Cross-Cutting Research and Training

Bala Subramaniam, Director
Center for Environmentally Beneficial Catalysis

Kansas Statewide EPSCoR Conference
Lawrence, KS
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Designing environmentally responsible molecules, products, and processes – from the molecular scale to the plant scale.

**Lead Institution:** University of Kansas (KU)

**Core Partners:** University of Iowa (UI); Washington University in St. Louis (WUSTL); Prairie View A&M University (PVAMU)

**Director:** Bala Subramaniam (KU); **Deputy Director:** Daryle Busch (KU)

**Associate Directors:** John Rosazza (UI); Milorad Dudukovic (WUSTL); Irvin Osborne-Lee (PVAMU)

**Education Director:** Joseph Heppert (KU); **Industrial Liaison:** Darryl Fahey
Sustainability Vision for the Chemical Industry
2005 NRC Report

Current Paradigm
- Fossil Fuels
- Energy-intensive Processes
- Waste Generating Chemistry
- Earth Systems Illiterate

Ideal Vision
- Renewable Feedstocks
- Renewable Energy
- Atom Economy (Zero Waste)
- Earth Systems Literate

2005 - 2025: Continued Use of Fossil Fuels
- Reduced Energy Intensity
- Carbon Management
- Sustainability Education

2025 - 2105: Phase out of Fossil Fuels
- Life Cycle Analysis
- Green Chemistry and Engineering
- Toxicology
- Renewable Chemical Feedstocks
- Renewable Fuels

Year
- 2005
- 2025
- 2105
**CEBC Thrust Groups**

**TG1: Catalyst Design, Discovery and Engineering**
- Active Site Design and Synthesis of Homogeneous and Enzymatic Catalysts
- Nano-scale Catalysts
- Tailored Catalysts Supports
- High Throughput Screening Methods
- Catalyst Characterization

**TG2: Media Design, Evaluation and Characterization**
- Selection and use of Benign Media
- Phase Behavior Involving Benign Media
- Solubility of Gases, Catalysts, and Substrates in Benign Media
- Physical and Transport Property Measurements of Media

**TG3: Advanced Measurements Pertaining to Reactions & Reactors**
- Structure Determination
- Catalyst Testing in Benign Media
- *In situ* Spectroscopic Studies to Probe Reaction Mechanisms
- *In situ* Measurements of Effective Transport Parameters in Reactors

**TG4: Molecular and Process Modeling/Optimization**
- Molecular Modeling
- Reactor Modeling
- Computational Fluid Dynamics
- Environmental Impact & Economic Analysis
- Scale-up and Optimization

**Disciplines Represented in TGs**
- **Engineering**: Chemical, Civil, Environmental
- **Sciences**: Chemistry, Biology

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**The Center for Environmentally Beneficial Catalysis**
# Current Industry Full Partners (12)

<table>
<thead>
<tr>
<th>Industry Partner</th>
<th>Areas of Relevance to CEBC</th>
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<tbody>
<tr>
<td>ADM</td>
<td>Crop Processing</td>
</tr>
<tr>
<td>BP Chemical</td>
<td>Energy, Chemicals</td>
</tr>
<tr>
<td>Chevron Phillips Chemical*</td>
<td>Chemicals and Polymers</td>
</tr>
<tr>
<td>ConocoPhillips</td>
<td>Energy</td>
</tr>
<tr>
<td>CritiTech (Small)</td>
<td>Pharma Start-up</td>
</tr>
<tr>
<td>DuPont*</td>
<td>Chemicals and Biosciences</td>
</tr>
<tr>
<td>Engelhard*</td>
<td>Catalysts and Diverse Chemicals</td>
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<tr>
<td>ExxonMobil Chemical</td>
<td>Energy, Chemicals</td>
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<tr>
<td>Kansas Technology Enterprise Corporation (KTEC) (Small)</td>
<td>Corp that promotes tech-based Economic Development</td>
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<tr>
<td>Novozymes</td>
<td>Biotech</td>
</tr>
<tr>
<td>Procter &amp; Gamble*</td>
<td>Consumer Products</td>
</tr>
<tr>
<td>UOP A Honeywell Company</td>
<td>Technology Supplier to Petrochem Industry</td>
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</tbody>
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*Charter Member*
Knowledge/Technology Deliverables From Core Projects

- Ionic Liquids
- CO₂ Expanded Liquids
- Synthesis Methods
- Supported Nanoparticulate Catalysts
- Supported Recyclable Homogenous Catalysts
- Media
- Modeling
- Multi-phase Processes
- Reaction/Catalyst Precipitation
- Enriched-O₂ Oxidation
- Liquid/Liquid Precipitation/Filtration

Tools:
- Computations
- Catalysts
- Reactor Designs
Education and Outreach Programs

- Undergraduates
- Graduate and Postdoctoral
- On-line Mentors
- K-12 Outreach Activities
- Research and Development
- Teaching Fellows
- Short Courses
- K-12 Students
- Professionals

Well-developed: Activities will continue
Being developed: Main focus during year 4
Periodic: Activities continue
Assembling Research Teams

• Critical mass of interdisciplinary researchers must exist
  - Mix of senior and junior faculty (core group of ten or so)
  - Kansas EPSCoR program helped nucleate interdisciplinary projects between chemists and engineers in catalysis

• Team Leadership
  - Senior researcher(s) with good reputation and commitment

• Leader(s) organize preliminary sessions
  - Core group should familiarize itself with ERC’s unique features
    • Systems-based industry-relevant research
  - Develop a preliminary theme/vision for a center

• Expand Research Team as Needed
  - Identify critical expertise gaps
  - Explore “core” and “flexible” partnerships with other universities
Details of Center Structure and Operation (Who? What? Why? How?)

• Ideation Session(s) with Core Team Members
  - Generate a compelling vision and rationale for center

• Areas of Expertise Needed to Achieve Vision
  - Research thrusts, thrust groups and thrust group leaders

• Develop a Strategic Research Plan
  - Describe process by which “engineered systems” will be developed with industry input and “testbeds”: 3-plane chart
  - Describe how research will be managed and integrated to achieve “engineered system” goals

• Refine Details based on Feedback
  - Organize focus groups involving a group of practitioners and academic researchers including those with ERC experience
  - Meet with ERC Program Officers to discuss proposal
Education, Outreach and Diversity

- Recruit education program director with a proven interest in pedagogical and human resource development matters
- Education/Outreach Strategic Plans
  - Must describe novel curricular, outreach and training aspects that recruit and produce uniquely trained engineers and scientists
  - Ideally, every center faculty must be involved in some (but not all) components of program (K-PhD and Life-long Learning)
  - Full-time education program coordinator desirable to coordinate logistics and assessment of multi-campus activities
- Diversity Strategic Plan
  - Form Diversity Advisory Board to help with planning and contacts
  - Must include targets for recruitment
  - Partnerships/linkages with minority serving institutions and organizations
Institutional Financial/Space Requirements

• Proposal Preparation Phase
  - Seed funds
    • To hire program assistant(s) to assist leader(s)
    • Industrial Liaison Coordinator
    • Consultants
    • To organize industry focus group meetings

• Commitments for Proposal
  - Headquarters space for administration, special research facilities, and industry projects
  - Cash match requirements
  - New faculty positions including startup packages
  - Cyberinfrastructure (video conferencing and class room facilities)