National Center for Clean Industrial and Treatment Technologies

Advancing the Science and Engineering of Pollution Prevention and Waste Minimization

Activities Report:
October 1998 - September 1999

http://cpas.mtu.edu/cencitt/

National Center for Clean Industrial and Treatment Technologies (CenCITT)

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We would also like to acknowledge and thank the Institutional Coordinators for their valuable guidance and assistance: C. Robert Baillod (Michigan Technological University); P. Mac Berthouex (former Coordinator, University of Wisconsin-Madison); Randy D. Cortright (current Coordinator, University of Wisconsin-Madison); and Michael J. Semmens (University of Minnesota-Twin Cities).

John C. Crittenden
CenCITT Director

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ACRONYM LIST FOR USE WITH THIS REPORT

AdDesignS	Adsorption Design Software
AdOx	Advanced Oxidation Process Software
AdRecover	Adsorption for the Recovery of Organics
AHP	Analytic Hierarchy Process
AIChE	American Institute of Chemical Engineers
ASAP	Aeration System Analysis Program
CDI	Continuous Deionization
CIPS	Chemical Industry Planning System
CPAS	Clean Process Advisory System
CReaTe	Clean Reaction Technologies
CWRT	Center for Waste Reduction Technologies
DEAR	Design Enhancement to AHP Ranking
DFD	Design for Disassembly
DFT	Density Functional Theory
DIPPR®	Design Institute for Physical Property Data
DORT	Design Options Ranking Tool
ECM	Environmentally Conscious Manufacturing
EFRAT	Environmental Fate and Risk Assessment Tool
EMU	Efficient Materials Utilization
ETDOT	Environmental Technologies Design Option Tool
FaVOr	Fate of Volatile Organics in Wastewater Treatment Plants
HARD	Heuristics and Reactor Design
HPV	High Production Volume
IIA	Innovative Industrial Applications
LCA	Life Cycle Assessment
MC-Dist	Multi-Component Distillation Software
MOSDAP	Molecular Structure Disassembly Program
NMR	Nuclear Magnetic Resonance
NPV	Net Present Values
OPPT	U.S. EPA Office of Pollution Prevention & Toxics
P2	Pollution Prevention
P2TRG	Physical Property and Thermodynamics Research Group
PBT Profiler	Persistence, Bioaccumulation, and Toxicity Profiler
PE Index	Product Environmental Index
PHA	Polyhydroxyalkanoate
PMN	Pre-Manufacture Notice
PPMS	Physical Property Management System
SAC	Science Advisory Committee
SCENE	Simultaneous Comparison of Environmental & Non-Environmental Process Criteria
SCMCR	Simulated Counter Current Moving Bed Chromatographic Reactor
SGA	Scaled Gradient Analysis
SMILES	Simplified Molecular Input Line Entry System
SQC	Statistical Quality Control
StEPP	Software to Estimate Physical Properties
VOC	Volatile Organic Compound

THE CENTER AT A GLANCE

The National Center for Clean Industrial and Treatment Technologies (CenCITT) is a collaborative effort between Michigan Technological University (MTU), the University of Wisconsin-Madison (UW), and the University of Minnesota-Twin Cities (UM). CenCITT was established as one of four exploratory environmental research centers (out of 89 proposers) through a competitive proposal process. Primary funding for the Center is provided by the U.S. Environmental Protection Agency, National Center for Environmental Research. The original grant was awarded in June 1992, and renewed in September 1996 for an additional four years.

CenCITT's mission is...

to assist industry in pollution prevention by devising clean technologies and process design tools, and by pursuing promising leads in treatment, beneficiation, and reuse where prevention is not feasible.

CenCITT's goal is...

to help create industrial facilities in which waste is minimized through the application of economically sound technologies, and a combination of optimized manufacturing processes, treatment operations, and reuse of materials.

CenCITT's goal, mission, and overall philosophy translate into a strategic objective of "developing and promoting tools and technologies for sustainability". This objective is addressed through individual research projects supported under the base grant within the following focus areas:

Clean Reaction Technologies (CReaTe)

The goal of CReaTe is to establish and integrate concepts for the purpose of producing chemicals in an environmentally benign manner. The concepts include green chemistry, catalysis, reactor technology, plant integration and control as well as stewardship of raw materials, final products, and intermediates.

The Clean Process Advisory System (CPAS)

The goal of CPAS is to develop a collection of pollution prevention design tools that will allow designers to integrate pollution prevention and environmental considerations into existing process and product design environments.

Environmentally Conscious Manufacturing (ECM)

ECM concentrates on the principles of disassembly simulation and environmental assessment of assembly and materials processing practices used in manufacturing.

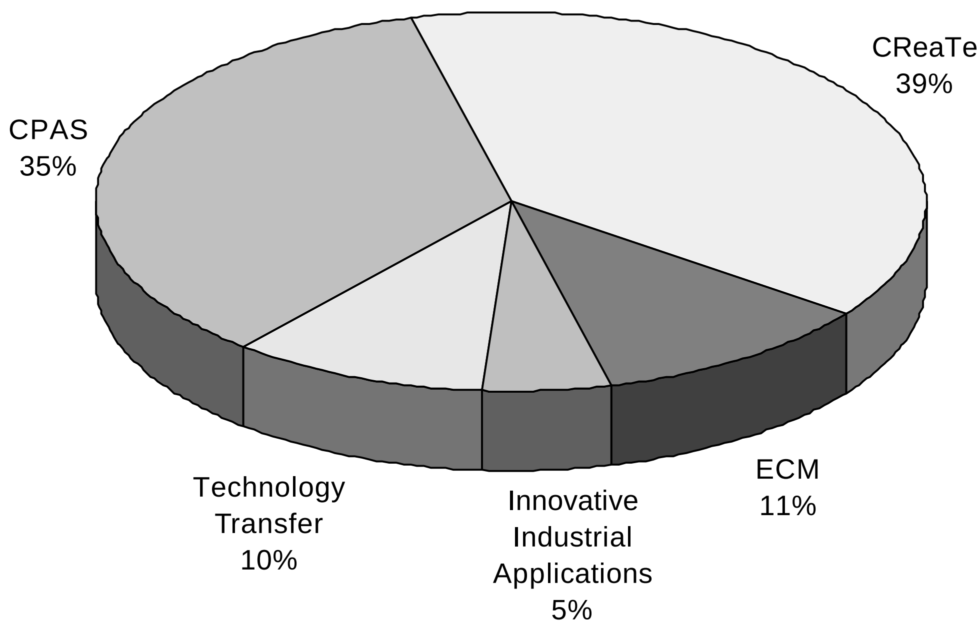
Innovative Industrial Applications (IIA)

This research area allows for flexibility beyond the specific focus areas stated above. Projects under this category include innovative technologies or applications that have a strong impact to industrial pollution prevention.

This report covers activities during the period of October 1998 through September 1999. Information regarding the Center's research activities between 1992 and 1998 may be found at http://cpas.mtu.edu/cencitt.

CenCITT Research Program Distribution

EPA FY1999 Allocation



Distribution of the U.S. Environmental Protection Agency FY1999 Allocation to CenCITT shown by Focus Area

DIRECTOR'S REPORT

Since the start of CenCITT in 1992, our primary objective has been to assist industry in pollution prevention by developing and promoting tools and novel clean technologies that lead to sustainability. As CenCITT nears the completion of its U.S. EPA base grant, we can all be proud that this objective is being met with much success. Our tools and clean technologies are providing industry with a means to enter a new era of sustainable manufacturing that is consistent with the needs of our society and the environment we live in.

Going into this final year, there is still much productive research and technology transfer activity in our focus areas as well as parallel activities. In the Clean Reaction Technologies (CreaTe) focus group, there is continued development of green chemical process technologies. The University of Wisconsin research groups are making advances in their development of green processes. Drs. Cortright and Dumesic successfully applied their microkinetic analysis to the development of a new catalytic process for the production of 1,2 propanediol by selective catalytic hydrogenation of lactic acid. Lactic acid can be easily obtained from renewable carbohydrate feedstocks instead of non-renewable petroleum. Dr. Root established the laboratory capabilities to synthesize novel silicalite catalysts. These catalysts are used with a benign co-reactant such as hydrogen peroxide to carry out the chemical synthesis reactions. Dr. Noguera is making strides in establishing the experimental protocol for evaluating the biosynthesis of polyhydroxyalkanoate polymers from industrial waste sludge. The MTU catalysis research group led by Drs. Chen, Hand, and myself successfully carried out the synthesis of methanol from methane gas using the photocatalytic oxidation process. Further work is ongoing to increase both the conversion and selectivity through catalyst modification and reactor operation.

In the area of Innovative Industrial Applications (IIA), MTU researcher Dr. Drelich is developing methods to recover waste polystyrene from metal casting processes. At the present time, his process is able to recover over 98% of the waste polystyrene. The University of Minnesota research groups are making advances in their development of innovative processes related to recovery and reuse of waste residuals. Dr. Sarkanen continues to have success in the development of biodegradable plastics using 100% Kraft Lignin-Based materials obtained from the Kraft black liquor byproducts generated at a Minnesota pulp mill. Dr. Semmens recently completed a study that recovered copper sulfate and purified water from acid copper electroplating rinse waters. Both of these Minnesota projects were originally funded under the former Efficient Materials Utilization focus area.

There is one project ongoing in the Environmentally Conscious Manufacturing area. Dr. Gadh's research group at the University of Wisconsin is developing a software package that can be used to assess the disassembly of manufactured products. His group is having significant interaction and exchange with several automotive and aerospace companies.

The Clean Process Advisory System (CPAS™) research area continues to make strides in software development and application. Drs. Rogers and Kline are creating a general software-based physical properties management data delivery system that will serve as an expandable framework for adding property estimation algorithms and third-party-generated data resources. This software will replace version one of StEPP and provide CPAS with physical property data.

Drs. Barna and Rogers completed the Design Options Ranking Tool (DORT) software which includes process economics and some environmental metrics. DORT software was completely redesigned and a licensing agreement with a value added reseller is near completion.

Drs. Shonnard, Barna, Kline, and Rogers are demonstrating the integrated assessment of chemical process economics (DORT) and environmental attributes (EFRAT) using the CPAS software. They are incorporating the CPAS process assessment tools with the optimizer in HYSIS chemical process simulator. These efforts successfully demonstrated input/output analyses and optimization by applying the integrated suite of CPAS tools to a case study.

Mr. Oman has been developing automated linkages between P2-related software design tools and the HYSIS chemical process simulator. This software incorporates linkages between DORT, EFRAT, U.S. EPA Office of Pollution Prevention and Toxics (OPPT) environmental tools, and HYSIS and is called Simultaneous Comparison of Environmental and Non-Environmental Process Criteria (SCENE). Version 1.0 of SCENE was developed and is presently being applied to a case study.

Drs. Mihelcic, Crittenden, and Hand and Mr. Hokanson are developing environmental indices for green chemical production and use. These indices enable the comparison of several existing risk assessment methods as applied to the High Production Volume (HPV) chemical manufacturing and use. The software will ultimately consider emission rates, toxicity, and more realistic attenuation mechanisms of chemicals will be developed to assist CPAS in evaluating the environmental performance of process alternatives.

Drs. Mullins, Kline, and Rogers developed a prototype Heuristics and Reactor Design algorithm to aid engineers in the conceptual design and engineering of clean chemical processes. This algorithm was applied to a catalytic membrane reactor model that is based upon a Stephan-Maxwell formulation for mass transfer, and incorporated into a radial reactor model. Comparisons to in-house permeation studies for zeolite membranes are being completed.

In addition to projects funded through the base grant, CenCITT researchers participate in several projects through external funding sources. These activities are consistently targeted toward addressing the general objective of “developing and promoting tools and technologies for sustainability”. An important distinction of these activities is that they typically have a high level of collaboration with other groups sharing similar objectives.

Examples include:

- Collaboration with the U.S. EPA Office of Pollution Prevention and Toxics (OPPT) in a Pollution Prevention Partnership Program - OPPT has developed many methods for screening the risk of chemicals in EPA's Pre-Market Notification Program. CenCITT is collaborating with OPPT to distribute and train several industrial groups in the application of the methods to screen chemical risk and identify pollution prevention opportunities. Use of the tools will result in companies making more environmentally responsible decisions when developing and selecting chemicals. Initial support for this activity was provided by EPA/OPPT. During the CenCITT 1998 proposal review cycle, this project was selected to receive support directly from the CenCITT/EPA grant to further the initial efforts.

- ChemAlliance - Since its launch on October 20, 1998, ChemAlliance, the compliance assistance web site for the chemical industry (www.chemalliance.org), continues to grow and provide useful information to the chemical sector. Readership continues to increase and includes a representative mixture of users from the regulated community as well as regulators and technical assistance providers. Demonstrating its value to the private sector, ChemAlliance was recently named a "select site" by the Dow Jones business directory.

- Continued development on pollution prevention decision making methodologies under a cooperative agreement with the U.S. EPA National Risk Management and Reduction Laboratory and the U.S. DOE Office of Industrial Technologies - This effort is entitled Pollution Assessment and Prevention Software for Chemical Industry Process Simulators. Under this effort, decision-making methodologies have been developed to allow process designers to quantitatively consider environmental, safety, and economic considerations during the design process. The prototype software tools have been transferred to the private sector through a Value Added Reseller agreement with Horizon Technologies of Littleton, Colorado. Horizon is currently working to commercialize and release the tools under the name DecisionMAPR™.

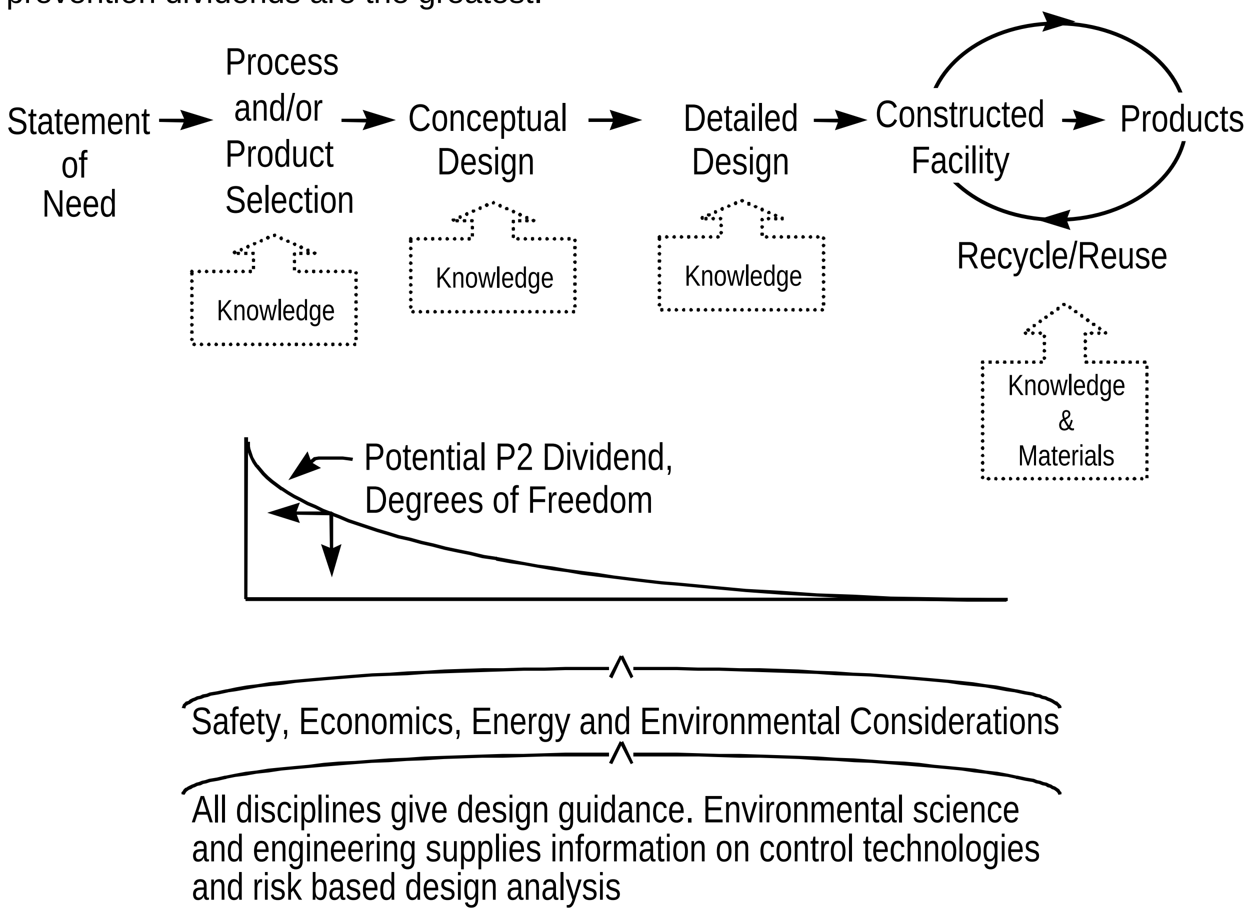
- The Department of Education funded a three-year project entitled: “Environmental Engineering Doctoral Fellowship Program for Risk Reduction of Persistent and Global Change Compounds”. This project will provide $478,125 in support for 5 Ph.D. students over a period of 3 years. This effort will undoubtedly aid in the development of the EFRAT software and environmental metrics for the CPAS effort.

- Jim Mihelcic and John Crittenden received additional funding from the City of Cedar Rapids to develop user friendly software for biofliters. This initiative will assist the Environmental Technologies Design Option Tool (ETDOT) effort. Currently, the City is operating a full scale biofilter which removes hydrogen sulfide (120,000 cfm of foul air, an influent concentration of 50 to 300 ppm and a treatment of objective of 0.5 ppm) and is experiencing occasional upsets. The purpose of the software is to develop strategies to predict and overcome these upsets.

These activities and other developing initiatives complement the efforts under CenCITT's base grant. The success of the projects within each Focus Area coupled with the external collaborative projects is extremely exciting as we look toward the future. These successes will ensure that the programs continue under alternate funding sources after the completion of the base grant.

Overview of Focus Areas

The following figure graphically represents the general design process that is followed by industry in translating societal statements of need into products that fulfill those needs. CenCITT's Focus Areas provide for pollution prevention research in issues throughout the entire design process. However, CenCITT's primary focus remains on the front-end, where the degrees of freedom for design and potential pollution prevention dividends are the greatest.



The primary input during most of the product development process is knowledge. Construction materials and chemical feedstocks are not considered until facility construction and product manufacturing. However, decisions regarding the input materials and feedstocks of choice are made during the process/product selection stage of the design process. Therefore, it is essential that environmental considerations be considered early in the design process before environmentally beneficial alternatives are eliminated.

Projects within the Clean Process Advisory System target the stages of process selection and conceptual design by developing design tools to identify and rank technology and design options. These tools will ultimately be able to rank options on the basis of environmental impact, and worker and consumer safety, and economics.

Projects within Environmentally Conscious Manufacturing (ECM) range from process/product selection to product recycle. The research underway in the area of dry-machining addresses process selection: "are traditional cutting fluid processes or dry-machining processes suitable for a given application?". In contrast, the ECM research in disassembly addresses the recycling of consumer products that are currently being manufactured.

Innovative Industrial Applications (IIA) is an adaptation of a previous Focus Area titled Efficient Material Utilization (EMU). IIA focuses on projects involving high volume industrial materials, potential waste stream elimination, and the development of methods to produce useful products from wastes.

Research in the Clean Reaction Technologies Focus Area has the strongest technology component and will result in the development of new technologies or processes (e.g. catalysts and reactors). These new technologies and processes will provide designers with more environmentally friendly options at the process selection stage.

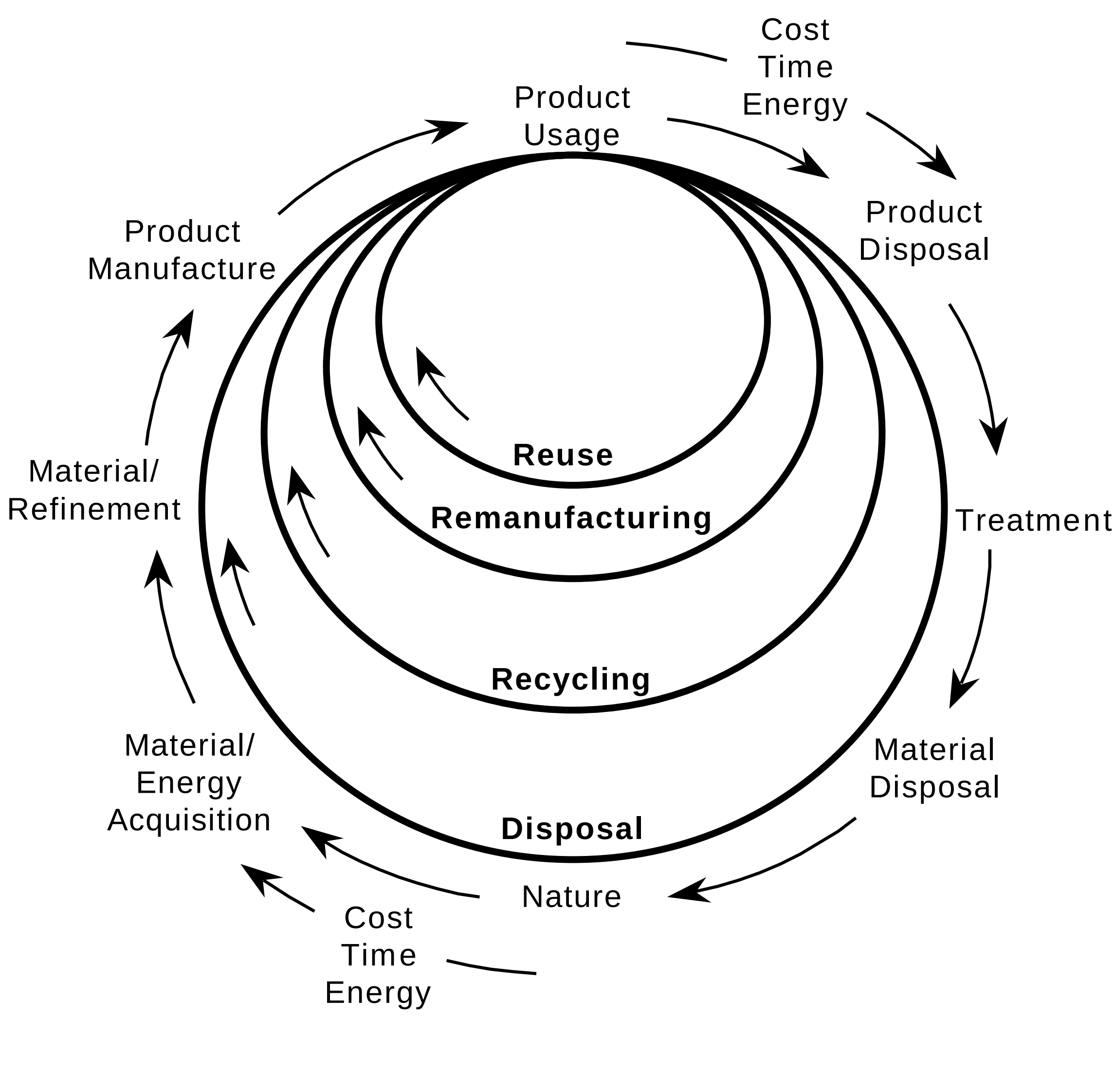
CenCITT's research program addresses the entire design in an effort to address both present and future P2 problems. By identifying product recycle and reuse opportunities near the end of the design line, CenCITT is reducing the burden of existing processes, products, and technologies on the environment. By developing new clean process technologies and decision-making tools for use early in the design process, CenCITT is helping to ensure that the products, processes, and technologies of the future will be more environmentally benign.

A detailed description of each Focus Area is presented below. Please refer to the Research Project Descriptions section of this report for summaries of each current CenCITT project.

Environmentally Conscious Manufacturing

The goal of the Environmentally Conscious Manufacturing (ECM) Focus Area is to develop tools and methods that characterize the environmental impact of product designs. With environmental information at their fingertips, designers may modify the design to reduce environmental impact while maintaining other product-related constraints.

ECM is directed at the environmental issues surrounding the life cycle of discrete products. The figure below has frequently been used to illustrate the life cycle for products such as automobiles, lawn mowers, blenders, and washing machines. The cycle begins with material extraction from nature, and includes the material processing, manufacture, use, and post-use handling of a product. Movement through the life cycle (clockwise motion) has costs (direct and societal) and energy consumption associated with it.



The life cycle illustrates that even the post-use handling of a product (including demanufacturing, treatment, and disposal) adds to the life cycle costs and energy consumption. The figure also indicates that in addition to the product disposal option, demanufacturing also considers reuse, remanufacturing, and recycling. These options are preferred over disposal since they increase the useful life of the product. It may also be noted that the inner loops are preferred over the outer loops because potentially less raw materials, energy, time and cost would be involved in manufacturing.

In responding to the needs of customers, product designers must carefully consider the life cycle depicted above. A variety of design-related decisions control the ability of the product to satisfy form, fit, function, cost constraints, production schedules, and environmental impact. These include:

- material selection
- part geometry and dimensions
- surface character
- component orientation and attachment to form and assembly
- manufacturing process plan
- process conditions
- demanufacturing (including disassembly-related issues and post-use processing choices)

While designers have become facile in making many of these decisions, they have little experience in terms of environmentally-responsible driven metrics. This Focus Area seeks to remedy this deficiency.

Clean Reaction Technologies

The Clean Reaction Technologies focus area (CReaTe) within CenCITT has been established to integrate concepts at different scales for the purpose of industrially sustainable pollution prevention. The CReaTe focus area consists of research projects involving:

1) the analysis of catalytic chemistry at the microscale for the rational design of selective catalyst required for green chemistry;
2) the development of microorganisms for benign biosyntheses;
3) the development and analysis at the micro- and mesoscale of separative reactors; and
4) at the macroscale, the stewardship of chemical raw materials, final products and intermediates.

CenCITT and several industrial and governmental partners are collaborating on the development of experimental and theoretical methods for the rational design of commercially competitive and less polluting catalytic reactions. Researchers within CenCITT have developed the concept of microkinetic analysis to combine the results from physical, chemical and spectroscopic measurements of a catalytic system to formulate molecular models that provide critical information of catalytic processes. This methodology has proven effective for the development of new highly selective hydrocarbon processing catalysts required for the production of components necessary for clean motor fuels. Furthermore, microkinetic analysis provides a chemical basis for kinetic expressions required in the design and modeling of chemical reactor technologies needed for the treatment of process streams containing ppm contaminant levels.

Microbial catalysts have great potential growth in the selective production of specialty chemicals. There are limits to what catalytic chemistry can do; consequently CenCITT is developing reactors that separate reactants and products during reaction thereby greatly improving the conversion of reactants to the desired products. Lastly, tracking the production of chemical feedstocks through the various intermediates allows CenCITT to compare the greenness of various approaches in producing chemical feedstocks and can be used to decide the needs for development of new chemical pathways and catalysts.

Clean Process Advisory System

The Clean Process Advisory System (CPAS) is an integrated system of software design tools which design engineers can use to incorporate pollution prevention (P2) methodologies into process and product design. The CPAS software tools provide the P2 component of an overall "Engineering Analysis Environment" as depicted in Figure 1. This "Engineering Analysis Environment" provides the following three-tiered approach: (1) **Find** candidate technologies; (2) **Simulate** and size equipment; and (3) **Compare** and rank candidate options. This conceptual structure allows designers to work with process simulation and design tools they are currently familiar with while supplying additional economic, environmental, and safety information through the CPAS tools.

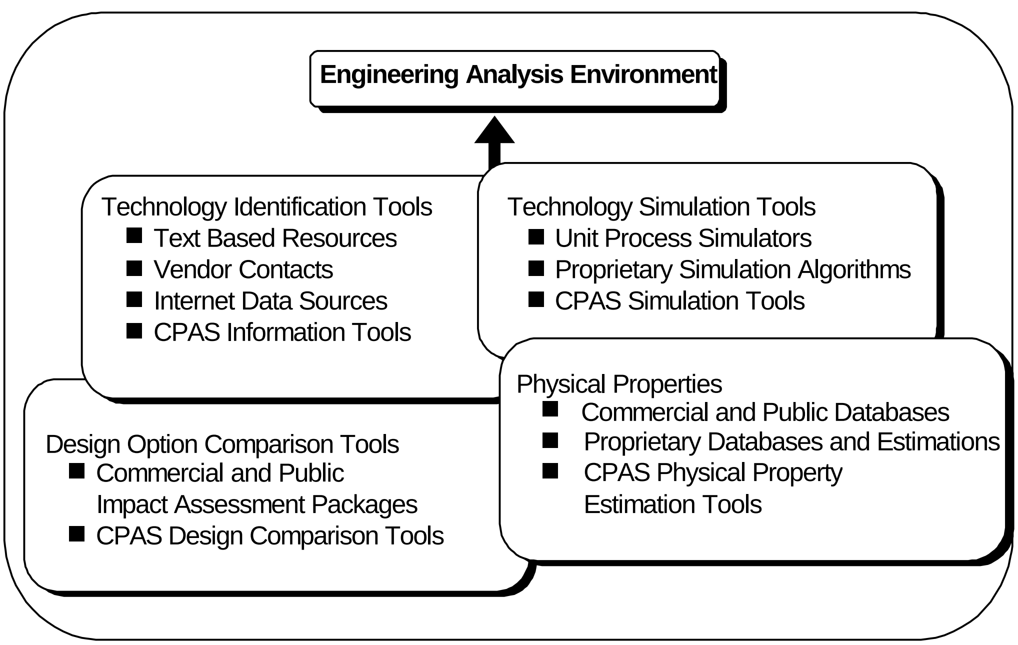


Figure 1. - Overall "Engineering Analysis Environment" that Encompasses CPAS

In previous years, several design tools have been completed under the CPAS banner. These include the Center for Waste Reduction Technologies (CWRT) Information Tools (Find) and Environmental Technologies Design Option Tools (Simulate). Two portions of the Compare aspect have been well-developed in earlier phases of the CPAS Focus Area efforts: economic considerations in the Design Options Ranking Tool (DORT) and process safety considerations. The Physical Properties Management System (PPMS) has fulfilled the need for accurate physical property values. The Environmental Fate and Risk Analysis Tool (EFRAT) which is used to evaluate the environmental impact of a process was completed. However; further refinements in EFRAT are being performed during this final funding cycle. In addition, the environmental and economic comparisons within CPAS are being optimized using the Analytical Hierarchy Process and scaled gradient analysis.

CPAS researchers are focusing their efforts on integration, demonstration and dissemination of all the CPAS tools. Under a current project entitled “Simultaneous Comparison of Environmental and Non-Environmental Process Criteria” (SCENE), automated linkages between all CPAS Tools are being established. In addition, automated linkages between CPAS tools and a Hyprotech commercial process simulator called HYSYS are being made. These linkages will enable industry and decision-makers to evaluate and integrate pollution prevention design practices and dividends into process design and operation. Demonstrations of CPAS applications are being developed and presented in this final year to demonstrate the benefits of incorporating pollution prevention decisions into product and process design.

Innovative Industrial Applications

To allow for flexibility beyond the Focus Areas described above, an additional general category was added to CenCITT's research program in 1998. This area is titled Innovative Industrial Applications (IIA). As the title suggests, projects in this area must constitute innovative technologies or applications that have a strong impact on industrial pollution prevention.

IIA is an adaptation of a previous Focus Area titled Efficient Material Utilization (EMU). EMU's objective was to produce step reductions in pollution generation by focusing on the production of useful products from high volume industrial materials currently thought of as wastes. IIA also seeks to focus on projects involving high volume industrial materials. However, the scope of IIA has been broadened to include potential waste stream elimination through innovative process changes and technology development in addition to the development of methods to produce useful products from wastes.

Technology Transfer

In the absence of technology transfer, the greatest discoveries and technical achievements have marginal value at best. Therefore, technology transfer continues to be an integral component of CenCITT's program. CenCITT firmly believes that technology transfer is a two-way street whereby the needs and existing capabilities of industry are actively pursued, and the technologies and concepts generated are transferred to address those needs. Each member of CenCITT's research program plays a key role in communicating the discoveries and technological advances generated.

The topic of technology transfer has recently begun to be referred to more broadly as "knowledge transfer". This broadening of scope is quite appropriate considering that technology itself is only one component of scientific discoveries. Communication of the knowledge and fundamental understandings that have resulted in and from the technology is commonly more important than the technology itself.

This concept is especially appropriate in the field of pollution prevention where there is a need for both: 1) the development of new technologies for process, material, and energy efficiency, and 2) a change in the culture of those who implement technology to produce consumer goods and services. This process of transferring knowledge in addition to transferring technology has been, and continues to be, a significant component of CenCITT's outreach efforts.

During this period, CenCITT researchers and staff have been involved in a number of technology transfer activities. The table below summarizes the activities during the FY 1999 period. For the complete listing, please see the bibliography section at the end of this report. A few events are highlighted on the following pages.

CenCITT Publications and Technology Transfer Activities - FY 1999

ACTIVITY TYPE	NUMBER
Refereed Journal Articles	8
Articles Submitted for Publication	4
Books, Chapters, or Bound Proceedings	11
Major Project Reports	1
Theses/Dissertations	6
Patent Disclosures	2
Research Presentations	31
Technology Transfer Meetings and Presentations	14
Conferences/Meetings Held	1
TOTAL	78

The CPAS Environmental Technologies Design Option Tool (ETDOT) is presently being developed and marketed. During 1999, 26 copies of ETDOT have been sold to several universities, consulting engineering firms, and industrial companies; including two academic 50-site licenses. Two new ETDOT components, Advanced Oxidation (AdOx™) and the Fate of Volatile Organics (FaVOr) software have been completed and will be released for sale in July, 2000.

CenCITT researcher James Baker gave a presentation, “Decision-Making Tools for the Chemical Process Industry", on February 18, 1999 at the Tools for Sustainability Workshop in Washington, DC, sponsored by the U.S. Environmental Protection Agency. Co-authors of this presentation, John Crittenden, and Eric Oman were also in attendance and participated in the workshop roundtable discussion and other activities.

CenCITT researchers made a significant contribution at the 1999 Annual Meeting of the American Institute of Chemical Engineers, Dallas, TX, October 31 - November 5, 1999. Three papers on CPAS applications were presented:

1) “Defining an Analytic Hierarchy Process (AHP)-based Approach for Simultaneous Consideration of Environmental and Economic Process Attributes”, presented by MTU graduate student Hui Chen and co-authored by MTU graduate student Brenden O’Donnell, Drs. David Shonnard, Tony Rogers, Bruce Barna and Andrew Kline, and Research Engineer Eric Oman.
2) “Environmental Assessment and Optimization of Chemical Process Designs”, presented by Dr. David Shonnard and co-authored by MTU graduate student Dennis Hiew.
3) “Integrated Assessment tools as Process Simulator Enhancements for Chemical Engineering Education presented by MTU graduate student Hui Chen and co-authored by MTU graduate student Dennis Hiew, Research Engineer Eric Oman and Drs. Andrew Kline, David Shonnard, Tony Rogers, Bruce Barna and Daniel Crowl.

A large group of CenCITT researchers participated in the week long United Engineering Foundation’s Clean Products and Processes II conference held November 14-19, 1999 in Lake Arrowhead, CA. The conference provided an opportunity for scientists and engineers to explore problems and issues of concern related to pollution prevention and sustainable manufacturing.

CenCITT Director John Crittenden chaired a session, “Applications of Life Cycle Assessment (LCA)”, co-chaired by MTU Research Engineer David Hokanson. MTU Associate Professor David Shonnard made a podium presentation in the LCA session entitled “An Environmental Assessment Framework for Chemical Process Designs,” co-authored by MTU graduate student Dennis Hiew (currently of Essential Technologies Incorporated) and MTU graduate student Hui Chen. University of Wisconsin Research Professor Randy Cortright made a podium presentation in the Cleaner Materials and Products session entitled “Selective Catalytic Processing of Lactic Acid to Commodity Chemicals”.

In addition to the talks mentioned above, several posters were also presented at the conference:

(1) "Use of Material Selection Target Plots for Screening Chemicals based on Environmental and Health Properties", co-authored by MTU graduate student Marcela Velazquez-Carillo, MTU Associate Professor James Mihelcic (presenter), and Crittenden.
(2) "P2 Workshop: An Internet-Based Workshop for Pollution Prevention Curriculum Development", co-authored by Shonnard and Stephen Beaudoin from Arizona State University.
(3) "Mathematical Modeling of Isothermal-Three Phase Separative Reactor Systems", co-authored by MTU graduate student Ji Yang, MTU Research Engineer Eric Oman, MTU Associate Professor and CenCITT Program Manager David Hand, Hokanson, and Crittenden (presenter).
(4) "Environmental Indices for Green Chemical Production and Use", co-authored by MTU graduate student Qiong Zhang, Crittenden, Hand, Mihelcic, and Hokanson (presenter).
(5) "CenCITT's Tools for Sustainability," co-authored by MTU Corporate Relations Associate Director James Baker, MTU Professor Bruce Barna, former MTU Research Engineer John Bulloch (currently of Trinity Consultants), Crittenden, MTU Professor Daniel Crowl, Hand (presenter), Hokanson, MTU Senior Research Engineer Andrew Kline, MTU Associate Professor Alex Mayer, Mihelcic, Oman, former MTU Assistant Professor Robert Patty (Brigham Young University), MTU Corporate Relations Director Peter Radecki, MTU Associate Professor Tony Rogers, Shonnard, University of Minnesota Professor Michael Semmens; Manager of Pollution Prevention and Value Engineering Darryl Hertz (Kellogg Brown and Root, Inc) and Senior Research Scientist Scott Butner (Batelle/Pacific Northwest National Laboratory).

CenCITT Researchers also presented two papers at the 22nd Annual Midwest Environmental Chemistry Workshop held at Michigan Tech University, October, 1999. Dr. Yongsheng Chen presented a paper entitled, "Advances in TiO_2 Photocatalytic Oxidation Process," co-authored by Drs. John Crittenden and David Hand and Research Scientist Volker Selzer. MTU Graduate Student Qiong Zhang presented a paper entitled, ""Environmental Indices for Green Chemical Production and Use," co-authored by Drs. John Crittenden, and James Mihelcic, and Research Engineer David Hokanson.

CenCITT has also held meetings to identify needs and/or collaborative opportunities with SASOL, Exxon, Texaco, Amway, Abbott Labs, Chrysler, Pratt & Whitney, United Technologies, Boeing, Ford, General Motors, and others. Continuing the philosophy that technology transfer is a two-way street, CenCITT continues to pursue venues with industrial consortia, individual companies, government agencies, and other stakeholders.

Quality Assurance/Quality Control

CenCITT's Quality Assurance/Quality Control (QA/QC) plan is implemented at the project level and is the responsibility of each Project Investigator. The general CenCITT plan is tailored to integrate with the needs, aim, and type of each project. For example, projects which do not include experimental data collection (e.g. modeling, process simulation, industrial needs surveys) will not have an experimental QA/QC plan. QA/QC procedures for projects which include experiments and data collection normally consider the accuracy of results required for the stated intention of the work. For example, a study to examine industrial feasibility of a new technology would normally not require reagent purities as high as those demanded by catalytic reaction product determinations. Screening experiments may not require as many repeat experiments as pure component property measurements.

The CenCITT internal Request for Proposals requires that each proposed project develop a QA/QC plan and appoint a QA/QC supervisor. The Science Advisory Committee reviews each plan as part of the proposal review process. Since almost all of CenCITT's research includes participation from graduate and undergraduate students, QA/QC is as much of an educational process as a set of experimental guidelines. CenCITT's goal is to emphasize quality in such a way that it becomes second nature to all students involved with its projects. Communication among students and faculty throughout CenCITT is encouraged so that plans and analytical procedures can be compared and constantly improved upon.

TECHNICAL HIGHLIGHTS

- CenCITT Researcher Dr. Daniel Crowl, the Herbert Henry Dow Professor of Chemical Process Safety at MTU, has received the 1999 Safety and Health in Chemical Engineering Education Award of Excellence from the Joint Council for Health, Safety, and Environmental Education of Professionals. Crowl was presented the $1,000 award at the November 1999 meeting of the American Institute of Chemical Engineers in Dallas. The joint council supports health, safety, and environmental education in post secondary schools and is made up of engineering and other professional societies, as well as related government agencies and organizations.

- CenCITT researchers Drs. Yongsheng Chen, David Hand, John Crittenden, and Research Scientist David Perram developed a photocatalytic partial oxidation process capable of conversion of methane gas to methanol. Their successful research efforts have led to filing a patent application. In addition, the process has gained the interest of three major oil companies and further development funding from a third party is under negotiation.

- CenCITT researcher Dr. Jaroslaw Drelich was appointed to the Editorial Advisory Board of the Journal of Adhesion Science and Technology. Dr. Drelich applies fundamental concepts of adhesion to separation of materials including separation of coatings from waste polymeric patterns.

- CenCITT researchers Randy Cortright, James Dumesic, and Dale Rudd at the University of Wisconsin have enjoyed great success in the field of catalysis using microkinetic analysis, which is now well established. More recently, their research has resulted in the invention of a new method to produce 1,2 propanediol through the catalytic hydrogenation of lactic acid. This vapor-phase method employs a copper-based catalyst and operates at atmospheric pressure in the presence of water vapor. Currently, a patent is being pursued for this technology through the Wisconsin Alumni Research Foundation.

- CenCITT Director John Crittenden's Editorialship with Environmental Science and Technology Journal was renewed for another two years.

- CenCITT Researcher and MTU Associate Professor Dr. James Mihelcic was lead author in a recently published text book entitled "Fundamentals of Environmental Engineering" for beginning Environmental Engineering undergraduates. The text is now being used at over 17 schools including Rensselaer Polytechnic Institute, Rutgers University, University of Michigan, and Michigan State University. The textbook is also being translated into Spanish for use in Latin America. In addition, Dr. Mihelcic was appointed to the Editorial Advisory Board of the Journal Chemosphere.

CenCITT 1998-99 PROJECT LISTING

Project Title w/Project Investigators	End Date	Current Budget	Total Budget *
Clean Reaction Technologies (CReaTe)			
Selective Catalytic Hydrogenation of Lactic Acid J.A. Dumesic, R.D. Cortright	2000	$90,790	$752,852
Biosynthesis of Polyhydroxyalkanoate Polymers from Industrial Wastewater D.R. Noguera	2000	$55,470	$55,470
Tin Zeolite Catalysts for Partial Oxidation with Hydrogen Peroxide T.W. Root	2000	$93,750	$93,750
Development of a High Performance Photocatalytic Reactor System for the Production of Methanol from Methane in the Gas Phase D.W. Hand, J.C. Crittenden, Y. Chen, D.L. Perram	2000	$103,112	$103,112
Partial Oxidation of Methane to Methanol R.W. Carr	1999	$71,978	$228,624
Heuristic Reactor Design for Clean Synthesis and Processing - Separative Reactors M.E. Mullins, A.A. Kline, T.N. Rogers	1999	$61,200	$115,725
Clean Process Advisory System (CPAS)			
Establishing Automated Linkages between Existing P2-Related Software Design Tools E.J. Oman, T.N. Rogers, B.A. Barna, J.C. Crittenden, D.R. Hokanson	2000	$104,143	$104,143
Development of Environmental Indices for Green Chemical Production and Use J.C. Crittenden, D.R. Hokanson, D.W. Hand, J.R. Mihelcic	2000	$58,775	$58,775
Industrial Implementation of the P2 Framework J.L. Bulloch, J.C. Crittenden, D.W. Hand, V.H. Selzer	2000	$55,177	$55,177
Integrated Applications of the Clean Process Advisory System to P2-Conscious Process Analysis and Improvement D.R. Shonnard, T.N. Rogers, B.A. Barna, A.A. Kline	2000	$111,229	$111,229
Clean Process Advisory System Core Activities J.R. Baker, B.A. Barna, P.P. Radecki, T.N. Rogers	1999	$124,270	$499,009
Development and Testing of Pollution Prevention Design Aids for Process Analysis and Decision Making B.A. Barna, T.N. Rogers, A.A. Kline	2000	$71,388	$426,521
Development and Demonstration of Environmental Technologies Design Option Tool (ETDOT) D.W. Hand, J.C. Crittenden, D.R. Hokanson, T.N. Rogers, A.S. Mayer, M.J. Semmens	2000	$153,949	$486,177
The Physical Properties Management System (PPMS): A P2 Engineering Aid to Support Process Design and Analysis T.N. Rogers, A.A. Kline	2000	$57,567	$398,117
Environmentally Conscious Manufacturing (ECM)			
Integration of Environmentally Conscious Manufacturing and De-manufacturing Through the Development and Use of a Product Environmental Index for Industrial Mechanical Assemblies and Their Constituent Components R. Gadh	2000	$93,750	$293,750

Project Title w/Project Investigators	End Date	Current Budget	Total Budget *

Innovative Industrial Applications

Recovery of Waste Polymer Generated by Lost Foam Technology in the Metalcasting Industry J.W. Drelich	2000	$57,209	$57,209
Means for Producing 100% Kraft Lignin-Based Biodegradable Plastics S. Sarkanen	1999	$54,236	$183,071
Assessment of an In-Line Copper Recovery Technology as a Waste Reduction Strategy for the Metal Finishing Industry M.J. Semmens	1999	$42,174	$84,348

CenCITT project accounts include cost share such as cash contributions, academic release time, and overhead reduction as validated by the research administrations of the consortium institutions. Many of the projects include additional cost sharing which are not a part of the CenCITT project accounts. Examples include industrial in-kind, such as access to equipment or data; visiting engineers; and parallel activities at sponsoring organizations.

* Several CenCITT projects have been funded for more than one funding cycle. Total budget column includes cumulative funding, including cost share, from multi-year projects.

RESEARCH PROJECT DESCRIPTIONS

Environmentally Conscious Manufacturing (ECM)

Design for Disassembly (DFD) in De-Manufacturing of Products Rajit Gadh, University of Wisconsin-Madison (References: Figueroa, 1999; Gadh, 1998; Gadh, 1999a,b,c,d,e; Lee and Gadh, 1998; Lee, 1998; Shyamsundar et al., 1998; Srinivasan and Gadh, 1999a,b,c,d,e; Srinivasan et al., 1999a,b,c;)

Goal: The research goals are:

1) Allow environmental engineers and designers at different locations to collaborate and design products that can be assembled in a cost-effective manner so that final disassembly and disposal of the materials and components in them can be effectively and economically achieved.
2) Generate automatically the disassembly and disposal instructions from the product design information, using the DFD tool, which can be accessed by the person in charge of disposing the product via the De-Manufacturing Web.
3) Empower the consumer to dispose the product in an environmentally sound manner, following the disassembly instruction on the web, in a way that would maximize reuse and minimize waste.

Rationale: Design for Disassembly (DFD) allows efficient separation of components for product recycling and disposal. Currently, products are acquired with no clear plan of disposal of the product. Often, consumers are left with no other choice at the end of a product's life but to dispose of it by throwing it in the trash.

The de-manufacturing program at the University of Wisconsin-Madison addresses the question of systematically designing for easier products dismantling and disposal. Moreover, financial measures for justification of de-manufacturing in the Product Life Cycle to companies encourages them to invest further in design for disassembly methodology.

Approach: This research develops a framework for allowing the investigation of the universal Product Environmental (PE) index for a given product directly during design and well before production. The PE index determines the environmental impact engendered by the creation and dismantling of mechanical product sub-assemblies, within automobile or aircraft. By comparing and contrasting different design alternative, the optimal PE index value design may be selected.

Status: The PE index is being defined that is valid within a given class of manufactured products. The definition of PE index is based partly on existing indices and partly on new research findings regarding the environmental effects of creating and dismantling products. While existing indices have relied primarily on the pollution due to the chemical constituents to measure environmental consequences, these definitions will be expanded to include mechanical component fabrication, assembly activities, disassembly activities, and component de-fabrication activities.

The first focus is on plastic assemblies, which have the following important characteristics with respect to mechanical de-manufacturing:

(I) Dies are expensive and have significant environmental implications.

(II) The following variables in a die are expected to be the most significant contributors to PE: (a) shape, (b) tolerance, and (c) weight/volume/size/bulk.

(III) The injection molding process has significant PE impact due to energy needed in manufacturing.

(IV) The assembly process requires energy and so will add to the PE.

(V) The disassembly process tends to be energy-expensive and is expected to contribute significantly to the de-manufacturing process. At the conclusion of the project, the effect of design decisions on the PE index contribution due to the above product life cycle steps will be determined.

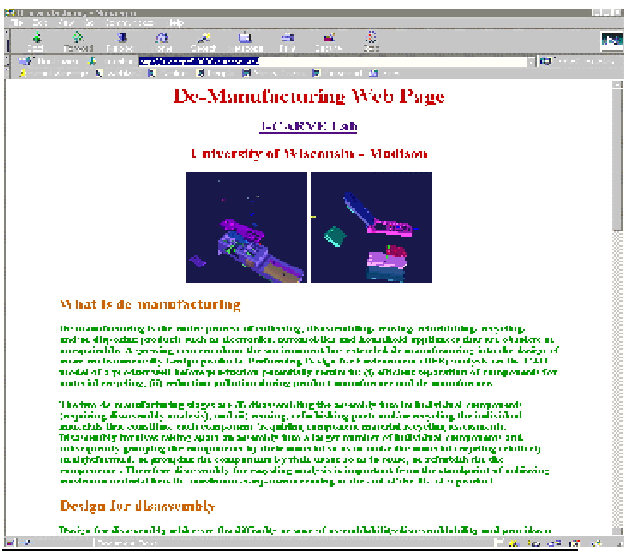


Figure 1. De-Manufacturing Web

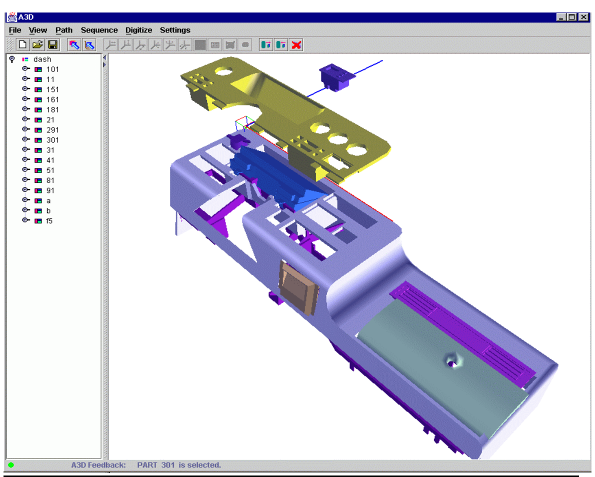


Figure 2: Example of Dashboard Disassembly

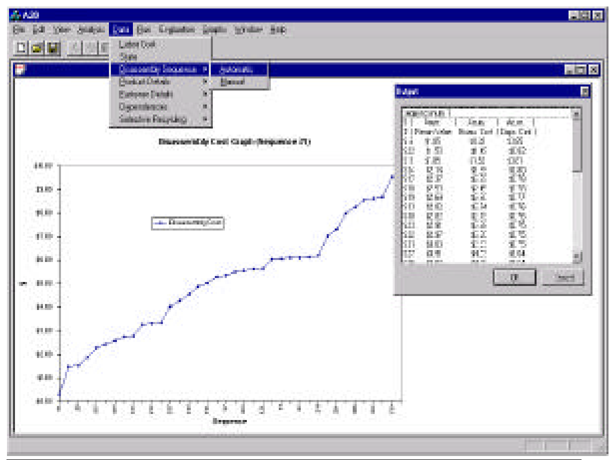


Figure 3. DFD Tool: Recycling Assessment

A web-based software tool called De-Manufacturing Web that supports collaborative de-manufacturing (dis-assembly, service, recycling and disposal) between manufacturer, de-manufacturer, disposer, customer and designer, is being developed. A web-enabled DFD software program has been developed for determining the disassembly sequence and cost of product assemblies utilizing the product domain, material, and environmental databases. Some of the Preliminary implementation results (including automotive and consumer electronics) of the DFD tool are presented in Figures 1-3.

Additional information on the De-manufacturing Web tool can be found at http://emedia_pc1.emedia.engr.wisc.edu/deman/. Additional information on the DFD tool can be found at http://smartcad.me.wisc.edu/groups/disassembly.

Application of software to real-world product designs: The research methodology and the software has been applied to two classes of products:

1) electro-mechanical assemblies - cellular phone and printer assemblies, and
2) large mechanical assemblies - dashboard subassembly, IC engine assembly, augmentor assembly, aircraft engine subassembly and conceptual aircraft assembly.

Collaboration with industry: Significant interaction and exchange has occurred with several automotive and aerospace companies. Currently, Prof. Gadh is having discussions with Ford, Hayes Lemmerz (an automotive supplier), and Pratt & Whitney on using the software developed for specific applications within each company.

The DFD software system has been demonstrated to the following industrial groups: Pratt & Whitney-Florida, United Technologies Engineering Coordinate Activities-Connecticut, and Stanford University workshop on Virtual Prototyping attended by several companies including Boeing, GM, and General Electric.

Graduate student Ramon Figueroa spent the summers of 1998 and 1999 with Pratt and Whitney/United Technologies, West Palm Beach, Florida. There, he investigated jointly with Pratt and Whitney the usage of the DFD software system within their Engineering Design and Manufacturing programs.

Clean Reaction Technologies (CReaTe)

Selective Catalytic Hydrogenation of Lactic Acid Randy D. Cortright and James A. Dumesic, University of Wisconsin-Madison

Goal: The goal of this project is to identify and develop methods for the selective catalytic processing of lactic acid to 1, 2-propanediol.

Rationale: Currently, a number of agriprocessing and chemical companies are entering the lactic acid market as they have or will soon be starting-up large scale fermentation processes to produce lactic acid from carbohydrates. The combination of fermentation processes and selective catalytic processes would provide a clean route for the production of 1,2-propanediol from renewable carbohydrates feedstocks instead of from non-renewable petroleum.

This project utilizes principles developed during previously funded CenCITT projects to investigate two possible catalytic reaction pathways:

(1) the direct hydrogenation of lactic acid to 1,2-propanediol over a supported metal catalyst and;
(2) the esterification of lactic acid to ethyl lactate over a solid-acid catalyst followed by the hydrogenation of ethyl lactate to 1,2-propanediol over a supported metal catalyst.

Approach: We are combining the results from microcalorimetric measurements, reaction kinetics studies, spectroscopic investigations, and density functional theory (DFT) calculations to elucidate pathways for the reactions of lactic acid, alcohols, diols, and esters over supported metal catalysts and solid-acid catalysts.

Catalysts will be characterized using transmission electron microscopy (TEM), FTIR, and chemisorption measurements. TEM measurements will supply information about the size and dispersion of metal particles on a given support. Chemisorption measurements will be used to count the numbers of sites on the various catalysts using standard probe molecules such as hydrogen, oxygen, carbon monoxide, and ammonia.

Status: This research has resulted in the invention of a new method to produce 1,2 propanediol through the catalytic hydrogenation of lactic acid. This vapor-phase method employs a copper-based catalyst and operates at atmospheric pressure in the presence of water vapor. Currently, a patent is being pursued for this technology through the Wisconsin Alumni Research Foundation.

Biosynthesis of Polyhydroxyalkanoate Polymers from Industrial Wastewater
Daniel R. Noguera, University of Wisconsin-Madison (References: Noguera and Drnevich, 1999)

Goal: The main goal of this project is to explore the use of industrial wastewater as an inexpensive food source for polyhydroxyalkanoate (PHA) accumulating bacteria. Specific objectives include:
1) evaluate the possibility of operating a biological process to maximize PHA production without compromising the quality of waste treatment,
2) test two different types of industrial wastewater for their potential utilization as raw material for PHA production, and
3) isolate and characterize efficient PHA-accumulating organisms from dual-purpose biological processes.

Rationale: PHAs are polymers of microbial origin that can be used for the manufacturing of biodegradable plastics. A significant cost in the commercial production of PHA-based plastics is the substrate used for the growth of the microorganisms. Thus, using industrial wastewater as the raw material could potentially reduce the cost of PHA production and increase the marketability of this environmentally benign product.

PHA accumulating bacteria are known to exist in biological wastewater treatment plants. The type of PHA stored depends on the characteristics of the food source. Thus, from biological processes fed with industrial wastewater it might be possible to isolate PHA-accumulating bacteria with unique PHA accumulating characteristics. These organisms might be of value for future biotechnological developments for PHA manufacturing.

Approach: The project is divided in four different tasks. During Task 1, analytical methods for PHA extraction and characterization will be implemented. Task 2 involves the operation of a bench-scale sequencing batch reactor to evaluate the operation of a biological process for the dual purpose of waste treatment and PHA recovery. The reactor will be maintained at a fixed solids retention time, but excess biomass will be removed at two different stages during the operational cycle, at the end of the anaerobic stage when cells are loaded with PHA, and at the end of the aerobic stage as is normally done in nutrient removal treatment processes.

During Task 3, the reactor will be operated with two different types of industrial wastewater, one simulating a carbon and nutrient-rich waste and the second one simulating a carbon-rich, nutrient-poor waste. During this operation, the accumulation of PHA will be characterized for different operational conditions (e.g., percent of wastage from anaerobic and aerobic stages will be varied). An alternative evaluation during this stage of the project will involve operation of the reactor with a pure culture of *Ralstonia eutrophus*, a known PHA-accumulating bacteria. The final task of the project is the isolation of microorganisms, from the bench-scale reactor, that are capable of storing PHA.

Status: A gas chromatographic technique for PHA quantification and characterization has been implemented. The bench scale sequencing batch reactor has been designed and constructed. The reactor was seeded with mixed liquor from a municipal wastewater treatment plant (Madison, WI) and has been in operation for about 40 days using synthetic wastewater. This start-up time was longer than originally expected. Experiments to characterize PHA recovery when sludge wastage is from the anaerobic and aerobic stages have been recently initiated. Because of unexpected delays during start-up, the schedule for reactor operation during Tasks 2 and 3 of the project will be modified. The isolation of PHA-accumulating microorganisms has not been initiated.

Tin Zeolites for Partial Oxidation Catalysis Thatcher W. Root, University of Wisconsin-Madison (References: Sever and Root, 1999)

Goal: This investigation of novel zeolites with tin framework substitution has the following two objectives:

1) exploration of reaction activity and selectivity for hydrogen peroxide partial oxidation of selected organic chemicals; and
2) mechanistic studies of tin active sites to define the limiting behavior possible with this class of catalysts.

Rationale: This research is significant for development of environmentally benign chemical processes. Partial oxidation reactions abound in the specialty chemicals, fine chemicals, and pharmaceuticals industries, and often use undesirable chlorinated reactants to activate the reactions, or have other inorganic co-reactants that produce substantial process waste. Replacement of these processes with new chemistry using the benign reactant hydrogen peroxide is desirable, but these new processes will require innovative catalysts that activate the peroxide and direct its selective oxidation reactions.

One successful example is the use of titanosilicalite TS-1 by an Enichem plant in Italy for the oxidation of phenol to hydroquinone and catechol (used in photography, pigments, and pharmaceuticals). Recent work has shown that substitution of tin, vanadium, or other reducible elements into silicalite can potentially produce new catalysts that allow control of the selectivity between products for these reactions. Other partial oxidation reactions using hydrogen peroxide, such as olefin expoxidation, are also possible with these catalysts, but have not yet been explored or developed into practical processes.

Approach: The project work plan involves several steps:

1) synthesis of novel tin-containing zeolites,
2) measurement of reaction kinetics and selectivities for candidate reaction systems, and
3) spectroscopic studies using a variety of sophisticated catalyst characterization techniques, including our specialty of solid-state multinuclear nuclear magnetic resonance (NMR) (for routine studies of Si, novel investigation of Sn).

Status: In our lab, we have established new capabilities for synthesizing silicalite and tin-containing silicalites. Several routine zeolite structural characterization or verification tools have been implemented, including XRD, FTIR, and ICP, which allow us to demonstrate critical tin incorporation into the zeolite lattice.

We have built, calibrated, and operated two batch microreactors that allow us to measure reaction kinetics and selectivities for our initial test reaction, oxidation of phenol to hydroquinone or catechol using hydrogen peroxide. We have also investigated the use of ethylbenzene oxidation as an alternative probe reaction. Now underway are experiments aimed at refining the zeolite synthesis, both to better control tin content and to extend products to other promising silicate lattices in addition to the MFI structure.

We are also improving reactor product analysis. Substantial effort is being focused on development of ^{119}Sn solid-state NMR as a novel probe of the active site in these poorly understood catalysts. Difficulties have been encountered in consistency of zeolite synthesis from batch to batch, especially in the crystal yield, so this is receiving ongoing attention as we strive to modify procedures to minimize variations and maximize yields.

Although this project contains funding for only one graduate student, there has been significant interest among our students and we have been able to collect a larger team using support from other sources:

- Robert Sever – third year graduate student pursuing Ph.D., focusing on reaction characterization, FTIR and NMR spectroscopy (NSF Fellow).
- Ulrich Hennings - second year graduate student pursuing an M.S., focusing on Sn-zeolite synthesis of MFI, MEL, and MTW frameworks, and associated characterization (XRD, ICP) (first-year support from German government on exchange program).
- Tutsomi Shimotoru - visiting student from Kyoto University's M.S. program, arrived September 1999 for nine months, focusing on preparing Sn-, Ti- and V-silicalite series, and adding porosity (gas sorption) characterization capabilities.
- Undergraduate Independent Study (ChE 599) students: Matt Kalscheur, Spring 1999 - initial zeolite synthesis; John Lin, Summer 1999 - hydrogen peroxide conversion analysis on reactor; and Erin Mehlis, Fall 1999 - test reactor operation.

Development of a High Performance Photocatalytic Reactor System for the Production of Methanol from Methane in the Gas Phase David W. Hand, John C. Crittenden, Yongsheng Chen, and Dave L. Perram, Michigan Technological University (References: Chen, Y., et al., 1998, 1999; Dechapanya, 1999)

Goal: The goal of this project is to investigate the potential of TiO_2 catalysts for a low temperature and low pressure chemical synthesis route to convert methane to methanol and to design a laboratory separative reactor system that can convert methane to methanol for use as a commercial grade feed.

Rationale: Worldwide reserves of methane are an underutilized resource. For example, substantial quantities of methane are usually associated with the extraction of crude oil. Methane is usually flared into the atmosphere because it is too expensive to transport for industrial and commercial use. The production of methanol from methane provides many economic and pollution-prevention dividends.

For instance, the use of methanol reduces greenhouse gases associated with the extraction of crude oil. Methanol is in demand as an inexpensive fuel oxygenate and a feed stock for commodity chemicals. It is being investigated as an alternative fuel for conventional auto engines, which will reduce CO, NO_x, volatile organics, and benzene emissions from automobiles making it a cleaner burning fuel than coal or petroleum.

Approach: We developed high performance photocatalytic catalysts using surface modifications such as metal semiconductor modification, surface sensitization, and transition metal doping. Conversion to the desired product methanol is adversely affected by further oxidation of methanol to species such as carbon monoxide or carbon dioxide, and this tendency must be reduced. One strategy for reducing this tendency is to remove the methanol from the reactive environment immediately upon formation.

This photocatalytic separative reactor system for partial oxidation of methane to methanol will be developed in this project.

Status: The energy requirements for conversion of methane to methanol using different processes including electrochemical process, solar process, and lamp process have been calculated. The energy required for production of one mole methanol from methane is 4.5 einstein (at 365nm).

The photoreactor system made from M_7 tubing and quartz tubing has been designed, built and preliminarily tested. The results in the fixed bed photoreactor system showed that the methane conversion, catalyst activity, and quantum efficiency were 8.2%, 2.935 µmol/g/min, and 49.5% respectively. Experiments are ongoing to increase the conversion rate and selectivity by optimizing the CH_4/O_2 ratio at influent stream, the relative humidity, the empty bed contact time (EBCT), and the reaction temperature, and by cycling the lights on and off to remove methanol while the lights are off before continuing the conversion with the lights on. A photocatalytic model is being developed to increase our understanding of the operation and optimization of our photocatalytic reactor system.

The explorations of adding alkali-metal ions including Li^+, Na^+, K^+, and Rb^+ to modify our silica-supported metal oxide catalysts are ongoing because alkali-metal ions have electron-donating ability, which leads to an enhancement of basicity of metal oxides. These investigations will be helpful in understanding the effect of an alkali-metal addition for partial oxidation of light alkanes. Furthermore, the addition of NO to increase the conversion and selectivity has been investigated.

Investigation of the Partial Oxidation of Methane to Methanol in a Simulated Countercurrent Moving Bed Chromatographic Reactor Robert W. Carr, University of Minnesota (References: Bjorklund, 1999; Carr, 1999a,b,c)

Goal: The goal of this project is to develop a simulated countercurrent moving bed chromatographic reactor (SCMCR) for the production of methanol from methane (natural gas).

Rationale: The partial oxidation of methane to methanol is a process that utilizes a clean source material in an energy efficient manner to produce a substance that is both a clean fuel and a useful chemical feedstock. Simulated countercurrent moving bed chromatographic reactors are chemical reactors in which reaction and separation occur simultaneously in integrated reactor/adsorbers.

The adsorptive separation has very low energy requirements, so the SCMCR is environmentally benign from the standpoint of CO_2 emissions. The separation of product(s) from reactant(s) enables equilibrium limited reactions to be carried to higher conversions than would be possible in conventional non-separative reactors. The

SCMCR is also capable of improving yields of other intrinsically low conversion processes.

The partial oxidation of methane to methanol is a low conversion process if it is carried out at conditions where deep oxidation to CO_2 and H_2O is minimized. The consequent low yields of methanol have made commercialization unattractive. The present investigation seeks to determine to what extent the SCMCR can improve methanol yields, and whether a commercially feasible process might result.

Approach: The homogeneous gas phase partial oxidation of methane was carried out at total pressures from 60 to 100 atm in a multiple column configuration SCMCR. The reactor design and operating conditions were optimized for methanol production on the basis of a program of experimentation. A mathematical model has been developed as a basis for refinement of the design and for potential scale-up.

Status: The SCMCR system has been designed, built, and operated. A suitable adsorbent that separates methane from methanol and does not significantly spread the methane block wave, (10% Carbowax on 80/100 Supelcoport) was selected and used in the adsorber columns. Parts of the system have been redesigned and replaced in order to reduce methane spreading due to dispersion. It was found that using nitrogen instead of helium as a carrier gas has a favorable effect on the viscosity and the flow characteristics of the mixture at high pressures.

The effect of temperature, total pressure, and methane to oxygen ratio in the make-up feed, on methane conversion, methanol selectivity, and methanol yield, have been determined. The optimum SCMCR performance was obtained at 477°C, 100 atm, and $CH_4/O_2 = 2$. For these conditions methane conversion is 50%, methanol selectivity is 50%, and the methanol yield is 25%. The per-pass methanol yield in the tubular reactor alone at these operating conditions is 3%. Thus, the SCMCR improves the methanol productivity by a factor of 8. Furthermore, the best methanol yields, from conventional tubular reactors, that have been reported in the literature are 6-8%. The SCMCR betters these reactors by a factor of 3 to 4.

Heuristic Reactor Design for Clean Synthesis and Processing - Separative Reactors Michael E. Mullins, Andrew A. Kline, and Tony N. Rogers, Michigan Technological University (References: Kallio, 1999; Kallio et al., 1999)

Goal: This project intends to develop a prototype Heuristics and Reactor Design (HARD) system to aid engineers in the conceptual design and engineering of clean chemical processes. There are two core tasks in the initial phase of the effort both aimed at separative reactor processes: the development of mathematical models for 1) the reactive distillation process and 2) catalytic membrane reactors.

The resulting models can be used as a screening tool to determine the suitability of a given reaction for these processes. The completed models will be integrated into an expert system resource along with other existing models for chemical reactor design.

Rationale: Currently there are no existing design models for catalytic membrane reactors; and although commercial software from several simulation companies is available for distillation related modeling, they are not specifically tailored to reactive distillation process. Therefore, it is important to construct a model based on the unique features of reactive distillation in a packed column. The reactive distillation model was completed in 1998. The work over the past year has focused on the development and analysis of models for catalytic membrane reactors; especially those based upon zeolite membrane systems.

Supported zeolite membranes can have high selectivity for the separation of gas mixtures, but typically have low permeation rates. Several methods have evolved for the preparation of continuous ZSM-5 membranes over the last ten years. Most of these are passive techniques that utilize precipitation onto the surface from dilute solutions or the surface application of gel precursors. We have investigated the use of an electrophoretic deposition method based on the *in-situ* hydrothermal method which was developed previously. Application of an electric potential across the support in solution allows for improved control of membrane density and thickness. The membranes have been characterized via SEM and X-ray diffraction. The rates of gas permeation through the membranes has been characterized using H_2, N_2, Ar, n- and iso-butane, SF_6 and toluene in a continuous flow system. The membranes have been determined to be crack free and have selectivity's similar to those published in the literature. The major difference between membranes prepared with the electrophoretic method and those prepared by existing methods is an improved overall transfer rate and better control over the membrane properties. Higher transfer rates in zeolite films may facilitate the use of these membranes in separative reactor systems.

Approach: Zeolite ZSM-5 is chemically and thermally stable and has previously been used as an adsorbent in pressure swing adsorption plants. However, the practical application of zeolites in the form of inorganic membranes has been limited due to low specific permeation rates that have been obtained. The rates of permeation, and hence the total molar fluxes, directly depend upon the membrane thickness. In turn, a requirement for producing a thin-film membrane is that the zeolite crystallite size should also be very small. Several techniques have been developed in order to obtain a thin, uniform zeolite layer on porous substrate materials. One of these methods is the dilute precursor solution synthesis, or sol-gel, process. Previous work using a hydrothermal synthesis method has produced supported zeolite films 10 microns thick with 2-micron crystals via precipitation. Our investigation has focused on modifying these dilute solution hydrothermal synthesis methods by using electrophoretic deposition. By its application we hope to control and reduce the membrane thickness and individual crystallite size. In this process an applied electric potential is used to attract the zeolite particles to a porous ceramic substrate surface prior to precipitation from solution.

A systematic study of the ZSM-5 films produced via electrophoretic deposition has been conducted. The physical and chemical composition of the membranes has been characterized via SEM and X-ray diffraction. The gas permeation characteristics for each membrane were characterized using H_2, Ar, N_2, n-butane, iso-butane, toluene, and SF_6. Residual ZSM-5 powder from the synthesis was also used to characterize the film material's adsorption and diffusion parameters.

To evaluate the membranes produced, a permeation cell apparatus was designed to hold the membrane tubes. It allows for two inlet streams, a sweep stream of pure argon and the feed containing the gas species of interest. One stream is directed down the axis of the membrane and the other stream flows around the outside of the tube, i.e.-the membrane side. Under normal operations the feed enters the system on the membrane side of the tube. Omega mass flow control valves maintain a steady flow on both streams. The cell is constructed of 316 stainless steel, approximately four inches in length and 1-3/4 inches in diameter. The cell is placed within an automatically controlled tube furnace allowing for isothermal diffusion studies at various temperatures. A sampling capillary for the mass spectrometer is inserted through septa at the two outlets of the permeation cell to provide "real-time" analysis of the outlet gases.

The approach used in the membrane reactor model is based upon a Stephan-Maxwell approach for mass transport. Since the diffusion in a microporous membrane can be in the form of discrete molecules, a continuum approach similar to Fick’s law is no longer appropriate. The inadequacy of the Fickian approach is particularly pronounced for multi-component flux analysis. An algorithm based on the Stephan-Maxwell model is used to predict the behavior observed in laboratory membrane permeation studies.

In order to explain the lower permeation rates a thermodynamic model of the transport process must be used. It is necessary to use a modeling system that can account for the non-Fickian thermodynamics of a zeolite system, such as the Maxwell-Stefan approach. Krishna and Wesselingh present an extensive review of this subject. This multicomponent form equates the vector of micropore molar fluxes, N^s. Here ρ is the fluid mixture density, ε is the porosity of the particles, and the total saturation concentration is q_{sat}. $[D^s]$ is the square matrix of Fick micropore diffusivities. Finally, ∇Q is the gradient of fractional surface occupancy across the membrane.

$$\left(N^s\right) = -\rho\varepsilon q_{sat}\left[D^s\right]\left(\nabla\Theta\right)$$

Status: A catalytic membrane reactor model has been developed based upon a Stephan-Maxwell formulation for mass transfer, and incorporated into a radial reactor model. Comparisons to in-house permeation studies for zeolite membranes are being completed. This algorithm was incorporated into a simple radial reactor model to predict the performance of tube-type catalytic membrane reactors. In the near future, a comparison of model results to actual data on dehydrogenation of toluene will be made.

Innovative Industrial Applications

Recovery of Waste Polymer Generated by Lost Foam Technology in the Metal Casting Industry Jeremy Pletka and Jaroslaw W. Drelich, Michigan Technological University (References: Pletka, 1999; Pletka and Drelich, 1999)

Goal: It is desirable to recover expanded polystyrene and dispose of only coating and glue components from scrapped lost foam patterns produced in automotive manufacturing. Although it is not an objective to circulate recovered polystyrene back into lost foam casting it is desirable to reclaim polystyrene of sufficient quality to return to the consumer market. Therefore, it is the goal of this project to develop a simple, inexpensive technology for the recovery of expanded polystyrene with a minimal amount of contaminants for further use.

Rationale: This research program was initiated to assist the metal casting industry in prevention of polymer waste disposal, and to promote engineering solutions leading to reuse of the polymer. In the automotive casting industry, lost foam casting is a process in which a polystyrene pattern is formed into the desired shape of the part to be cast. More complex parts are fabricated by simply gluing several pattern pieces together. The final pattern is then coated with a refractory material consisting of a mineral mixture and binders. Hot metal is then poured into the patterns, evaporating the polystyrene, and taking shape of the mineral coating shell.

Inevitably, pattern fabrication introduces a waste stream as a result of subsequent handling or from degradation of the casting in storage. The damaged patterns are not reusable, creating a potential disposal problem, as lost foam casting is becoming more prevalent in the automotive casting industry. The potential volumes of scrap therefore prompt the development of an effective, inexpensive technology for the recovery of the recyclable material (polystyrene) as an alternative to waste disposal.

Approach: Our strategy adapts the principles of modern mineral processing technology to polymer recovery. The two-year program includes particulate characterization, examination of surface-interfacial properties of the pattern components, development of an analytical technique for contaminant concentration measurements, shredding and size reduction, and selective separation testing based on component density.

Additionally, in the initial phase of the program we observed that component separation based on size compliments density separation, and therefore our approach also includes a fundamental investigation of component size segregation resulting from rotary shredding and impact comminution.

Status: Investigation of component size segregation, impact comminution, and initial separation tests have yielded positive results. It was observed that almost complete release of coating from polystyrene occurs during shredding with a rotary blade shredder allowing for differential size segregation of the components. Shredded material was first screened and next separated by density using float-sink or cyclone testing. Separation testing recovered as high as 98% of the polystyrene, while the level of coating contaminants did not exceed 5%wt in the final product.

Additionally, impact comminution has succeeded in decreasing the coating contamination level to 2%wt. These experiments have indicated that an extensive investigation of a separation process based on component density and size is justifiable and will be continued in the second phase of the project.

Predictive Tool for Ultrafiltration Performance Michael J. Semmens and Brian Huff, University of Minnesota (References: Huff, 1999)

Goal: To create a computer model to help design engineers predict ultrafiltration membrane performance using global and empirical models.

Rationale: Ultrafiltration is a highly efficient separation process. It can be used in a variety of industrial applications, such as electroplating and painting, to recover products for reuse, or separate them for resale. In the future, when pollution prevention planning exists throughout industry, ultrafiltration is expected to be widely implemented. If a waste stream cannot be reused, then in most cases its volume can be reduced by separating the water and thickening the waste. This will facilitate better treatment or disposal.

Lastly, ultrafiltration is becoming more popular in water and wastewater treatment plants to separate organics from feed waters, thereby reducing the number of trihalomethane (THM) precursors. If ultrafiltration is to have such a prominent place in the future, then we need to create better tools to predict its performance.

Approach: A comprehensive literature review was performed, in search of articles related to current ultrafiltration prediction models. Each model's strengths and weaknesses was then analyzed. Several different models were selected, each requiring different input from the user. To make the tool as versatile as possible several different models were incorporated into the program. For example, if the user has little information about the system, a mechanistic model may be used to approximate flux values. If more information is known, the user may input experimental data into the computer. Using this data, the program will determine the empirical coefficients, and then allow the user to alter the model parameters to predict flux with greater accuracy. Extensive help files are available on each model's strengths and limitations.

Status: Stand-alone elements of the model have been completed that may be used by other investigators. The computational aspects of the software tool was completed and the model has the ability to predict membrane flux with both mechanistic and empirical models. The flux prediction with empirical models is not as powerful as originally hoped for, due to difficulties in modeling arbitrarily entered data sets. Nevertheless, the user interface was completed and tested.

In-Line Copper Recovery Technology Michael J. Semmens and Carla Dillon, University of Minnesota (References: Dillon, 1999)

Goal: The objective of this project was to investigate the ability of Continuous Deionization (CDI) to recover copper sulfate and purified water from acid copper electroplating rinse waters for reuse within the same process.

Rationale: Copper electroplating is a common metal finishing process. Copper plating from copper sulfate solutions is a primary and integral process in the manufacture of printed circuit media. These copper electroplating operations involve the generation of copper contaminated rinse waters that usually cannot be discharged without undergoing some form of treatment. Presently, two common types of treatment processes for copper-laden rinse water are hydroxide precipitation and ion exchange.

Hydroxide precipitation requires the addition of polymers, acids, and a hydroxide source. Wastewater and sludge are generated. Typically, the sludge will require disposal as a hazardous waste. Treatment by ion exchange will require regeneration of the resin by acids that will require additional treatment prior to disposal.

Successful use of the CDI process for copper sulfate and purified water recovery would allow the discharge of pollutants from acid copper electroplating rinses to be eliminated. It would also eliminate the need to purchase, handle, and eventually dispose of treatment chemicals presently used in conventional and ion exchange treatment of these rinse waters.

Approach: To meet the project objectives, the following tasks were identified:

1) Process Review – Review operating parameters and current literature.
2) Bench-scale Testing – Run experiments using a bench-scale CDI unit under various conditions of operation. The solutions for testing will be those typically encountered in printed circuit media fabrication facilities.
3) Final Report Preparation – Prepare a detailed report of the technical and economic feasibility of CDI for in-line copper recovery.

Status: This project has been completed. A literature review of the CDI process review was completed and the operating parameters and treatment objectives for high strength plating rinse waters was determined. Bench-scale experiments for both batch and single-pass flow regimes were designed and completed using synthetic copper sulfate rinse waters. Three different modules of varying configurations were tested under different conditions to identify the influence of the ion exchange resins. A pilot study was also completed to evaluate the effectiveness of the process on a real plating rinse water.

Means for Producing 100% Kraft Lignin-Based Biodegradable Plastics Simo Sarkanen, University of Minnesota (References: Li and Sarkanen, 1999a,b; Sarkanen, 1999a,b,c,d,e; Sarkanen and Li, 1999)

Goal: This project is dedicated to developing technology for establishing a plant where the first truly lignin-based biodegradable plastics can be manufactured. The industrial byproduct lignin for producing these plastics was isolated from kraft black liquor generated by a pulp mill in International Falls, Minnesota.

Rationale: The conversion of wood chips to pulp for manufacturing paper generates huge quantities of byproduct lignins annually in the United States. The best estimates indicate that more than 26 million tons of kraft lignins are generated as byproducts of such pulping operations every year. As steps have been taken to maximize production, the recovery furnaces in an ever-increasing number of mills have become overloaded; the result is that all the byproduct lignin can no longer be used in its traditional role as a fuel.

Unfortunately the necessary capital investment usually precludes construction of a new recovery furnace so there is little prospect of rectifying the situation in the majority of recovery-loaded mills. Even though untreated black liquor cannot be discharged directly into rivers, an exacerbation of pollution originating from pulp mills is likely to occur. A compelling way of responding to the problem may be found in creating biodegradable plastics from the kraft lignin in surplus black liquor.

Intensive efforts have been under way for twenty years to incorporate surplus byproduct lignins from pulp mills into useful plastics. Until 1994 it had been thought that most polymeric materials inevitably become brittle and weak when their lignin contents exceed 25-40%. However, the first 85% industrial kraft lignin-based thermoplastics with promising tensile strengths were reported by the principal investigator in 1995 and a more detailed description of this work appeared two years later.

Then, through CenCITT funded work, alkylated 100% kraft lignin-based plastics with tensile properties very similar to those of polystyrene were produced. Thus the proposed work has sought to develop feedstocks suitable for injection-molding biodegradable plastic components composed solely of simple industrial kraft lignin derivatives in blends with commercially available plasticizers.

Approach: Ultrafiltration has been employed to purify and fractionate industrial kraft lignin samples that, after simple derivatization, could be extrusion-molded into strong plastic components. The compositions of the preparations have been evaluated through chromatographic analyses and molecular weight determinations. The plasticizers sought for use with the new alkylated kraft lignin-based plastics were to be commercially available and inexpensive (not more than about $1.50 per lb). A low threshold for effectiveness in blends with the alkylated kraft lignin preparations was centrally important. The final step in making these new biodegradable plastics was to involve spray-drying aqueous suspensions of the kraft lignin derivatives to produce powders that would be pelletized for extrusion-molding purposes.

Status: In the quest to broaden the range of thermoplastic formulations with very high lignin contents, the feasibility of creating polymeric materials composed exclusively of alkylated kraft lignin was fully established during the previous reporting period. In the absence of plasticizers, these new materials exhibited tensile behavior very similar to that of polystyrene.

In the first instance, kraft lignin preparations had been alkylated with the corresponding dialkyl sulfates in solution at pH 11-12. Solvent-casting from DMSO of the alkylated derivatives thus produced had yielded plastics containing 95-100% alkylated kraft lignin that exhibited very encouraging mechanical properties. In contrast to the earlier results with 85% kraft lignin-based plastics, variations in the degree of association between the individual molecular components before derivatization seemed to have no effect upon the tensile properties of the corresponding alkylated kraft lignin-based polymeric materials. This arose from the casting conditions employed, where heavy association was promoted.

It was then found that removal of the low molecular weight kraft lignin components by ultrafiltration improved the successful polymeric material formulations. This first became evident with an ethylated higher molecular weight kraft lignin fraction obtained by ultrafiltration through a 10,000 nominal molecular weight cutoff membrane, which exhibited substantially better tensile behavior than the parent preparation. When compared with common synthetic polymeric materials, alkylated kraft lignin preparations were closest to polystyrene as far as tensile strength (37 MPa), Young's modulus (1.9 GPa) and elongation to failure (2%) were concerned. In regard to the relatively low elongation to failure, alkylated 100% kraft lignin-based polymeric materials were quite brittle and therefore needed to be plasticized or toughened if the goal of injection-molding useful components from them was to be realized.

For the first time ever, extensive plasticization of alkylated 100% kraft lignin-based polymeric materials was achieved in 1998 with commercially available aliphatic polyesters. By blending with such components at levels ranging to 30 - 40%, alkylated kraft lignin-based polymeric materials were progressively plasticized and exhibited extensive plastic deformation before fracture. The ultimate strains could extend comfortably beyond 60%. The poly(1,4-butylene adipate), poly(1,3-propylene adipate), poly(1,3-propylene succinate), poly(diethyleneglycol adipate) and poly(trimethylene glutarate) used for the purpose did not themselves have any measurable tensile strengths and therefore they acted as true plasticizers, presumably separating the macromolecular lignin chains so as to facilitate chain segmental mobility. A 30% plasticizer content may be higher than desirable from an economic point of view, and so a major effort was mounted to attain adequate degrees of plasticization using only 10 - 15% blend component levels. This part of the enterprise has so far not succeeded.

The final phase of the project has involved extrusion-molding studies with the plasticized alkylated 100% kraft lignin-based polymeric materials. This work has focused upon making tensile test pieces with a Randcastle RC-0250 single screw extrusion-molding unit. Hereby the feasibility of extrusion/injection-molding components and/or parts from these thermoplastic formulations has been clearly demonstrated. However, the configuration of the apparatus employed for the purpose has tended to engender the appearance of voids in the test pieces that have been produced. The cause of the problem is under investigation.

Clean Process Advisory System (CPAS)

Industrial Implementation of the P2 Framework John L. Bulloch, John C. Crittenden, David W. Hand, and Volker H. Selzer, Michigan Technological University (References: Bulloch, 1999; Crittenden, 1999a,c,d,e,f; Crittenden and Bulloch, 1999a,b; Selzer et al., 1999)

Goal: The scope of this research activity is to promote U.S. EPA developed toxicological, environmental, and ecological estimation software for the use in industry. More specifically, the two main objectives of this project are:
1) to make a wide variety of industrial organizations aware of the Pollution Prevention Assessment Framework (P2 Framework) and CenCITT's software P2 tools, and
2) to assist several companies (primarily related to chemical manufacturing industries, but also other sectors) in successfully using the P2 Framework as an information resource in risk assessment and in identifying pollution prevention opportunities.

Rationale: During the last two decades the U.S. EPA Office of Pollution Prevention and Toxics (OPPT) has developed computer-based methods that derive important risk assessment information based on the atomic connectivity of organic chemicals. These methods provide information on carcinogenicity, toxicity to aquatic organisms, worker and general population exposures, bioconcentration, and environmental fate, among other data. OPPT routinely uses these methods to highlight chemicals of concern, to identify safer substitutes, and to reduce or eliminate risks.

Although originally developed by U.S. EPA to estimate the properties of chemicals submitted under the Pre-Manufacture Notice (PMN) approval process, EPA has recently considered using these tools for pollution prevention. The purpose of this project is to promote these tools as beta test versions to industry, in order to identify their applicability, weaknesses, and strengths. Further, we will utilize this opportunity to promote CenCITT's software P2 tools.

The Pollution Prevention Assessment Framework (P2 Framework) is a document that contains many of OPPT's most important computer-based methods for assessing risk based on chemical structure. The P2 Framework provides important risk-related information not previously available. Its purpose is to provide information that can inform decision making and help promote the design, development, and application of safer chemicals and processes. The document describes each assessment methodology and the importance of the data generated, and provides case studies showing how methods can be used collectively to answer complicated risk assessment questions and identify pollution prevention opportunities. The P2 Framework, as currently constructed, does not address all biological endpoints. It is a screening-level methodology that is of value when chemical-specific data are lacking.

The principal investigators of this project have identified the P2 Framework tools to be particularly beneficial in three areas: 1) on the side of the chemical manufacturer early on in the development of a new chemical (basic R&D work), 2) facilitating the PMN process by understanding risk estimations, and 3) on the side of the chemical formulators choosing between different chemicals based on risk and environmental properties. The following figure may illustrate this conceptually.

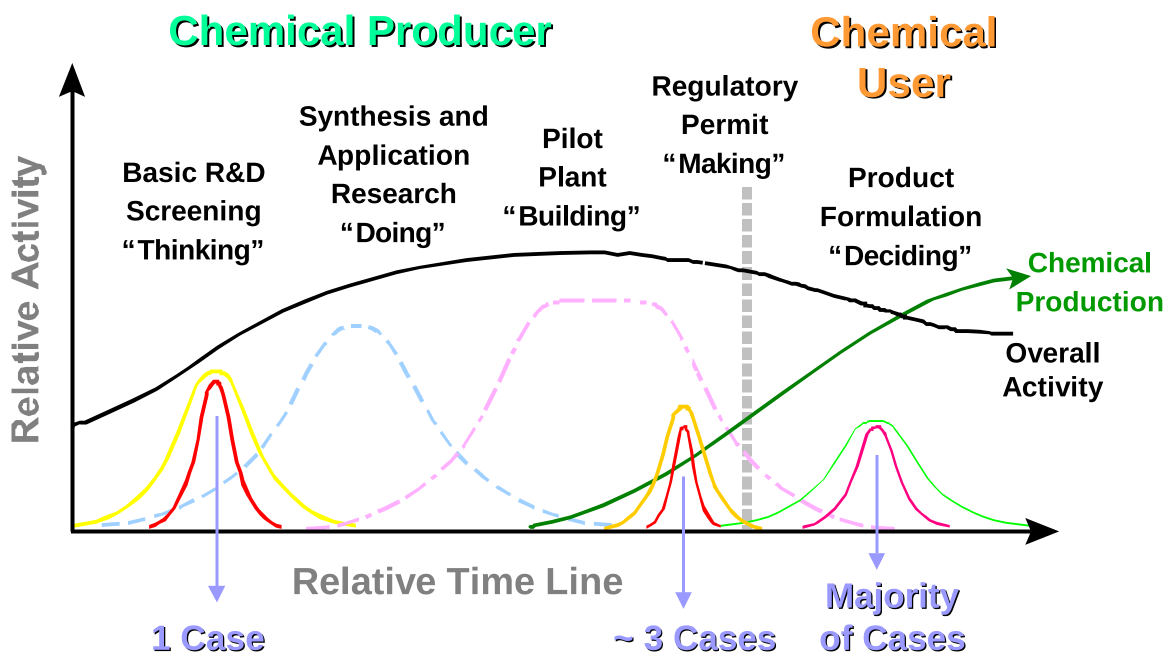


Figure 1. *Conceptual illustration of the industrial P2 Framework implementation process and its potential applicability to the chemical industry and the chemical supply chain. Notice that the tools can be used in three different areas, CenCITT researchers have conducted actual implementation studies with industry in all three of these areas.*

Approach: Specific tasks of this activity include presenting the software tools to industry and identifying partners for pilot studies. During the pilot study period the principal investigators assist industry in the use of the software tools through their own calculations and technical expertise. Concluding a test period, the industrial partner and CenCITT staff are to assess the P2 and potential economic effectiveness of the software tools. Suggestions for improvement are encouraged.

Status: Current achievements and results towards project deliverables include:

- CenCITT has interacted with eight organizations listed in the table below as part of the P2 Framework Assessment Partnership.
- CenCITT staff has made calculations for over 80 molecules and submitted them to corporate partners mostly in the form of Confidential Business Reports (based on their confidential submittals of the “problem” molecules).
- CenCITT has developed qualitative and quantitative area resolute multi-objective plots (scaled and normalized) to demonstrate selected environmental scenarios of interest to less technically inclined personnel.
- CenCITT has recently begun using the PBT-Profiler (Persistence, Bioaccumulation, and Toxicity) as part of this project.
- Extensive discussions have been initiated with the following companies regarding the use of the P2 Framework or the PBT Profiler: Herman Miller (Furniture Manufacturer, Coatings), Ashland Chemicals (Pre-Polymers, Petroleum Products, and Fine Chemicals), C. K. Witco (Organo-Silicone Compounds, problem solving with PMNs), and the National Council for Air and Stream Improvement (NCASI).

Previous and Current Industrial Partners Using the P2 Framework Tools

Organization:	Estimations Performed for:	Results:
General Motors	10 Molecules	10 Successful
BASF USA	1 Polymer + 3 Intermediates	Limited Success
Shell, Inc.	12 Molecules	Mostly Successful
Amway Corporation	3 Molecules	2 Very Successful
National Council for Air and Stream Improvement (NCASI)	2 Molecules	Successful (Preliminary Study)
Stepan Corporation	42 Molecules	~ 30 Successful
Dell Engineering	3 Molecules	(Ongoing Work)
Confidential Partner	1 Design Molecule	15 Suggested Derivatives Very Successful

Establishing Automated Linkages Between Existing P2-Related Software Design Tools Eric J. Oman, Tony N. Rogers, Bruce A. Barna, John C. Crittenden, and David R. Hokanson, Michigan Technological University (References: Baker et al., 1999a,b; Crittenden et al., 1999a,b,c,d; Hand et al., 1999a,b; Oman and Crittenden, 1999; Oman et al., 1999a,b,c; Yang et al., 1999)

Goal: (1) To construct rapid design assistance software (DAS) that links existing P2-related design comparison tools with existing economic, environmental risk, and safety modules; (2) To construct an automated client/server feedback loop with an existing chemical process simulator to automate the economic-environmental-safety optimization procedure; and (3) To provide software support for the investigators of other projects in their development of case studies to demonstrate the completed software deliverable.

Rationale: Within industrial settings, design engineers planning new processes and the retrofitting of existing processes are typically required to make quick decisions due to a short development cycle. Traditional process design decision-making tools include chemical process simulators and economic analysis, which are well-developed technologies capable of providing information in a timely manner. Currently, no similar rapid design assistance software is available for consideration of P2 opportunities.

Approach: In order to ensure that P2 opportunities are factored into the design process, this project has focused on the generation of rapid design assistance software.

Specific aspects of this work include:

- Design the main software deliverable known as Simultaneous Comparison of Environmental and Non-Environmental Process Criteria (SCENE) to facilitate the linking of SCENE with existing and future P2-related design comparison tools.
- Construct a core comparison engine in SCENE that permits the comparison of completely different processes (e.g. adsorption versus steam stripping) or slightly different processes (e.g. a continuum of reflux ratios or oil flow rates) based on a wide selection of process attributes. This comparison engine is derived from the Design Enhancement to AHP Ranking (DEAR) software.
- Link the SCENE comparison engine with the CPAS economic tool (DORT), the CPAS environmental tool (EFRAT), and the Office of Pollution Prevention and Toxics (OPPT) environmental tools.
- Create an automated client/server link between SCENE and a commercial chemical process simulator (e.g. HYSYS from Hyprotech) to automate the optimization of a given process based on economic, environmental, and other attributes.
- Provide software support to the investigators of other CenCITT projects to aid in the development of case studies to demonstrate the completed SCENE software deliverable.

Status: A preliminary version of the SCENE software has been constructed. The preliminary version includes links between SCENE, DORT, EFRAT, and the HYSYS chemical process simulator. No links with the OPPT environmental tools have been constructed at this time. Discussions with the U.S. EPA and Syracuse Research Corporation are currently underway to make such links possible.

A preliminary version of the SCENE software was made available in September 1999. A case study for SCENE was generated that determines the optimal oil flow rate for an absorption process, based on economic and environmental process attributes. This case study will be demonstrated in a paper and in presentations.

The SCENE program will undergo several planned revisions in the future. SCENE will be revised in response to feedback from various sources, including students who have used the program in their classes, researchers responding to presentations and publications, and software beta-testers. The program will be renovated or perhaps rewritten in order to improve its ease of use. Finally, SCENE will be modified to permit the use of chemical process simulators other than HYSYS.

Several ancillary tasks are also planned. The first task is to merge all of the CPAS physical property data and estimation techniques into a single program known as Software to Estimate Physical Properties (StEPP) Version 2. The second task is to work with the authors of Environmental Indices for Green Chemical Production and Use to merge their tool with the EFRAT and SCENE programs. The third task is to rewrite the Chemical Industry Planning System (CIPS) and merge it with the SCENE comparison engine.

Development and Testing of Pollution Prevention Design Aids for Process Analysis and Decision Making Bruce A. Barna and Tony N. Rogers; Michigan Technological University (References: Atkins, 1999; Chen, H., et al., 1999a,b)

Goals: This project is to create the evaluation and analysis module that will serve as the engine for design comparison in the CPAS Focus Area. The current title for this module is the Design Options Ranking Tool or DORT.

Rationale: The DORT module is a necessary component of CPAS. DORT implements the "compare" phase of the three-tiered approach to information delivery and P2 analysis implemented by CPAS:

- Find Candidate Technologies, Processes or Retrofits
- Simulate and Size Equipment
- Compare and Rank Candidate Options

DORT is envisioned as the analysis and comparison engine within CPAS that will help the designer to rank the multiple design alternatives using the various performance measures generated by CPAS. Ultimately these performance measures will include economics, environmental impact, and safety.

The DORT module is intended to be a prototype of the information flow and algorithms necessary to develop a pollution-conscious process design and retrofit capability. This is intended to occur through software module linkages to other CPAS design aids and existing commercial process simulator programs.

Approach: Through the use of case studies, we intend to demonstrate the use of the DORT module as the analysis engine for a variety of cost and non-cost measures which are being developed under CPAS or elsewhere. For example, the CPAS Environmental Fate and Risk Assessment Tool (EFRAT) and Safety Tool (Dow Indices Tools) are index generators that can be used to rank processes with respect to environmental fate and safety. These process attributes can then be combined with cost or other performance measures to provide an overall rank of process options based on usersupplied index weightings. Ideally this information will be provided to the designer incrementally as the conceptual process design is being developed.

The present approach is to conduct a systematic evaluation of the necessary components of a general P2 assessment algorithm and the information flow between the pieces. A paradigm process (case study) will illustrate the application of the tools and techniques. A P2 assessment methodology will be developed which illustrates the logical ordering of the calculation steps necessary to process the information being passed between components and identifies what needed information and data are not being provided by process simulators or other sources.

Status: This project is in its final stages and all objectives have been met or exceeded. The software prototype has been completely redesigned and a licensing agreement with a value added reseller is near completion.

The first case study, an analysis of cogeneration options, is complete as reported in the last annual report. The second case study, a solvent recovery design problem, is also complete with respect to this project but continues to provide useful analysis opportunities for further study of P2 design methodology. Results were presented in several forums at the AIChE Annual meeting in the Fall of 1999.

Another significant success of this project was not a specific part of the original objectives. A methodology has been created for identifying and ranking multi-criteria, optimization opportunities in process analysis. The methodology can be applied to both existing and conceptual designs and has been proven to be very effective in helping even highly experienced design engineers to identify opportunities. In addition, the procedure has been proven to be very useful in the classroom in teaching inexperienced engineers to perform process analysis. For the time being the procedure is called “Process Diagnostics.” Initial efforts in this area have been summarized in a master’s thesis (Atkins, 1999). Current research under different funding will attempt to automate the generation of the diagnostic tools from process simulator output and to further develop the techniques.

Integrated Applications of the Clean Process Advisory System to P2-Conscious Process Analysis and Improvement David R. Shonnard, Bruce A. Barna, Andrew A. Kline, and Tony N. Rogers, Michigan Technological University (References: Atkins, 1999; Hiew and Shonnard, 1999; Raymond et al., 1999; Shonnard and Hiew, 1999; Shonnard et al., 1999)

Goal: The purpose of this research project is to design cleaner and more profitable chemical processes through the application of rigorous optimization techniques. We intend to show that methods currently used to judge optimization performance on a monetary scale may be applied to judge a process on a non-monetary basis (environmental). Another goal is to demonstrate integrated assessment of chemical process economic and environmental attributes using CPAS™ software already developed from prior CenCITT and other EPA support. The specific objectives are:

1) Develop a rigorous chemical process design and improvement methodology for integrating environmental and economic measures of performance.
2) Further demonstrate the applications of multiple CPAS™ tools (EFRAT, DORT, and DEAR) by applying them in close coordination with a chemical process simulator (HYSYS™) for design evaluation of a suite of case studies.
3) Evaluate the influences of model uncertainty on the process optimization methodology. We will set up the framework for this analysis and apply it to a small number of model parameters.
4) Disseminate the results from these case study applications by publishing the results in peer-reviewed journals and presentation of results at national meetings.

Rationale: Efficient chemical process designs are the key to future economic success and environmental protection. The chemical process and allied products industries, including petroleum refining, have provided innovative products and processes for the economy of the United States and for the global economy as well. However, estimates show that these industries are responsible for up to 80% of the industrial hazardous waste generated, treated, and disposed of in the U.S. each year. It has been estimated that approximately 5% of the raw materials entering these processes exit as waste stream components.

Previous process improvement methodologies minimized equipment and operating costs under the constraints of imposed emissions reduction targets. Unfortunately, focusing on single environmental or economic endpoints neglects the reality that there are multiple environmental and human health impacts, which are affected by process optimization. The application of simultaneous economic and environmental optimization will address this important need for improving chemical process design based on multiple evaluation criteria.

Approach: We propose a three-step method for rigorous process optimization as shown in Figure 1. In the first step, which is termed "Input/Output Screening," an initial critical examination of the process is performed resulting in a set of "Process Diagnosis Summaries". A process flowsheet is created and material and energy balances are performed using a commercial process simulator (HYSYS™ for our study). Then input/output tables for energy consumption and process emissions are created to spot process improvement opportunities. This step leads to an initial set of process parameters for consideration and process simulation.

The second step is referred to as "Parameter Identification". The objective functions, which are selected as the basis of the optimization, can consist of total annual cost, environmental impact indexes, or net present value. The process simulator and the CPAS™ software will again interact very closely to generate economic and environmental performance curves for each parameter studied. A Scaled Gradient

Analysis is performed to identify a reduced parameter set to carry forward to the last step in the procedure.

In the last step of the project, “Multi-Variable Optimization”, we will utilize the optimization capabilities within HYSYS and couple that capability with the assessment function of the SCENE software. This will allow us the flexibility to optimize on any single objective function, economic or environmental, or to utilize Analytic Hierarchic Processing (AHP) through the DEAR software as a method to generate a single objective function from multiple indexes of process performance.

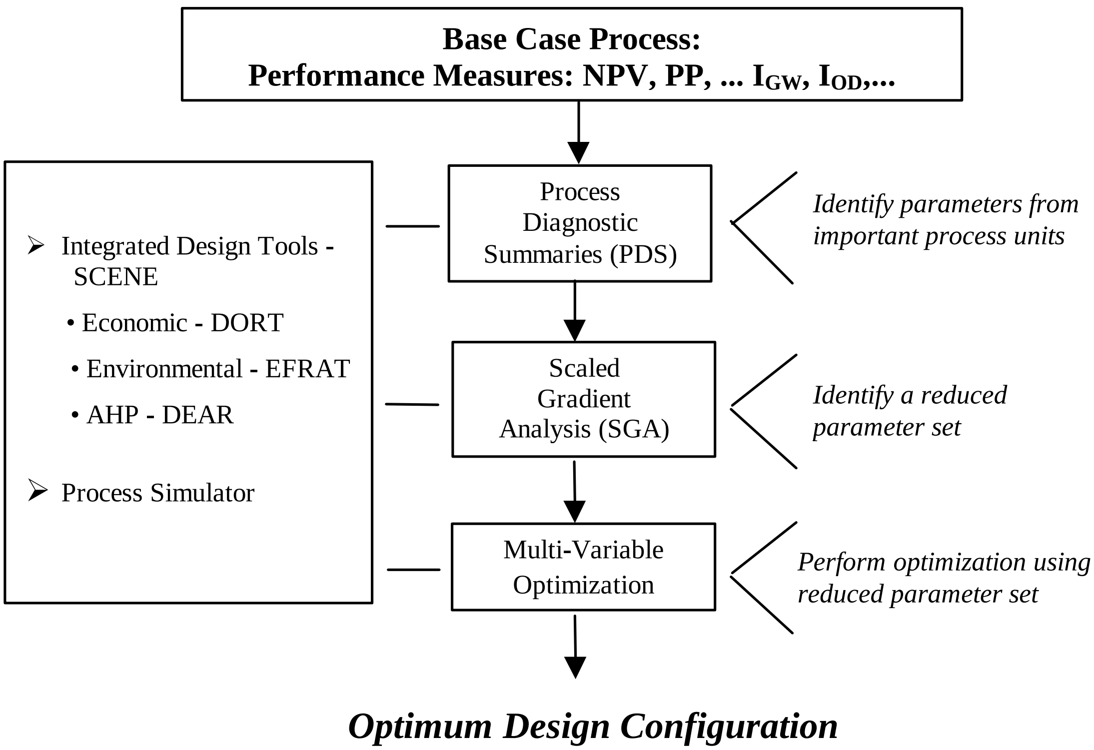


Figure 1. Generalized optimization method for integrating environmental and economic objectives into process design. SCENE is a software package for interfacing the environmental and economic assessments with a commercial process simulator; EFRAT is the Environmental Fate and Risk Assessment Tool which is a software that calculates 9 environmental risk indexes; DORT (Design Options Ranking Tool) is the economic index calculator; and DEAR is the AHP process design decision software tool.

Status: Through the efforts of Mr. Eric Oman and his parallel project “Establishing Automated Linkages Between Existing P2-Related software Design Tools”, we have an integrated software tool for automated assessments of economic and environmental process attributes, and this capability has been linked to a commercial process simulator, HYSYS. There are three graduate students working on this project at the present time. Hui Chen is a student in Chemical Engineering working toward a Ph.D. degree. Ms. Chen is leading the environmental assessment efforts using the EFRAT software within SCENE. Brendan O’Donnell is a M.S. student in Chemical Engineering and is in charge of the economic assessments using the DORT software within SCENE.

Prasad Patgaonkar is a M.S. student in Chemical Engineering and is working on the optimizer in HYSYS with the process assessment software tools.

Thus far, we have successfully demonstrated the input/output analyses and scaled gradient analysis (SGA) by applying the integrated suite of tools to a single case study process; VOC recovery and recycle from a gaseous waste stream using absorption into a heavy oil followed by distillation. We have verified that the SGA leads logically a reduced parameter set for subsequent optimization activities and that economic and environmental indices provide similar and consistent information to the scaled gradient analysis. We intend to have the optimization of the gaseous waste stream finished in the near future.

The Physical Properties Management System (PPMS): A P2 Engineering Aid to Support Process Design and Analysis Tony N. Rogers and Andrew A. Kline, Michigan Technological University (References: Chatkunnaayuttaya, 1999; Dechapanya et al., 1999; Kline et al., 1998; Raymond and Rogers, 1999; Raymond et al., 1999)

Goals: This project continues to be the primary physical and chemical property resource for CPAS tools. The project provides supporting consultation and data resources on an as-needed basis. Results are available through a stand-alone tool called "Software to Estimate Physical Properties" (StEPP), which is being extended to a second version, "StEPP2," in this project.

The project also facilitates data exchange between various other CPAS tools. Ultimately, the goal is to create a general software-based data delivery system that will serve as an expandable framework for adding property estimation algorithms and third-party-generated data resources.

Rationale: Physical and chemical property measurements and estimations are central to virtually all environmental assessment and process design decisions. Despite the importance of property data, expertise in physical and chemical properties tends to be a specialization beyond the capabilities of most process and product designers. By being closely aligned with the Physical Property and Thermodynamics Research Group (P2TRG) in the MTU Chemical Engineering Department, this project continues to insure that this expertise is available and becomes incorporated into CPAS tools. The P2TRG also conducts two programs dealing with chemicals of environmental interest for the Design Institute for Physical Property Data (DIPPR®) of the American Institute of Chemical Engineers (AIChE).

Approach: The first-generation version of the software being developed under CPAS, called StEPP Version 1.0, has already been designed to provide data support to the Adsorption Design Software (AdDesignS) and Aeration Systems Analysis Program (ASAP) modules under the Environmental Technologies Design Option Tool (ETDOT) initiative led by Dr. David Hand of MTU. StEPP, an acronym for "Software to Estimate Physical Properties," will ultimately link to every other tool and module within CPAS that needs data for its calculations. Many of the CPAS tool development efforts now underway rely on a working, expanded StEPP program for their development, testing, and release. StEPP will also have value, apart from CPAS support, as a stand-alone program that efficiently and rapidly supplies engineers, scientists, and process designers with necessary physical property data.

To support the Adsorption for Recovery (AdRecover) and Multi-Component Distillation (MC-Dist) modules, StEPP2 (an updated version of the original StEPP program) will be linked to provide vapor pressures, activity coefficients, and Henry's constants for relative volatility calculations. StEPP2 also includes chemical, physical, and environmental reactivity data that will be useful in computing design comparison indices in the Environmental Fate and Risk Assessment Tool (EFRAT) being developed by Dr. David Shonnard.

Status: The StEPP2 project team has supported the data requirements of the AdDesignS, ASAP, AdRecover, MC-Dist and EFRAT development projects throughout the project's existence. Data exchange has been promoted between the various CPAS tools, facilitating rapid evaluation of "clean" process designs.

The StEPP2 module under development will also feature stand-alone data display. Data sources for StEPP2 include tables of discrete data from AIChE/DIPPR Project 801, as well as data calculation and extrapolation methods, with a broad capability that includes infinite dilution thermodynamics, polarizability estimates, phase equilibrium algorithms, and transport properties. Among the pure component properties available in StEPP2 are: vapor pressure, molar volume at the normal boiling point, liquid density, activity coefficient, Henry's law constant, aqueous solubility, octanol-water partition coefficient, soil-water partition coefficient, and partitioning onto the organic carbon portion of biomass. The extent of use of DIPPR Project 801 data within StEPP2 is limited and conforms to licensing agreements between CenCITT and DIPPR.

Beta Version 2.0 of StEPP is nearing completion as the primary physical property server for CPAS. It will have the following features:

- Generic protocol for data delivery/export (export feature is now working and needs to be expanded to specific CPAS modules)
- On-line Help system (almost completed, being examined for errors)
- Fill database gaps with estimated values (ongoing)
- Test structure disassembly from SMILES (MOSDAP, “Molecular Structure Disassembly Program”, completed; UNIFAC, Hine & Mookerjee, Lydersen, and Benson groups will be supported)
- Incorporate group contribution vapor pressure module developed by Andrew Loll, M.S. Graduate
- Database scrutiny (Statistical Quality Control, SQC, data checking to proceed through Spring 2000)
- Partial licensing of AIChE/DIPPR data for incorporation within StEPP2
- Supply physical property needs of the ETDOTs, EFRAT, and other CPAS modules (ongoing)

Development of Environmental Indices for Green Chemical Production and Use
John C. Crittenden, David W. Hand, James R. Mihelcic, and David R. Hokanson, Michigan Technological University (References: Qiong et al., 1999; Velazquez-Carillo, et al., 1999; Zhang et al., 1999a,b)

Goal: This project intends to develop practical methods for predicting the potential risk from chemical manufacturing and use. The initial phase of this effort will provide a comparison of several existing risk assessment methods for different application scenarios: (1) Pollution Prevention (P2) Assessment Framework stage I risk analysis method, (2) Toxicity-based method, (3) Toxicity/Persistence Index, (4) Partitioning Persistence/Toxicity Index, and (5) Concentration/Toxicity method. This comparison will illustrate the influence of simplifications of transport and exposure estimation on risk prediction. Ultimately, a model that considers emission rates, toxicity, and more realistic attenuation mechanisms of chemicals will be developed to evaluate the environmental performance of process alternatives.

Rationale: Chemical production, use and disposal cause adverse impacts on the environment. Consequently, much research has been conducted to develop methods for estimating the risk of chemicals and to screen them based on environmental impact. Risk assessment may be subdivided into two categories: environmental fate and exposure assessment, and adverse effect assessment. It is difficult to estimate the exposure level using complex fate and exposure models because many input parameters are not known. Due to the lack of reliable data and estimation techniques for determining input parameters, past research efforts in the field of risk assessment incorporate simplifying assumptions into the fate and exposure assessment that can result in poor decisions, even wrong decisions.

This project will seek a middle ground to evaluate risks for chemical production and use. It will provide industry with environmental impact information. This knowledge will be applied in the conceptual design phase such that not only economic and safety factors are considered, but also environmental factors. This project will help the government to evaluate the environmental performance of high-production-volume (HPV) chemicals and their manufacturing pathways not only based on the total release, but also their adverse effects.

Approach: The approach in this project is to compare several existing risk assessment methods and to develop a software design tool that requires minimal user input. The methods will be compared in the manufacture and use of chemicals. The Chemical Industry Planning System (CIPS) will be used to identify a number of production facility options. CIPS is a database developed by CenCITT investigators to link hydrocarbon feedstock to end products through industrially proven chemical technologies. The software package will consist of a multimedia environmental fate model and a risk index calculator. A sensitivity analysis for the fate model will be conducted to determine the dominant attenuation mechanisms and the important parameters to simplify the fate equations and direct future work in parameter estimation.

The risk-related information obtained by the EPA's Office of Pollution Prevention and Toxics (OPPT) Pollution Prevention (P2) Assessment Framework is used to conduct stage I risk analysis for chemicals of concern. The P2 Framework also provides risk-related information for other methods. Toxicity-based method, Toxicity/Persistence method, Partitioning Persistence/Toxicity Index (PPTI) and the Concentration/Toxicity method have been compared for solvent selection, reaction pathway selection, and risk evaluation among facilities and industries. This comparison demonstrates that ignoring or simplifying transport and exposure estimation will result in decreasing reliability of risk assessment.

The multimedia environmental fate model to be developed consists of main compartments and considers important attenuation mechanisms. The magnitude of the risks is expressed as the equal risk release of a reference chemical for different environmental impact categories. Under standard exposure scenario, the ratio of exposure level is equal to the ratio of the ambient concentration of the chemical in question to the concentration of the reference chemical. The risk index calculator portion of the model calculates the dimensionless risk indices based on a combination of the adverse effects and the concentration.

Status: Several existing risk assessment methods have been compared for example cases: green solvent selection, green reaction pathway decision-making, and risk evaluation for industries (or facilities, states). The different results obtained using different methods show that ignoring or simplifying exposure will result in decreasing reliability of risk assessment. It is concluded that toxicity is a key component to predict risk for chemicals with similar physical chemical properties and the fate of chemicals is very important in developing process risk potentials, especially when there is not a large difference in toxicity among chemicals used in different reaction pathways. It was found that the environmental impact assessment based only on total release may be misleading for industry (or facility, state) risk analysis.

The multimedia environmental fate model that has been developed consists of 6 compartments: air (troposphere and stratosphere subcompartment), surface water, sediment, soil (surface soil and vadose subcompartment), ground water, and vegetation (foliage and root subcompartment). The attenuation mechanisms considered in the fate model include advection, diffusive and non-diffusive mass transfer, and reaction. The model provides steady-state and dynamic simulation capabilities. In addition, the default values of landscape properties for one location are available for use in the model input. The model has been verified by comparing the steady-state concentrations with the reported data and the results from Mackay Level III fate model under the same input scenario (no mass transfer into the additional compartment – ground water and vegetation in the model).

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Program Manager
Dr. David W. Hand - MTU

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Dr. Michael J. Semmens - UM
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Dr. Edward L. Cussler	Chemical Engineering/Materials Science
Dr. Prodromos Daoutidis	Chemical Engineering/Materials Science
Dr. Malcolm T. Hepworth	Civil Engineering
Dr. Simo Sarkanen	Forest Products

University of Wisconsin – Madison

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Dr. Randy D. Cortright	Chemical Engineering
Dr. James A. Dumesic	Chemical Engineering
Dr. Rajit Gadh	Mechanical Engineering
Dr. Daniel R. Noguera	Civil and Environmental Engineering
Dr. John T. Quigley	Engineering Professional Development
Dr. Thatcher W. Root	Chemical Engineering
Dr. Dale F. Rudd	Chemical Engineering (retired)

Michigan Technological University

Dr. Martin T. Auer	Civil and Environmental Engineering
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Dr. John W. Sutherland	Mechanical Engineering

RESEARCH AND TECHNOLOGY TRANSFER PARTNERS

Industrial Alliances and Memberships

- Center for Waste Reduction Technologies of the American Institute of Chemical Engineers
- National Center for Manufacturing Sciences
- National Pollution Prevention Roundtable

Industry and Government Collaboration and Cooperation

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Air Products & Chemicals, Inc.
ALCOA
American Energy Technologies, Inc.
Amoco
Amway
Arizona State University
Ashland Chemical Limited
AT&T
Barneby-Sutcliffe
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Trojan Industries
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U.S. EPA National Risk Management Research Lab.
U.S. Filter Recovery Services, Inc.
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University of Nebraska
University of Sonora, Mexico
Versar, Inc.
Water Environment Research Foundation
Whirlpool Corporation
W.R. Grace Company

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Barbara Karn, PhD (non-voting member)	U.S. EPA Office of Research and Development	EPA/CenCITT Project Officer
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William E. Thacker, PhD	National Council for Air and Stream Improvement (NCASI)	Pulp and Paper Waste Minimization and Hazardous Waste Management
William Tumas, PhD	Los Alamos National Laboratory	Chemical and Industrial Processes
Clare Vinton	Vinton, Inc.	Environmentally Conscious Manufacturing
Edward A. Weinbrecht (former member)	Sandia National Laboratories	Environmentally Conscious Manufacturing

CENTER FUNDING AND STUDENT SUPPORT

CENTER FUNDING *	**Program Funds FY 1999**	**Total Funding 6/1/92 through 9/30/99 FY 1992 – FY 1999**
EPA core funding	$ 1,000,000	$ 7,915,000
EPA, other	$ 0	$ 175,000
Other federal	$ 0	$ 0
State/local	$ 83,632	$ 326,484
University Cost Share	$ 197,315	$ 1,762,409
Private Sector	$ 20,000	$ 373,069
Total Funds Received through 9/30/99		$ 10,551,962
Total Funds Expended through 9/30/99		$ 9,801,108

STUDENT SUPPORT **	**Students Funded FY 1999**	**Students Funded to Date**	**Funds Expended FY 1999**	**Funds Expended To Date**
Graduate	25	206	$ 219,337	$ 1,671,036
Post Doctoral	7	18	$ 86,916	$ 204,853
Undergraduate	6	112	$ 21,684	$ 182,279
Total	38	336	$ 327,937	$ 2,058,168

* Figures shown include cost share contributions such as academic release time, in-kind, and other forms which are validated by the research administrations of the consortium institutions. In addition, many of the research projects include collaboration with industrial and other organizations. The value of these parallel activities is not shown in the figures above; CenCITT estimates this level of effort to be in excess of $917,500. Examples include visiting engineers; joint projects; access to data; and access to facilities and equipment. Without these additional contributions by external partners, the broad scope of many of our projects would not be possible.

** Total Student Support to date for the Center has amounted to approximately 29% of the total program value, including the indirect costs associated with student support. These funds have been utilized to educate students out of the classroom, thereby giving them hands-on experience in their chosen discipline. Student Support dollars shown do not include indirect costs. Over the entire life of the Center some students may have been counted more than once, due to multiple reporting periods.

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RESEARCH PRESENTATIONS:

Baker, J.R., B.A. Barna, J.L. Bulloch, J.C. Crittenden, D.A. Crowl, D.W. Hand (presenter), D.R. Hokanson, A.A. Kline, A.S. Mayer, J.R. Mihelcic, E.J. Oman, R.M. Patty, P.P. Radecki, T.N. Rogers, D.R. Shonnard, M.J. Semmens, D.W. Hertz, and S. Butner, “CenCITT’s Tools for Sustainability”, poster presentation, United Engineering Foundation’s Clean Products and Processes II Conference, Lake Arrowhead, CA, November, 1999a.

Baker, J.R., J.C. Crittenden, and E.J. Oman, “Decision-Making Tools for the Chemical Process Industry”, U.S. Environmental Protection Agency Tools for Sustainability Workshop, Washington, DC, February, 1999b.

Bulloch, J.L. "The Pollution Prevention Assessment Framework (P2 Framework): Tech Transfer from EPA to Industry", National Pollution Prevention Roundtable, Washington, DC, April, 1999.

Carr, R.W., “Adsorptive Chemical Reactors”, AIChE Annual Meeting, Dallas, TX, October-November, 1999a.

Carr, R.W., “Adsorptive Chemical Reactors”, invited presentation, NICHE Conference (sponsored by Chemical Research Council), Marco Island, FL, June, 1999b.

Carr, R.W., “Partial Oxidations with a Simulated Countercurrent Moving Bed Chromatographic Reactor”, invited presentation, 4th International Conference on Environmental Catalysis, Tokyo, Japan, January, 1999c.

Chatkunnaayuttaya, P., T.N. Rogers, A.M. Provost, M.E. Mullins, and D.S. Hiew, “Thermodynamic Study of Dilute Organic-Water Mixtures: A Proposed Model of Henry's Law Constant at Elevated Temperatures”, Session 01A17: Posters--General Papers on Thermodynamics and Transport Properties I, Paper 86J, AIChE Annual Meeting, Dallas, TX, October-November, 1999.

Chen, H., B.R. O'Donnell, E.J. Oman, A.A. Kline, D.R. Shonnard, T.N. Rogers, B.A. Barna, and D.A. Crowl, "Integrated Assessment Tools as Process Simulator Enhancements for Chemical Engineering Education", poster presentation, AIChE Annual Meeting, Dallas, TX, October-November, 1999b.

Chen, Y., J.C. Crittenden, D.W. Hand, and V.H. Selzer, "Advances in TiO_2 Photocatalytic Oxidation Process", 22nd Annual Midwest Environmental Chemistry Workshop, Houghton, MI, October, 1999.

Crittenden, J.C., "Economic and Environmental Conscious Decision-Making Through the Use of Pollution Prevention Assessment Tools", Michigan Sustainable Business Forum, Grand Rapids, MI, July, 1999a.

Crittenden, J.C., Session Chair, "Applications of Life Cycle Assessment", United Engineering Foundation's Clean Products and Processes II Conference, Lake Arrowhead, CA, November, 1999b.

Crittenden, J.C. and J.L. Bulloch, "The Pollution Prevention Assessment Framework (P2 Framework)", 2nd AIChE Pollution Prevention Topical Workshop, Houston, TX, March, 1999a.

Crittenden, J.C., H. Hautakangas, J.R. Mihelcic, H. Li, E.J. Oman, "Optimization and Modeling of Biofiltration for Odor Control", presented at the WEFTEC '99, 72nd Annual Water Environment Federation (WEF) Conference and Exposition, New Orleans, LA, October, 1999d.

Kallio, E. and M. E. Mullins, "Synthesis and Application of a Novel Zeolite Membrane Reactor", ACS Annual Meeting, Anaheim, CA, March, 1999.

Kallio, E., B. Oonkhanond, and M.E. Mullins, "Preparation of ZSM-5 Membranes on Porous Alumina via Electrophoretic Deposition", AIChE Annual Meeting, Dallas, TX, October-November, 1999.

Oman E.J. and J.C. Crittenden, "Application of Process Design Tools for Pollution Prevention", U.S. Environmental Protection Agency Tools for Sustainability Workshop, Washington, DC, February, 1999.

Oman, E.J., D. Audeves, D.R. Hokanson, D.W. Hand, J.C. Crittenden, and T.N. Rogers, "Modeling and Optimization of a Catalytic Wet-Oxidation Process Used for Water Recycling Applications", presented at WEFTEC '99, 72nd Annual Water Environment Federation (WEF) Conference and Exposition, New Orleans, LA, October, 1999b.

Oman, E.J., D.W. Hand, J.C. Crittenden, D.R. Hokanson, D.L. Carter, and C.E. Martin, "Characterization and Optimization of Three Phase Catalytic Oxidation Processes in the International Space Station (ISS) Water Processor", presented at the 29th International Conference on Environmental Systems (ICES), Denver, CO, July 1999c.

Pletka, J., "Recovery of Waste Polymer Generated by Lost Foam Technology in the Metal Casting Industry", seminar at General Motors Powertrain, AMDC, Saginaw, MI, August, 1999.

Pletka, J. and J. Drelich, "Recovery of Waste Polymer Generated by Lost Foam Technology in the Metal Casting Industry", poster presentation, Michigan Technological University's Graduate Student Council, Houghton, MI, October, 1999.

Qiong Z., J.C. Crittenden, D.W. Hand, J.R. Mihelcic, and D.R. Hokanson, "Environmental Indices for Green Chemical Production and Use", 22nd Midwest Environmental Chemistry Workshop, Houghton, MI, October, 1999.

Sarkanen, S., "Plasticization of Alkylated 100% Kraft Lignin-Based Biodegradable Polymeric Materials", 217th American Chemical Society National Meeting, Anaheim, CA, March, 1999b.

Sarkanen, S., "Plasticizers that Transform Alkylated Kraft Lignins into Thermoplastics", Fourth Biomass Conference of the Americas, Oakland, CA, September, 1999c.

Sarkanen, S., "Plasticizers that Transform Alkylated Kraft Lignins into Versatile Thermoplastics", invited seminar, Westvaco Corporation, Charleston, SC, September, 1999d.

Sarkanen, S., "Plasticizers that Transform Alkylated Kraft Lignins into Versatile Thermoplastics", Tenth International Symposium on Wood and Pulping Chemistry, Yokohama, Japan, June, 1999e.

Selzer, V.H., J.L. Bulloch, and J.C. Crittenden, "The Pollution Prevention Partnership: Environmentally Conscious Decision-Making", Workshop of the Cleveland Area Manufacturing Program (CAMP), Cleveland, OH, May, 1999.

Sever R.R. and T.W. Root, "Environmentally Benign Processing with Hydrogen Peroxide", poster presentation, University of Wisconsin-Madison Chemical Engineering Graduate Recruiting Festival, Madison, WI, February-March, 1999.

Velazquez-Carillo, M., J.R. Mihelcic (presenter), and J.C. Crittenden, "Use of Material Selection Target Plots for Screening Chemicals based on Environmental and Health Properties", poster presentation, United Engineering Foundation's Clean Products and Processes II Conference, Lake Arrowhead, CA, November, 1999.

Yang, Ji, E.J. Oman, D.W. Hand, D.R. Hokanson, and J.C. Crittenden (presenter), "Mathematical Modeling of Isothermal-Three Phase Separative Reactor Systems", poster presentation, United Engineering Foundation's Clean Products and Processes II Conference, Lake Arrowhead, CA, November, 1999.

Zhang, Q., J.C. Crittenden, D.W. Hand, J.R. Mihelcic, and D.R. Hokanson, "Environmental Indices for Green Chemical Production and Use", 22nd Annual Midwest Environmental Chemistry Workshop, Houghton, MI, October, 1999a.

Zhang, Q., J.C. Crittenden, D.W. Hand, J.R. Mihelcic, and D.R. Hokanson (presenter), "Environmental Indices for Green Chemical Production and Use", poster presentation, United Engineering Foundation's Clean Products and Processes II Conference, Lake Arrowhead, CA, November, 1999b.

TECHNOLOGY TRANSFER MEETINGS AND PRESENTATIONS:

Crittenden, J.C., presentation and collaborative project discussions, U.S. EPA National Risk Management Research Laboratory, Cincinnati, OH, December, 1998.

Crittenden, J.C., presentation and collaborative project discussions, Abbott Laboratories, Chicago, IL, April, 1999c.

Crittenden, J.C., presentation and collaborative project discussions, Stephan Company, Chicago, IL, April, 1999d.

Crittenden, J.C., presentation and collaborative project discussions, Dell Engineering, Grand Rapids, MI, July, 1999e.

Crittenden, J.C., presentation and collaborative project discussions, National Council for Air and Stream Improvement, Kalamazoo, MI, July, 1999f.

Crittenden, J.C. and J.L. Bulloch, presentation and collaborative project discussions, Amway Corporation, Grand Rapids, MI, February, 1999b.

Gadh, R., UW laboratory tour and collaborative project discussions, Chrysler Corporation, Madison, WI, October, 1998.

Gadh, R., demonstration of Design for Disassembly (DFD) software and collaborative project discussions, Pratt & Whitney, Florida, 1999a.

Gadh, R., demonstration of Design for Disassembly (DFD) software and collaborative project discussions, United Technologies Engineering Coordinate Activities, Connecticut, 1999b.

Gadh, R., demonstration of Design for Disassembly (DFD) software at Stanford University workshop on Virtual Prototyping, attended by companies such as Boeing, General Motors, and General Electric, 1999c.

Gadh, R., industry seminars presented at various companies: United Technologies, Unigraphics Solutions, Ford Motor Company, Hayes & Lemmerz, Boeing, IBM Research Laboratories, and Lucent Technologies, 1999d.

Gadh, R., organized I-CARVE workshop for potential industrial collaborators, attended by companies such as Pratt & Whitney, Boeing, Ford Motor Company, General Motors, Caterpillar, Hayes & Lemmerz, Detroit, MI, July, 1999e.

Srinivasan, H., C.C. Chu, and R. Gadh, “Virtual Reality for Design and Manufacturing”, Appliance Manufacturer Magazine, pp. 23-25, May, 1999b.

Srinivasan, H., J. Mo, R. Figueroa, and R. Gadh, “Virtual Analysis, I-CARVE’s A3D Aid CAD Projects”, Silicon Graphics World Magazine, pp. 13-14, June, 1999c.

CONFERENCES/MEETINGS HELD:

CenCITT Science Advisory Committee Meeting, Project Review and Poster Session, Michigan Technological University Campus, Houghton, MI, September, 1999.