- Insufficent database on polymer/IL interactions
- Uncertainty around which ILs to select, due to unknown properties (transport, physical)
- Many other solvents to choose from with better known properties, lack of properties knowledge
- Do we get unique polymer properties?
- Value – data to help define, improved properties of polymers
- Ionic residuals not acceptable for electronics
- Lacking compatibility know how of ionic liquid and polymers (additives)
- Technology unknown, demand unknown

Engineering Processes (6)
- Separation of solvent from ionic liquid is different from conventional processing (i.e. evaporation)
- Unknown process advantages/disadvantages
- Entrainment
- Is a solvent necessary? Competing methodology
- Processing modes need to be changed (risk of change tradeoff)

Philosophy (1)
- What is the ionic liquid used for? Solvent? Monomer?
- Define what polymer processes need to be improved. What are the Holy Grails of polymer chemistry? (1)

Performance (6)
- Performance of ILs for/in polymerization reaction
- Must show new material properties
- Thermal stability insufficient for various applications
- Processing modes need to be changed

Toxicity (1)
- Bring impurity with known or unknown toxicity to polymer products (HSE)
- Food and personal care applications
- Environmental effect/safety

Cost/Benefits (4)
- Risk-Benefits: 1) polymerization - with/in IL, 2) as polymer additive
- What should be the advantage of ILs?
- Reluctance to change existing process. Risks (economic, technical) v. benefits (uncertain)
- If making monomers, must be economical
- Cost, many done in $H_2O$

Chemistry Processes (2)

- Fundamental polymer chemistry – what won't work, what will? What are the unique attributes? How do the polymer physical properties differ?
- Mechanistic information
- Define polymer chemistry: 1) making? 2) dissolution? 3) modifying?
- Have samples on hand for testing special solubilities for polymer modifications
- Viscosity, unknown parameter, product separation
- Database on different polymerization processes

Communication (5)

- ID major polymer issues, methacrylites
- Transparency
- Thermal stability
- Surface properties

<u>Polymer Strategies</u>

<u>What are the Strategies Needed to Overcome the Barriers to Use of Ionic Liquids in Polymer Production?</u>

Communications

Cost and Benefits

- Ionic liquids workshop for polymer experts: - course style at AIChE meeting, - tutorial at a university (U. Alabama)
- Identify top 50 polymers and processes and list problems associated with them: - write a technical paper for CEP/C&E News, - create a team that visits companies "fact finding" mission
- Facilitate cross-fertilization of ionic liquid and polymer chemists/engineers
- Communications: need to being people together from ILs and polymer areas (including academia and industry)
- Bring polymer chemistry experts together with ionic liquid industry and academics
- Communication: Create a roadmap (technical plan) for commercialization of ionic liquids, for polymers – convene a group to do this
- Successful demonstration of ionic liquid technology at an industrially relevant key example
- Communication: communicate new successes
- Key demonstration projects: collaboration between industry, national lab, and university. Identify key problems in specific polymer process (Holy Grails) – industry defines the problem. Work with knowledgeable experts in IL, business, polymer chemistry. Answer the questions
- Collaborate, demonstrate examples
- IL additions create higher Tg (glass transition temperature) → change = $+
- Focus: 1) limited needs – identify, 2) performance advantages – define
- Communication: alliance. University/business, B to B

- Collaboration/alliance between suppliers and users
- Prioritize most important polymer problem to be solved
- Material selection for critical processes
- ILs journal, web page

Data/Properties
- Create a physical properties consortium tied in with NIST/IUPAC database effort.  Industry, academia, national labs
- Center of Excellence
- New modifications through increased solubility in ionic liquid or mixing thereof
- Old monomers, new geometries, molecular weight, architecture, etc.

Engineering Processes
- Examine the major processes for the major polymers and identify the major desired/needed improvements
- Material selection to adapted process

Performance
- Collect literature data on solvent/performance relationships
- Address key problems of polymers/polymerizations and identify
- Laboratory demonstration on clear benefit of using ILs for polymerization process.  High throughput testing.  List positives and negatives and evaluate killer parameters
- Develop new ILs with low viscosity and tailored properties

Polymers R&D Players/Supporters
- Major polymer producers
- Merck KGaA, Germany
- ORNL
- Eric Beckman
- Peter Wasserscheid
- U. South Alabama
- Doug McFarland, Australia
- U. Belfast
- U. Alabama
- Jimmy Mays, ORNL
- U. Notre Dame
- LANL
- Dave Hadilton
- Experts: Europe, Japan, US