

University of Notre Dame

Notre Dame Energy Center

HELPING TO BUILD A BETTER ENVIRONMENT WITH ENERGY RESEARCH

2006-2007
Annual Report

Activity Period
July 1, 2006—June 30, 2007

August 2007

Dear Friends and Colleagues,

It gives me great pleasure to present to you the 2006-2007 Annual Report of the Notre Dame Energy Center. Now in its second year, the Energy Center has experienced significant growth and notoriety for the research and educational programs it provides to our students and to the members of our local, state, and national communities.



Joan F. Brennecke

I am especially grateful to the Energy Center faculty for their numerous contributions to the success of the Center. Many of these faculty have received new awards this year in support of energy-related research. This is a true testament of the dedication and commitment we have had and continue to have from our faculty researchers to address world-wide issues and policies related to energy.

I would also like to thank the members of the newly comprised Notre Dame Energy Center Student Advisory Board. This 14-member board was established in January 2007 for the purpose of developing new programs and initiatives in support of the Energy Center's mission. They have worked hard and have accomplished a lot in a short period of time. You will read more about their efforts in the coming pages. Also new to the management team this year is Barbara Villarosa, Programs and Research Specialist. Barbara provides part-time support for the administrative and management functions associated with a productive and successful Center. Please join me in welcoming our newest members to the Energy Center family.

Overall, the Energy Center has had a very successful year, and I hope you will enjoy reading, in more detail, about the many activities and initiatives that have contributed to our success.

Best regards,

A handwritten signature in black ink that reads "Joan F. Brennecke". The signature is written in a cursive, flowing style.

Joan F. Brennecke
Keating-Crawford Professor of Chemical and Biomolecular Engineering
Director, Notre Dame Energy Center

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Faculty Involvement and Research

In the past year, faculty participation in the Center has increased from 15 to 35. Many of the additions have been in the College of Arts and Letters and the Mendoza College of Business.

2006-2007 Energy Related External Awards

It is difficult to track energy research at Notre Dame solely by the use of the Center code since many faculty use their departmental codes when submitting proposals. Please note that there was significant energy-related work going on at Notre Dame even before the establishment of the Center. Although we anticipate that this is an underestimate, self-identified new awards for energy-related projects in 2006-2007 are:

| PI (Co-PIs) | Project Title | Sponsor | Total Award |
|---|---|-----------------------------------|--------------------|
| Mark McCready | Entrainment in two-phase gas-liquid flows | Chevron Energy Technology Company | \$82,500 |
| Patrick Fay | Solar arrays with high specific power | NASA | \$24,263 |
| William Schneider | Towards realistic models of heterogeneous catalysis: simulations of redox catalysis from first principles | DOE BES | \$420,000 |
| Joan Brennecke | Ionic liquids for CO ₂ capture from advanced post-combustion or advanced pre-combustion gases | GE | \$300,000 |
| Joan Brennecke (Mihir Sen, Ed Maginn, Samuel Paolucci and Mark Stadtherr) | Ionic liquids for utilization of waste heat from distributed power generation systems | DOE | \$1,425,000 |
| Ed Maginn (Joan Brennecke and William Schneider) | Ionic liquids: breakthrough technology for post-combustion CO ₂ capture | DOE NETL | \$2,214,591 |
| Ed Maginn | Determination of physical properties of ionic liquids using molecular simulations | AFOSR | \$399,498 |
| Ed Maginn | GAOLI - Atomistic simulations of the physical properties and phase behavior of ionic liquid/gas mixtures | NSF | \$109,321 |
| Vikas Tomar (John Renaud) | Computer aided multi-scale design of SiC-Si ₃ N ₄ nanoceramic composites for high-temperature structural applications | DOE NETL | \$300,000 |
| John Renaud (Vikas Tomar) | Multiscale design tool development for high performance nanocomposites | NSF | \$320,000 |
| Paul Bohn | Molecular aspects of transport in thin films of controlled architecture | DOE BES | \$375,000 |
| Joseph Powers (Samuel Paolucci, Andrew Sommese, Charles Wampler) | Slow invariant manifolds for spatially homogeneous and inhomogeneous combustion systems with detailed kinetics | NSF | \$299,998 |
| Joseph Powers (Samuel Paolucci) | Advanced multi-scale computational methods for hypersonic propulsion | NASA | \$361,154 |
| Robert Nerenberg | Hollow-fiber membrane microbial fuel cells (HFM-MFCs) for electricity production from wastewater | NSF | \$75,000 |
| TOTAL | | | \$6,706,325 |

Faculty Involvement and Research (continued)

VINCENT P. SLATT UNDERGRADUATE RESEARCH FELLOWSHIP

In March 2007, undergraduate students were invited to submit proposals for consideration of financial support up to \$5,000 under the Vincent P. Slatt Fellowship, to conduct hands-on research in energy-related areas. Six proposals were received and, of those, five fellowships were awarded to students in various amounts totaling \$20,000. The 2007 Vincent P. Slatt Fellows are:

- Joseph Basconi, sophomore in the Department of Chemical and Biomolecular Engineering. Basconi plans to analyze the impact of Daylight Savings Time on energy consumption in Indiana. His adviser is Jeffrey C. Kantor, professor of chemical and biomolecular engineering.
- Patrick Brown, a sophomore from the Department of Chemistry and Biochemistry. Collaborating with his adviser Prashant V. Kamat, professor of chemistry and biochemistry, Brown will study single-wall carbon nanotube based photochemical solar cells, focusing on the desired properties for harvesting light energy.
- Shawn Coleman, sophomore in the Department of Chemical and Biomolecular Engineering. Coleman will investigate first-principles prediction of active sites for catalytic hydrogenation, which will provide insight into the development of improved catalytic materials and processes. His adviser is William F. Schneider, associate professor of chemical and biomolecular engineering.
- Kyle Kron, a sophomore in the Department of Aerospace and Mechanical Engineering. Guided by John E. Renaud, professor of aerospace and mechanical engineering, and Vikas Tomar, assistant professor of aerospace and mechanical engineering, Kron will perform finite element analyses of SiC-Si₃N₄ nanoceramic composites for high-temperature structural applications, such as earth and space based power generation systems.
- Felipe Witchger, a junior pursuing energy studies and economics. Biofuel development and sustainability in Latin America is the focus of Witchger's project. His adviser is David F. Ruccio, professor of economics and policy studies.



Joseph Basconi



Patrick Brown



Shawn Coleman



Kyle Kron



Felipe Witchger

Slatt Fellowship funds can be used for the student's stipend, incidental expenses associated with research, and travel expenses to a conference at which the student would present results of the research. Research projects are slated to begin summer 2007 and run through the academic year or until each project is completed.

Educational Programs

ENERGY CENTER DISCUSSION GROUP PROGRAM

The Energy Center hosted several discussion groups with Notre Dame faculty, graduate students, and undergraduate students from various disciplines during the months of April and May 2007. The Energy Center Discussion Group Program was developed for the purpose of bringing together faculty and students in an informal setting to discuss energy-related courses currently being offered within specific departments and, if possible, to address ways in which additional courses could be developed.

The following faculty members were lead participants in this year's discussion groups:

- April 5: George S. Howard, Department of Psychology
- April 19: Prashant Kamat, Department of Chemistry and Biochemistry
- April 25: Kenneth Sayre, Department of Philosophy
- April 26: Robert Nerenberg, Department of Civil Engineering and Geological Sciences
- April 27: Matthew Doppke, College Seminars — Arts and Letters
- May 3: Norman Crowe, School of Architecture

ENERGY CENTER COURSE DEVELOPMENT GRANT PROGRAM

The newly developed Energy Center Course Development Grant Program was designed to promote and increase the number of energy-related courses offered at the University of Notre Dame. Grants would be awarded to faculty, ranging from \$2,500 to \$5,000, and to graduate students, from \$1,000 to \$2,000, to help fund the development of a new energy-related course or to significantly redesign an existing course.

In April 2007, faculty, special professional faculty, and graduate students were invited to submit a two-page proposal, identifying course content and objectives, and including a brief statement from the department chair indicating approval of the course and verification that the course would be offered at least once during the upcoming two academic years. Grants were awarded in various amounts totaling \$6,500. The 2007 awardees are:

- Robert Nerenberg, Assistant Professor in the Department of Civil Engineering and Geological Sciences. Dr. Nerenberg will redesign two existing courses, CE40340 Wastewater Design and CE60330 Environmental Biotechnology, to incorporate energy efficiency, renewable energy production, and carbon sequestration.
- John Simon, graduate student in the Department of Electrical Engineering. Under the direction of Alan Seabaugh, Professor of Electrical Engineering, Simon will develop a new course entitled "Electrical Energy Extraction," teaching the physics of energy conversion devices.
- Alexandre Chapeaux, graduate student in the Department of Chemical and Biomolecular Engineering. Under the direction of Angela Miller McGraw, Director of Seminars and Educational Immersions in the Center of Social Concerns, Chapeaux will develop a seminar entitled "Energy Policy, the Environment, and Social Change," focusing on the scientific, environmental, economic, geopolitical, and social implications of current energy technologies.

Educational Programs (continued)

NOTRE DAME ENERGY CENTER STUDENT ADVISORY BOARD

A 14-member Student Advisory Board, chaired by Notre Dame Energy Center Director Joan F. Brennecke, was established in January 2007. Members were appointed for a one-year term and met regularly (every two weeks) to discuss energy-related topics and issues in support of the Notre Dame Energy Center's mission.

Members of the Student Advisory Board are: Kyle Bibby (Civil Engineering), Patrick Brown (Physics/Chemistry), Erin Dineen Burns (History/Science, Technology, and Values), Matthew Cahill (Marketing), Kimberly Churbock (Biological Sciences/Spanish and Catholic Social Tradition), Thomas Furlong (Mechanical Engineering/Science, Technology and Values), Courtney Haven (Chemical Engineering), Zachary Jara (Economics), Brianna Klco (Environmental Studies/Peace Studies), Mark Koegel (Civil Engineering), Lourdes Long (Anthropology and History/Business), Christina Marzo (ALPP/Film), Kristopher Tracy (Computer Engineering), and Felipe Witchger (Energy Studies/Economics).

Since its inception, the advisory board has either spearheaded or developed the following initiatives on behalf of the Notre Dame Energy Center:

- The Green Contract was presented for review and approval to the Energy and Environmental Issues Committee and was developed for the purpose of seeking student support throughout the academic year to conserve energy, recycle, and to be environmentally conscientious. The agreement will be given to freshman during orientation and introduced throughout the residence halls in August 2007.
- A list of energy-related courses currently being offered at the University of Notre Dame was compiled and made available on the Notre Dame Energy Center web site.
- Power Plant Tours were arranged for the following campus groups: Energy Center Student Advisory Board, Biology Club, and Student Environmental Action Committee.
- Energy Center Discussion Groups were held with several faculty members from various disciplines to promote open discussion on energy-related courses currently being offered at Notre Dame and to discuss ways in which additional courses could be developed. A list of questions was developed and distributed in advance to each lead participant to help guide and frame the discussion.
- The Energy Center Course Development Grant Program was developed to provide financial support to faculty and graduate students interested in developing new energy-related courses or significantly re-designing existing courses.

Announcing . . .

2007 NDEER

Notre Dame Environmental Education and Research Conference
sponsored by the Notre Dame Energy Center

October 10, 2007 * McKenna Hall

Administration

INDUSTRIAL ADVISORY BOARD

An Industrial Advisory Board was formed in Fall 2006 to provide advice and guidance to the Energy Center. Members are: Tom Degnan (ExxonMobil), Mike O'Sullivan (Florida Power and Light), and Anthony Early (DTE Energy).

PROGRAMS AND RESEARCH SPECIALIST

Barbara Villarosa was hired in October 2006 as a Programs and Research Specialist to assist part-time with the running of the Center.

FACILITIES

The Energy Center will occupy four laboratories and an office covering approximate 5600 ft² in the new engineering building. The Energy Center has been working with the architects throughout the year to ensure high quality, visible space for the Energy Center activities.

The Energy Center has worked actively with Development and the University architects to secure a donation of solar panels for the roof of the new engineering building. The estimated value of this donation is \$400,000.

The Energy Center has worked to secure the donation of a 30 kW microturbine from NiSource. The current plan is for this microturbine to be operated continuously in the new building, where it will generate electricity and provide heating for warm water. It will be located in the basement, with sufficient room for attachment of an anticipated experimental absorption cooling system. The microturbine will be fully instrumented and will be easily controlled for use in numerous student experimental studies. The estimated value of this donation is \$50,000.

NEWS AND NOTEWORTHY ITEMS

Joan F. Brennecke, Keating-Crawford Professor of Chemical and Biomolecular Engineering and Director of the Notre Dame Energy Center, was awarded the 2007 John M. Prausnitz Award for outstanding achievement in applied chemical thermodynamics by the Conference on Properties and Phase Equilibria for Product and Process Design. The award was presented in May 2007 at the 11th International Conference.

Brennecke also received the 2006 Professional Progress Award by the American Institute of Chemical Engineers and was presented the award at the AIChE Annual Conference on November 12, 2006.

The Notre Dame Energy Center developed a tri-fold, color brochure, which is being used to promote the Energy Center's research and education programs and initiatives to internal and external constituents. Additionally, a business card was developed to complement the brochure and to provide additional Energy Center contact information. Copies of these publications may be obtained by contacting Barbara Villarosa at villarosa.2@nd.edu.

On behalf of the Energy Center, the Director gave the following presentations and interviews:

| | |
|--------------------------------|---|
| MBA class, 10/12/06 | Chicago Area ND Chemistry/Engineering Mtg., 3/27/07 |
| Senator Lugar staffer, 1/24/07 | Tau Beta Pi initiation, 3/28/07 |
| Theology on Tap, 1/31/07 | Biology Club, 3/29/07 |
| WSBT interview, 2/8/07 | Introduction to Engineering Program, 6/21/07 |
| Washington Program, 2/27/07 | |

University of Notre Dame Energy Center

Helping to Build a Better Environment with Energy Research

Mission

The University of Notre Dame Energy Center was formed in 2005 to develop new technologies for energy efficiency, CO₂ separation and sequestration, and alternative energy sources. The Center also aspires to play a key role in energy education and literacy, affecting energy policy and exploring the ethical implications associated with energy sources, availability, and policy.

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Web Site

<http://energycenter.nd.edu>

Contacts

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RESEARCH AREAS

Energy Efficiency*CO₂ Separation, Storage, Sequestration, and Use*Safe Nuclear Waste Storage*Clean Coal Utilization*Solar and Other Renewables