National Center for Clean Industrial and Treatment Technologies

Advancing the Science and Engineering of Pollution Prevention and Waste Minimization

Activities Report:

January 1997 - September 1997

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

National Center for Clean Industrial and Treatment Technologies (CenCITT)

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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	Advanced Hierarchical Procedure
AIChE	American Institute of Chemical Engineers
AOP	Advanced Oxidation Process
ASAP	Aeration Simulation Analysis Program
CatReac	Multi-Phase Multi-Component Catalytic Reactor Software
CDI	Continuous Deionization
CMA	Chemical Manufacturers Association
CPAS	Clean Process Advisory System
CReaTe	Clean Reaction Technologies
CWRT	Center for Waste Reduction Technologies
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
EPAS	Expert Process Advisory System
ERIC	Environmental Risk Index Calculator
ETDOTs	Environmental Technologies Design Options Tools
FaMe	Fate of Metals in Wastewater Treatment Plants
FaVOr	Fate of Volatile Organics in Wastewater Treatment Plants
GUI	Graphical User Interface
HARD	Heuristics and Reactor Design
IonEx	Ion Exchange Process Model Software
IPES	Isotherm Parameter Estimation Software
MC-Dist	Multi-Component Distillation Software
MPMS	Membrane Process Model Software
MTAMRI	Machine Tool Agile Manufacturing Research Institute
NCMS	National Center for Manufacturing Sciences
NPPR	National Pollution Prevention Roundtable
P2	Pollution Prevention
P2TRG	Physical Property and Thermodynamics Research Group
PPMS	Physical Property Management System
SAC	Science Advisory Committee
SAM	Stochastic Analysis Module
SCMCR	Simulated Counter Current Moving Bed Chromatographic Reactor
StEPP	Software to Estimate Physical Properties
TAP	Technical Assistance Provider
TSA	Thermal Swing Adsorption
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 and Quality Assurance. The original grant was awarded in June 1992, and renewed in September 1996 for an additional 4 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.

Efficient Materials Utilization (EMU)

EMU seeks ways to develop and improve industrial technologies and processes that use materials more efficiently, thereby reducing the production and/or emission of wastes that become environmental pollutants.

Environmentally Conscious Manufacturing (ECM)

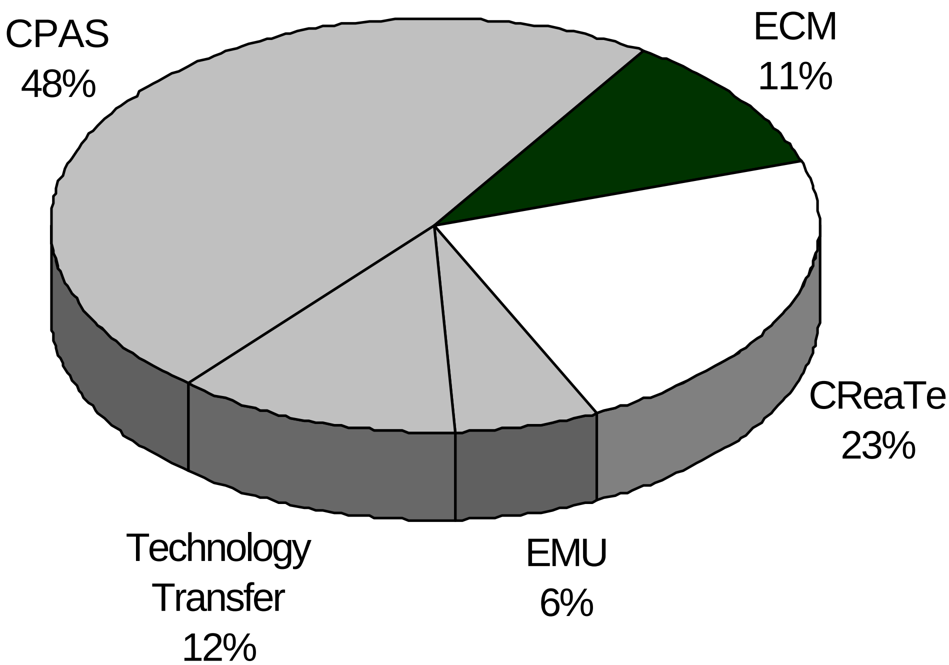
ECM concentrates on the principles of disassembly simulation and environmental assessment of assembly and materials processing practices used in the manufacturing industry.

In addition to advancing technology in each of these areas, CenCITT strives to foster industrial collaboration through the development and promotion of clean technologies and pollution prevention information systems. CenCITT researchers feel strongly that collaboration is truly the “key to success”. Accordingly, CenCITT places significant value in its relationships with industry trade associations, private companies, government agencies, and other universities. Through these relationships, all participants receive mutual benefit and the greatest impact can be achieved from the Center’s research activities.

This report covers activities during the period of January 1997 through September 1997. Information regarding the Center’s research activities between 1992 and 1996 may be found at our web site - http://cpas.mtu.edu/cencitt.

CenCITT Research Program Distribution
EPA FY1997 Allocation

Distribution of the U.S. Environmental Protection Agency's
FY1997 Allocation to CenCITT shown by Focus Area



DIRECTOR'S REPORT

During this years funding cycle CenCITT has supported 12 projects from its base grant. These projects cover a broad range of pollution prevention topics represented in each of CenCITT's Focus Areas. The research activities are consistent with the recommendations of the Science Advisory Committee (SAC) and include:

- ✓ A focused, results-oriented agenda for the Clean Process Advisory System Focus Area, targeted toward outreach and completion of developing design tools.

- ✓ A targeted scope for the Clean Reaction Technologies Focus Area including partial oxidation of methane to methanol, rational design of catalytic reactions, and heuristics for separative reactor design and selection.

- ✓ A maturing Focus Area in Environmentally Conscious Manufacturing which is investigating product disassembly and waste stream prediction.

- ✓ Support for the Efficient Materials Utilization Focus Area in the development of biodegradable plastics manufactured from waste lignin.

In addition to projects funded through the base-grant, CenCITT participates in a growing number of parallel activities. These activities are consistently targeted toward addressing the general objective of "developing and promoting tools and technologies for sustainability". Through this diversification, CenCITT can leverage base grant resources with other public and private funding sources to reach objectives that would not otherwise be possible.

Examples of these activities include:

- A cooperative agreement with the U.S. EPA Office of Enforcement and Compliance Assurance for the creation of a Compliance Assistance Center for the Chemical Industry. This activity will provide a bridge between pollution prevention, clean technology, and compliance with environmental regulations. This effort will provide CenCITT with an opportunity to further its objectives of assisting the chemical industry and promoting pollution prevention concepts and technologies.

- The development of an Expert Process Advisory System (EPAS™) in collaboration with Boeing (formerly McDonnell Douglas Helicopter Systems) and Arizona State University. The expected outcome of this activity is the development of a broad based design package for discrete part manufacturers to routinely evaluate design specifications on the basis of technical, economic, and environmental criteria. The environmental assessment and physical properties contribution of CenCITT in this effort will go a long way in assisting product designers in making more environmentally friendly decisions.

- A cooperative agreement with U.S. EPA National Risk Management and Reduction Laboratory and the Office of Industrial Technologies of the Department of Energy. This effort is titled Pollution Prevention Software for Chemical Industry Process Simulators. Work under this cooperative agreement will develop logical linkages between pollution prevention design tools under development by CenCITT and commercial unit process simulators commonly used in chemical process design. The ultimate result of this effort is expected to be a mechanism by which designers can routinely compare economic, environmental, and worker safety implications of design decisions.

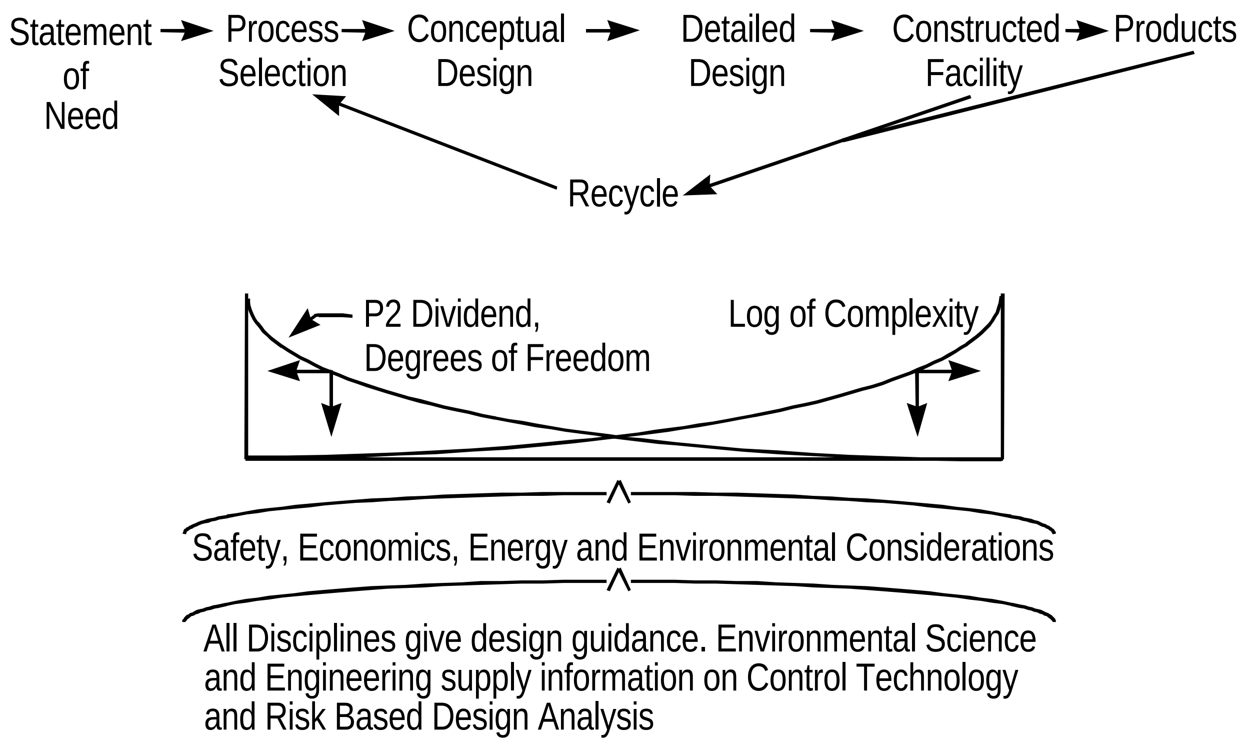
- Participation with the National Pollution Prevention Roundtable (NPPR) and the Machine Tool Agile Manufacturing Research Institute (MTAMRI) in the advancement and execution of a national research agenda in dry machining. This effort will build upon the significant work of the MTAMRI participants and others toward the elimination of cutting fluids for certain machining operations.

- Collaboration with the Center for Waste Reduction Technologies (CWRT) in the creation of a monograph on Emerging Separation Technologies and Separative-Reactors for Industrial Pollution Prevention. This document will explore industrial pollution prevention opportunities that may result from judiciously applying adsorption technologies, membranes and separative-reactors. A workshop on the topic will be sponsored by CWRT, CenCITT, and the Department of Energy February 4-6, 1998 in New Orleans, Louisiana. The workshop will bring together recognized experts (including monograph authors) to provide technology review, input for the monograph, and devise a road-map for the development and implementation of advanced separation and separative-reactor technology in industrial settings.

These activities and other developing initiatives complement the efforts under CenCITT's base grant. Together, they are all part of the mosaic of clean technology that CenCITT is creating through its national leadership in the development and promotion of clean technologies and pollution prevention information systems.

Overview of Focus Areas

The figure below presents a design line that is followed in translating societal statements of need into products and services that address those needs. CenCITT's research in each of the four Focus Areas continues to address issues along this line while maintaining primary focus on the front-end where the degrees of freedom and subsequent pollution prevention dividends are the greatest.



For example, projects under the Clean Process Advisory System Focus Area strongly target the stages of process selection and conceptual design by developing design tools that quickly identify and rank technology and design options. These tools will ultimately be able to rank options on the basis of economics, environmental impact, and worker and consumer safety.

Projects in the Environmentally Conscious Manufacturing (ECM) Focus Area travel across the design line and cover the range from statement of need through product recycle. The research underway in the area of cutting fluids addresses the statement of need: "are cutting fluids necessary for a given operation?". In contrast, the ECM research in disassembly recognizes that an industrial society requires consumer products that are currently being manufactured. Efficient and economical disassembly approaches will increase the amount of material that can be recycled from these products, thereby reducing the burden on natural resources and landfill space.

Similarly, research in the Efficient Materials Utilization Focus Area recognizes that there are currently bulk streams of waste material that could be manufactured into consumer products. Research in biodegradable lignin based plastics addresses the issues of waste reuse and product environmental impact. By both making use of a voluminous waste stream and generating a biodegradable product there are significant potential impacts in reducing stress on waste processing and storage facilities.

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

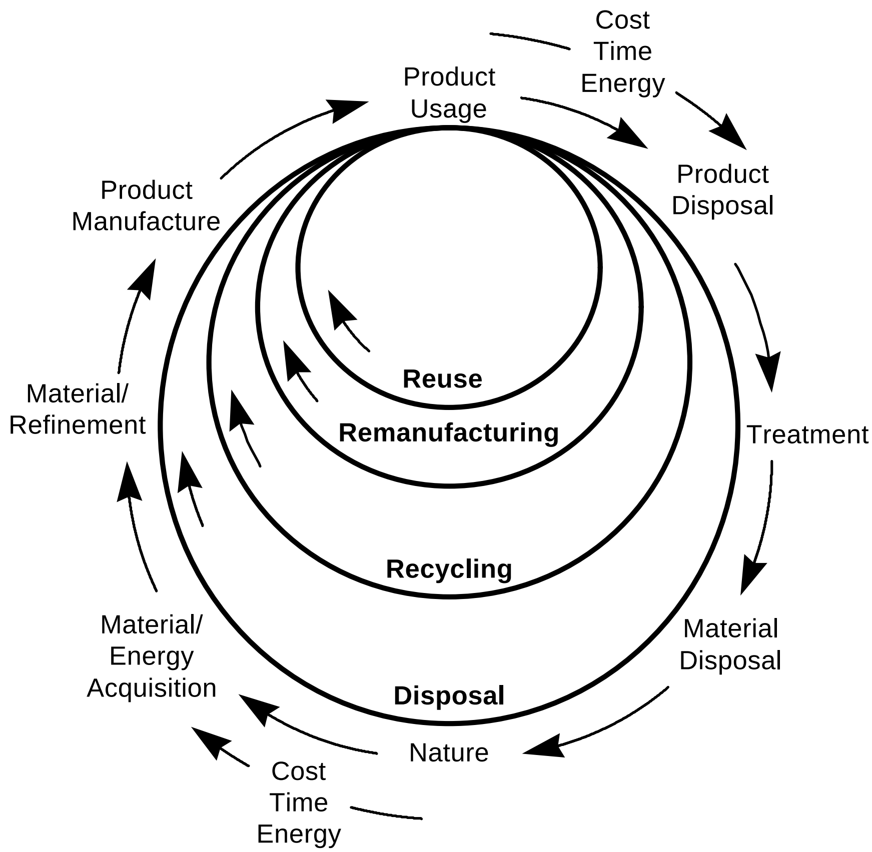
Through this approach of addressing needs along the entire design line, CenCITT researchers are working to solve the problems of the present and the future. By identifying product recycle and reuse opportunities near the end of the design line, they are reducing the burden of existing processes, products, and technologies on the environment. By developing new technologies and decision-making tools at the beginning of the design line, they are helping to ensure that the products, processes, and technologies of the future will be more environmentally benign.

A more detailed description of each focus area is presented below. Please see the Research Project Descriptions section of this report for summaries of each current CenCITT project.

Environmentally Conscious Manufacturing

The Environmentally Conscious Manufacturing (ECM) Focus Area develops tools and methods that can 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. This Focus Area seeks to identify product design strategies that are environmentally benign (or nearly so) and therefore prevent/reduce pollution.

ECM is directed at the environmental issues surrounding the life cycle of discrete products. The figure on the next page 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 suggests 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.

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 at making many of these decisions, they have little experience in terms of environment-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 catalysts that focus the reactions and improve selectivity at high conversions,
2) the development of microorganisms for benign biosynthesis,
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 is collaborating with several industrial and governmental partners 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.

Benign biosynthesis has great potential growth in the selective production of specialty chemicals from renewable carbon sources especially chemicals with chiral centers. Moreover there is a great potential for the interaction between chiral centers which are created from biosynthesis and subsequent chemical synthesis. During this reporting period, no projects in benign biosynthesis were funded. However, CenCITT may fund projects in this area in the next funding cycle.

There are limits to what catalytic chemistry can do. End products from chemical reactions build up and their production ceases. Consequently, CenCITT is developing reactors that separate reactants and products as the reaction proceeds; 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. The feedstock stewardship activity assists in identifying where new catalyst chemistry may be applied as it is discovered.

Efficient Materials Utilization
The Efficient Material Utilization (EMU) Focus Area has the global objective of producing step reductions in pollution generation by focusing on high volume industrial materials currently thought of as wastes. This Focus Area seeks to identify these high volume streams and either eliminate them through process changes and technology development, or develop methods to produce useful products from these wastes.

Examples of past EMU project objectives are: the reuse of foundry wastes, combustion residuals, and the development of a no-VOC inking system for specialty printing. Because combustion residual activities are being supported by other organizations with greater resources, SAC has recently suggested a reduced scope for EMU which does not include combustion residuals. The current scope of EMU includes lignin-based biodegradable plastics which utilize a high volume waste stream (kraft lignins) and produce a useful, biodegradable product.

Clean Process Advisory System
The Clean Process Advisory System (CPAS) is developing as a system of software and design aids for efficiently delivering information on clean technologies and pollution prevention methodologies to the conceptual process and product designer. The system is meant to address the challenge of incorporating environmental considerations into conceptual process and product design, where the majority of the waste can be reduced in a cost effective manner.

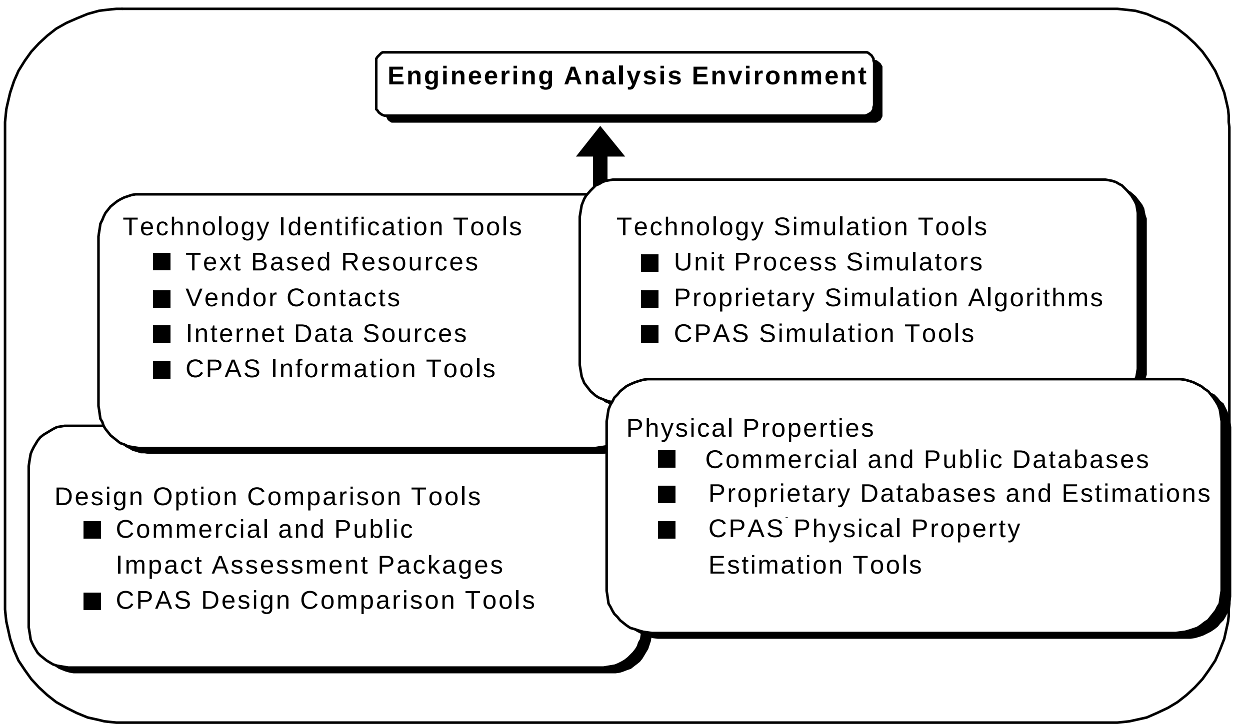
CPAS has been a co-development effort involving CenCITT, the Center for Waste Reduction Technologies (CWRT), and the National Center for Manufacturing Sciences (NCMS). CenCITT holds strategic alliances with CWRT and NCMS which were put in place to facilitate and encourage continued collaboration in the development of CPAS and more broadly in the advancement of clean technologies and information systems. Collaboration is the cornerstone of CPAS development and the developers understand that its continued success depends on the mutual involvement of industry, government, and universities.

While one of the fundamental goals of CPAS is the generation of pollution prevention design tools (e.g. software), it is important to note that CPAS is not just about software. CPAS is about process and product design in general. The CPAS vision is: creating a means for companies to make routine decisions inherently "green", inherently safe, and still cost effective. This requires the linking of a diverse collection of engineering design expertise; operations and construction know-how; and value engineering.

In many ways, CPAS can also be thought of as a technology transfer device for technologies that CenCITT and its partners discover and invent. For example, once a technology is proven, it can be immediately merged into CPAS. CPAS can also be used in the class room for educational purposes and could become an agent of change for the next generation of engineers.

Integrating pollution prevention concepts into the industrial environment requires a culture shift which will result in designers, operators, and managers thinking of opportunities for pollution prevention implementation at all times. This culture shift is currently occurring for a number of reasons from economics, to altruism, to compliance enforcement. CPAS has and will continue to act as a catalyst that continually accelerates this shift.

It is important to stress that CPAS is not intended to be a panacea for any and all green design issues, but rather one component of an overall "Engineering Analysis Environment". The following figure depicts this environment graphically. This conceptual structure allows designers to work with tools they are currently familiar with while supplying additional economic, environmental, and safety information through individual CPAS tools.



This framework also allows for the most efficient leveraging with existing and developing initiatives and programs in process and product design.

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 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. The notion of "knowledge transfer" recognizes and advances the culture change necessary to move toward a sustainable environment. This process of transferring knowledge in addition to transferring technology has been and continues to be a significant component of CenCITT's outreach efforts.

CenCITT Publications and Technology Transfer Activities - FY 1997

ACTIVITY TYPE	NUMBER
Refereed Journal Articles	13
Articles Submitted for Publication	16
Books, Chapters, or Bound Proceedings	10
Major Project Reports	1
Theses/Dissertations	7
Research Presentations Made	23
Technology Transfer Meetings and Presentations	23
Conferences/Meetings Held	3
TOTAL R&D RESULTS CONVEYANCES	**96**

During this period, CenCITT researchers and staff have been involved in a number of technology transfer events. Several CenCITT researchers participated in the 1997 ACS Green Chemistry and Engineering Conference. This participation included session chairs in Biosynthesis and Chemical Processing and Modeling, a poster presentation in the rational design of catalytic reactions, and a table top display for the Clean Process Advisory System (CPAS).

A representative from CenCITT also participated in a workshop on the Role of Modeling and Simulation in Environmental Management sponsored by U.S. EPA and DOE. The intent of this workshop was to direct DOE's research programs in the area of modeling and simulation for environmental management. The workgroup on manufacturing and pollution prevention provided several recommendations for the use of modeling and simulation in pollution prevention. Among these recommendations was a call for DOE to evaluate, utilize, and support existing environmental modeling and simulation efforts such as those under development by the CPAS Focus Area.

In June, 1997, CenCITT participated in an Engineering Foundation Conference on Clean Products and Processes. This participation included an invited presentation on Computer-Based Methods for Design of Clean Products and Processes and co-chairing a session on Computer-Based Design Tools.

CenCITT also continues to participate in the National Pollution Prevention Roundtable (NPPR). NPPR is a national organization consisting primarily of State Technical Assistance Providers (TAPs). These TAPs are instrumental in transferring technological information to small and medium sized businesses for economic and environmental sustainability. CenCITT maintains representation in the Information Technology and Research and Technology Transfer workgroups. This participation offers a conduit for CenCITT to transfer technologies and methodologies related to both information systems (e.g. CPAS) and technologies (e.g. EMU, CReaTe, and ECM) directly to small and medium sized companies throughout the country.

CenCITT also looks forward to increased participation with the Chemical Manufacturers Association (CMA). During this period, a presentation was made at a CMA Responsible Care Conference, "Delivering on the Promise". With the operation of the Chemical Industry Compliance Assistance Center, CenCITT anticipates a more significant level of collaboration in the areas of compliance assistance and technology development.

CenCITT has held meetings to identify needs and/or collaborative opportunities with: Air Products and Chemicals, Dow Corning, Calgon Carbon Corporation, Chemical Manufacturers Association, OLI Systems Inc., Detroit Edison, Libbey Owens Ford, Whirlpool Corporation, Velsicol Chemical Company, Caterpillar, 3M, Mercury Marine, Chrysler Corporation, IBM, Cleveland-Cliffs, Industrial Piping Inc., 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 (RFP) 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. Rajit Gadh, of the University of Wisconsin has received a Second Year Continuing Award for the NSF Industrial Ecology Fellowships Funded by Lucent Technologies Foundation. The National Science Foundation (NSF) and the Lucent Technologies Foundation have awarded 18 grants to researchers across the nation to advance the emerging field of industrial ecology and to encourage businesses to integrate pollution prevention practices into their day-to-day operations. The grants will support an individual or group of researchers focusing on research or teaching to help industry design processes that prevent pollution and create environmentally friendly products. (see page 45)

- Beta versions of the CenCITT/MTU/M.W. Kellogg Constructability Tool have been completed and approved at The M.W. Kellogg Company. This tool is a multimedia system that will allow designers and construction manager teams to consider on site environmental issues during facility planning and design while simultaneously evaluating facility performance criteria. In addition, collaborative efforts related to The M.W. Kellogg/MTU Environmentally Conscious Design for Construction Tool have resulted in the establishment of a team and track record which is attracting new data sources and funding to expand the database with environmental/ safety/constructability technology appropriate for use by practicing facilities planners and designers. (see page 36)

- The Boiler/Combustion Analysis software has been applied to the analysis of the Hillman Power Company facility which is a 20 MW generating plant fired with a combination of wood waste and tire derived fuel (TDF). The software was particularly useful in performing parametric studies related to the percentage of TDF in the fuel and the effect of the fuel composition on predicted sulfur dioxide emissions and fuel cost. Results of the study were reported at the 32nd Intersociety Energy Conversion Conference in July 1997. (see page 24)

- Significant progress has been made in the development of the Environmental Technologies Design Options Tools (ETDOTs™) for CPAS. The ETDOTs contain several important treatment technologies that are used in CPAS to determine whether it is more economical to treat or prevent waste streams. The Adsorption Design Software (AdDesignS™), Aeration System Analysis Program (ASAP™), Software to Estimate Physical Properties (StEPP™), and Fate of Volatile Organic compounds in wastewater treatment facilities (FaVOr™) tools are in final external beta testing stage by over 70 professionals from industry, academia and government. Pending necessary revisions due to Beta Tester comments, these tools will be ready for commercial release in the spring of 1998. (see page 26)

- Additional ETDOT tools which are under development are showing great potential for application in environmentally friendly process and reactor research and design: Adsorption for the Recovery of Organics (AdRecover™), Advanced Oxidation Process Software (AdOx™), Multi-Phase Multi-Component Catalytic Reactor Software (CatReac™) , and Ion Exchange Process Model Software(IonEx™). AdOx may be used to estimate the chemical dosages, power and reactor sizes needed to destroy toxic organics in water. IonEx may be used to make routine calculations to evaluate this water treatment technology for reuse. CatReac may be used to design two and three phase separative reactors and it considers parallel and series reactions of multiple components. CatReac is an unsteady state model which can consider dispersion, external and internal diffusion within a catalyst particle. AdRecover may be used to design adsorption systems to recover organics from dilute fluid streams. (see page 26)

- The combination of theoretical and experimental methods for the elucidation of catalytic chemistry and design of catalysts is a top goal according to the report: Technology Vision 2020 - The U.S. Chemical Industry. Continued support of research toward the rational design of catalytic reactions has placed the research group of Dumesic, Cortright, and Rudd as leaders in achieving this goal. (see page 19)

- The activation of alkanes and in particular the partial oxidation of methane to methanol is also a top goal according to the report: Technology Vision 2020 - The U.S. Chemical Industry. CenCITT is funding Carr's Group at Minnesota and they have developed a separative reactor that has more than doubled the previously observed selectivity for methanol production. This work builds on Carr's previous success in developing a separative reactor for the oxidative coupling of methane to make ethene. (see page 18)

- Continued research has increased the fraction of lignin to 100% in kraft lignin-based plastics. These plastics have tensile properties comparable to those produced earlier under CenCITT research with only 85% kraft lignin. (see page 39)

- Beta Versions of databases to provide failure rate data for various pieces of equipment and failure mode information for major process equipment have been completed. These tools will provide accident probability that is essential in estimating risk. These tools will supplement the Fire and Explosion Index software reported previously and under evaluation by Dow Chemical Company. (see page 33)

- Results in the disassembly of a dash board from a Ford Taurus have revealed that by appropriately sequencing the disassembly, the disassembly cost could be reduced, thereby resulting in more economically attractive recycling. (see page 45)

CenCITT PROJECT LISTING 1997

Principal Investigators	Project Title	End Date	Current Budget	Total Budget *
CLEAN REACTION TECHNOLOGIES (CReaTe)				
Carr	Partial Oxidation of Methane to Methanol	1998	$70,247	$156,646
Mullins, Kline, Rogers	Heuristic Reactor Design for Clean Synthesis and Processing - Separative Reactors	1998	$54,533	$54,533
Cortright, Rudd, Dumesic	Characterization of Selective Solid Acid Catalysts Toward the Rational Design of Catalytic Reactions	1998	$75,000	$587,062
CLEAN PROCESS ADVISORY SYSTEM (CPAS)				
Baker, Barna, Radecki, Rogers	Clean Process Advisory System Core Activities	1998	$124,131	$374,739
Barna, Rogers, Kline	Development and Testing of Pollution Prevention Design Aids for Process Analysis and Decision Making	1998	$74,665	$355,133
Crittenden, Hand, Rogers, Kline	Recovery of Organics from Fluid Streams Using Adsorption and Distillation	1997	$42,312	$84,624
Crowl	Design Tools for Chemical Process Safety: Accident Probability	1998	$31,760	$68,511
Hand, Crittenden, Hokanson, Rogers, Mayer, Semmens	Development and Demonstration of Environmental Technologies Design Options Tools (ETDOTs)	1998	$151,468	$332,847
Patty	Environmentally Conscious Design for Construction: Phase II	1998	$44,942	$198,776
Rogers, Kline	The Physical Properties Management System (PPMS): A P2 Engineering Aid to Support Process Design and Analysis	1998	$71,064	$340,549
Shonnard, Mayer, Paterson, Auer	Environmental Fate and Risk Assessment Tool (EFRAT)	1997	$55,043	$134,270
EFFICIENT MATERIALS UTILIZATION (EMU)				
Sarkanen	Means for Producing 100% Kraft Lignin-Based Biodegradable Plastics	1998	$53,459	$128,835
Semmens	Oil Recovery and Reuse in the Machining and Metal Fabrication Industries	1997	$22,044	$44,089

Principal Investigators	Project Title	End Date	Current Budget	Total Budget *
Semmens, Riley	Assessment of an In-Line Copper Recovery Technology as a Waste Reduction Strategy for the Metal Finishing Industry	1997	$42,174	$84,348

ENVIRONMENTALLY CONSCIOUS MANUFACTURING (ECM)

Gadh	Design for Disassembly to Support Demanufacturing	1998	$68,750	$131,250
Sutherland, Olson	Environmentally Conscious Manufacturing: Prediction of Manufacturing Process Waste Streams for Discrete Products	1998	$28,695	$144,322

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 multiple year projects.

RESEARCH PROJECT DESCRIPTIONS

Clean Reaction Technologies (CReaTe)

The Partial Oxidation of Methane to Methanol in a Simulated Countercurrent Moving Bed Chromatographic Reactor Robert W. Carr; University of Minnesota (References: Bjorklund and Carr, 1997)

Goal: The goal of this CenCITT funded 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 which 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 is being carried out at total pressures from 30 to 100 atm in a multiple column configuration SCMCR. The reactor design, including number of columns and operating conditions, are being optimized for methanol production on the basis of a program of experimentation. A mathematical model will be developed as a basis for refinement of the design, and for potential scale-up.

Status: A program of experimentation to characterize the performance of the adsorber beds, and to determine the methanol selectivity as a function of experimental conditions has been going forward. Attention has been paid to methanol desorption and recovery as a key to reactor performance.

An investigation of the homogeneous partial oxidation itself (no separation) has been carried out as a function of temperature, pressure and reactor residence time in a tubular reactor in order to optimize methanol selectivity. Selectivities from 0.5 to 0.8 have been found. We have found that adding a preheater to the methane feed line has a positive effect on selectivity.

We have also investigated the relationship between switching time (switching of the feed flow from one adsorber to the next) and residence time in the tubular reactor, finding that failure to pay attention to this aspect of the design may result in unexpectedly low conversion. The findings from these experiments have been used to make design decisions. These decisions are being implemented in modifications that are currently being incorporated into the SCMCR. Experiments to test the performance of the modified SCMCR are expected to commence by November 1997.

Characterization of Selective Solid Acid Catalysts Towards the Rational Design of Catalytic Reactions Randy D. Cortright, Dale F. Rudd, and James A. Dumesic; University of Wisconsin-Madison (References: Cortright and Dumesic, 1996; Cortright et al., 1997a,b,c; Natal-Santiago and Dumesic, 1997; Natal-Santiago et al., 1997; Watwe et al., 1997)

Goal: The goal of this project is the linking of microkinetic analysis and computational chemistry for the investigation of catalytic chemistry at the molecular level. Initially, this project investigated the interactions of hydrocarbons with solid-acid catalysts, but the scope of this project has been expanded to investigate the interactions of hydrocarbons and oxygenated hydrocarbons on supported metals catalysts.

Rationale: This project is part of a long-range research campaign to develop principles for the rational design of economically and environmentally sustainable catalytic reactions. The campaign involves two phases: 1) the development of the field of microkinetics of heterogeneous catalysis to elucidate the essential catalytic chemistry of existing heterogeneous catalysts and 2) the application of principles of computational chemistry to explore for new and improved catalysts. This research seeks to further develop the linking of microkinetic analysis and computational chemistry and use the resulting principles for the rational design of new catalytic systems.

Approach: We proposed an investigation that involves the combination of results from spectroscopic, microcalorimetric, kinetic, and quantum chemical studies to describe the interaction of gaseous molecules with catalytic sites. Structural, chemical, and catalytic information about the catalytic sites may be obtained from the combination of results from spectroscopic, microcalorimetric, and kinetic studies. Quantum chemistry techniques may be used to predict properties such as molecular energies and structures, vibrational frequencies, bond and reaction energies, as well as reaction pathways.

Importantly, these techniques may be applied to stable structures (*i.e.*, consisting of all positive eigenvalues for force-constants) and to transition states (*i.e.*, consisting of one negative eigenvalue for force-constants). In general, these calculations may be calibrated using spectroscopic and microcalorimetric measurements that determine the bond energies and structures of stable probe molecules on catalyst surfaces. The quantum mechanical calculations can then be used to predict the bond energies of reactive intermediates and transition states that cannot be measured directly.

Status: We are currently conducting experimental and theoretical studies for the reactions of hydrocarbons over a variety of solid-acid materials. We have developed quantitative kinetic models based on carbenium ion chemistry to describe the reaction pathways of the reactions of butanes and butenes on solid-acid catalysts. This modeling effort is being supplemented using theoretical calculations performed on the basis of Density-Functional Theory (DFT) to probe the role of carbenium ions in: (1) the isomerization of gaseous n-butyl to iso-butyl carbenium ions, (2) the protonation of alkenes by the highly-acidic hydronium ion and further isomerization of the resulting species, and (3) the interaction of alkenes with weakly-acidic silanol groups and further isomerization of the resulting species.

We are currently investigating the hydrogenolysis of ethyl acetate over copper-based catalysts using microcalorimetry, FTIR, kinetics measurements, and DFT calculations. The combined results from our microcalorimetric and FTIR studies indicate that methanol and ethanol adsorb dissociatively on silica-supported copper at 300 K to form alkoxy species, with heats of interaction of 115-140 kJ/mol. Predictions from DFT calculations on 10-atom Cu clusters are in agreement with these experimental results. Furthermore, we have observed that methoxy and ethoxy species decompose on copper at 400 K. Importantly, we have recently used DFT calculations to identify the transition states for these reactions. The activation energies for the decomposition of adsorbed methoxy and ethoxy species to produce hydrogen and the corresponding adsorbed aldehydes are predicted by DFT to be 110 and 95 kJ/mol, respectively, in agreement with our experimentally determined trends.

Finally, we are investigating the interaction of hydrocarbons with platinum-based materials using ethane hydrogenolysis as a probe reaction. This reaction has been widely employed for investigations of supported metal catalysts. Microcalorimetric investigations above provide enthalpies of adsorbed intermediates involved in the ethane hydrogenolysis pathways such as atomic hydrogen, adsorbed ethylene species, ethylidyne species, and adsorbed acetylene species.

Furthermore, we have conducted DFT calculations to provide enthalpies for CH_x intermediates as well as adsorbed ethyl species. Thus, our combined studies involving microcalorimetric measurements and DFT calculations for C_2H_y and CH_x species form an initial basis from which to begin kinetic analyses of our reaction kinetics data for ethane hydrogenolysis. Accordingly, we have combined the results of our microcalorimetric measurements and DFT calculations with the results of our kinetics studies to develop a quantitative description of ethane hydrogenolysis over supported Pt and Pt/Sn catalysts.

Heuristic Reactor Design for Clean Synthesis and Processing - Separative Reactors

Michael E. Mullins and Huidong Zhang; Michigan Technological University

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 (1) for the reactive distillation process, and (2) for 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.

Rational: 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.

Reactive distillation is a unit operation which combines a chemical reaction with a multistage distillation in one step simultaneously. This technique has two important advantages compared with conventional reaction and distillation processes: (1) energy savings and (2) reduction of capital investment. With reactive distillation, the heat generated by chemical reaction can be utilized directly for the separation of products. At any point in the reactive zone, the reaction heat will cause additional mass transfer between vapor and liquid phases.

Another benefit of this process is to reduce both hardware investment and operation costs. Combining the reactor and distillation column in one vessel, one process step is eliminated along with its associated pumps, piping, and instrumentation. In some situations, this elimination results a 30 - 40% reduction of hardware investment. Unfortunately, not all industrial processes are suitable for reactive distillation. One of the drawbacks of reactive distillation is that the temperature control in reactive zone is more difficult than conventional distillation, and it is also difficult to modify the process after it has been designed.

Approach: Our modeling approach is to consider the packed reactor column as a series of discrete stages, and model it the same way as a tray column. In this way, the resulting model equations are a set of non-linear algebraic equations. The composition and temperature profiles can be obtained after solving these equations simultaneously. Due to the small liquid hold-up in trays (pseudo-trays), the chemical reactions are assumed to reach equilibrium. Hence, we adopted a rigorous, non-equilibrium stage model which assumes vapor-liquid phase equilibrium is only established at the interface rather than over the whole stage.

The equations of Mass balance, Energy balance, Rate of mass and energy transfer, and eQuilibrium (so called MERQ model) are written for each phase separately. The Newton-Raphson method will be used to solve the equations, and the technique of line search and backtracking is incorporated into the algorithm to achieve global convergence. Therefore, the solution of the model does not totally depend on the initial estimate, which compensates for a major drawback of the Newton-Raphson method.

We will first develop this model with C++, and a Graphic User Interface (GUI) will be constructed afterwards. Basically, the model consists of four classes: a thermodynamic class which is designed to calculate all thermodynamic properties; a matrix class which does block matrix manipulation; a solver class which implements the Newton-Raphson method with line search and backtracking techniques; and a main program which simply incorporate other classes.

Status: Currently, the thermodynamic and matrix blocks have been done, and the creation of the solver block is ongoing. In the thermodynamic class, the activity coefficient in liquid phase is calculated by UNIFAC method. An advantage of the UNIFAC method is that the fragment parameters needed in the calculation are readily tabulated in the literature for a vast number of chemicals. The disadvantage is that UNIFAC is the most complex model and therefore needs more computation time. The fugacity coefficients in the gas phase are computed using the Souve-Redlich-Kwong equation. The application of cubic equations of state to mixtures requires that the parameters be expressed as functions of composition, and the Van der Waals mixing rule is used here. The vapor pressures are obtained by either the Lee-Kesler or Antoine equation, depending on the availability of parameters used in the correlations. The enthalpy calculation is divided into two parts. In the vapor phase, the enthalpy of non-ideal vapor mixture at temperature T is the summation of the ideal vapor mixture enthalpy (H^{ig}) at T and the residual enthalpy (H^R). H^{ig} is calculated with the standard enthalpy of formation at 298^0K and the mean heat capacity. The residual enthalpy is computed using the Soave-Redlich-Kwong equation. For the calculation of the enthalpy for non-ideal liquid mixtures, we first compute the enthalpy of the vapor mixture with liquid phase molar fractions, then deduct the individual enthalpies of vaporization. The partial molar enthalpy for every component is found from an appropriate form of the Gibbs-Helmholtz equation. The liquid phase of mixing is neglected since little basis exists for evaluation of this term, and the contribution of this term is usually not large.

A critical step in this model is to compute the Jacobian matrix for each individual stage. For separation of four components, there are 21 independent variables and corresponding equations for each stage. The Jacobian matrix in this model is usually ill conditioned, badly scaled, and quite sparse. The value of its elements could be from 10^{-5} to 10^5. The matrix class supports basic matrix manipulation such as addition, subtraction, multiplication, and transposition. The most important and difficult operation this block is the computation of the inverse matrix. It is frequently used in the solver block, and must be guaranteed to work properly. Two algorithms, Gauss-Jordan decomposition and Singular Value Decomposition, are combined to ensure it works successfully.

Clean Process Advisory System (CPAS)

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: Luehrs et al., 1997; Mullins and Rogers, 1997a,b; Rogers et al., 1997a,b)

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 generally available through a stand-alone tool called the Physical Property Management System (PPMS) and in various supplemental modules. The project also facilitates data exchange between various other CPAS tools. Ultimately, the goal of this ongoing support project is the creation of a general PPMS data delivery system that will serve as an expandable framework for adding 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 PPMS Version 1.0, has been designed to provide data support to the Adsorption Design Software (AdDesignS) and Aeration Systems Analysis Program (ASAP) modules under the Environmental Technologies Design Options Tools (ETDOTs) initiative led by Dr. David Hand of MTU. PPMS, originally called Software to Estimate Physical Properties (StEPP), may ultimately link to every other tool and module within CPAS. Many of the tool development efforts now underway (or newly proposed) rely on a working PPMS program for their development, testing, and release. PPMS 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, PPMS will be linked to provide vapor pressures, activity coefficients, and Henry's constants for relative volatility calculations. PPMS 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, and The safety assessment software of Dr. Daniel Crowl.

Status: The PPMS 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 PPMS module also features stand-alone data display. Data sources for PPMS include tables of discrete data, 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. A number of pure component properties are also available in the PPMS module, including: 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.

Beta Version 2.0 of PPMS is nearing completion as a physical property server for CPAS, with a target Beta-test release date around early Spring 1998. It will have the following features:

- Generic protocol for data delivery/export (developed in principle; test 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)
- Complete and test structure disassembly from SMILES (test module working by mid-November 1997)
- Incorporate group contribution vapor pressure module developed by Andrew Loll, M.S. Graduate (test module working by mid-November 1997)
- Database scrutiny (Statistical Process Control data checking to proceed in Spring 1998)
- Support properties needed by ETDOT, EFRAT, and Safety modules (ongoing)

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: Figuerora et al., 1997)

Goals: This project is to create the evaluation and analysis module which 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 which 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 user-supplied 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: The component parts of the DORT project are:

1. Economic Evaluation Aide
2. Costing Database
3. Graphical Interface
4. Stochastic Model
5. Advanced Hierarchical Procedure (AHP) Decision Making Aide

As stated in previous status reports, “items 1, 2, and 3, above, are generally complete as the centerpiece of a master's thesis (Toth, October 1995), they require substantial professional programmer time during the next budget cycle to convert them to a commercially viable software product." At this time the professional programmer effort is well underway and the software prototype is being completely redesigned both to increase the stability and user-friendliness of the code.

The first case study, an analysis of cogeneration options, is complete and documented in an MS thesis at MTU (Herlevich, 1996). To better illustrate P2 options and more fully understand the necessary information flow, a second case study, a solvent recovery design problem, is currently being studied. Multiple processing options have been prepared for this case study and simulations are complete for several of these. Performance indices for environmental fate and safety are being generated along with economic indices. Efforts on the Stochastic Analysis Module (SAM) and the Multi-attribute Decision Making Aide are awaiting suitable progress on the second case study.

An additional component of this effort, the Boiler/Combustion Analysis task is in the process of being closed out under previous funding. The final version of the tool will be delivered to CenCITT shortly. Results were presented to the Science Advisory Committee in September, 1997.

Development of the Environmental Technologies Design Options Tools (ETDOTs)
David W. Hand, John C. Crittenden, David R. Hokanson, Alex S. Mayer, James R. Mihelcic, and Tony N. Rogers; Michigan Technological University; and Michael J. Semmens; University of Minnesota (References: Bulloch et al., 1997a,b; Crittenden et al., 1997b; Hand et al., 1997a,b; Hu, 1997; Hu et al., 1997)

Goal: The Environmental Technologies Design Options Tools (ETDOTs) are a compilation of self-contained tools for use in assessing and implementing effective treatment strategies for gaseous, aqueous, organic, and solid waste by-product streams. ETDOT will assist CPAS in evaluating the technical and economic feasibility of source reduction, versus end-of-pipe treatment and waste segregation, versus treatment at a central facility. It is envisioned that eventually ETDOT or its component parts will be integrated with process simulators, or other manufacturing design tools, to provide more effective analysis evaluation and incentive for source reduction for pollution prevention.

Rationale: Currently, there is much interest by the industrial and regulatory communities in quantifying air, water, and solid pollutant emissions from waste treatment facilities, and in estimating the fate and treatability of specific potential pollutants produced during the manufacturing process. The goal of both communities is to effectively reduce generation of difficult and costly-to-treat pollutants, and optimize destruction of easy-to-treat pollutants in a cost effective and environmentally safe manner.

Before this goal can be achieved, reliable mathematical models, which describe industrial manufacturing and pollution treatment processes, must be developed and coupled into a user-friendly modular form. This project is aimed at developing advanced pollution treatment models, and integrating them with industrial manufacturing process simulators.

Approach: Models are being developed for metal and organic chemical fate during conventional wastewater treatment, air stripping and carbon adsorption. The software is being developed for each unit process as a stand alone package with the ultimate goal of linking them into the overall framework of CPAS. Software is being validated from plant data including different industrial sources.

Status: This project is undertaking the development of a total of nine software tools. Five of these tools have been completed or nearly completed during the past year: 1) Fate of Volatile Organic (FaVOr) compounds in wastewater treatment facilities; 2) Fate of Metals (FaMe) in wastewater treatment facilities; 3) gas- and liquid-phase Adsorption Design Software (AdDesignS); 4) Software to Estimate Physical Properties (StEPP); and 5) Aeration System Analysis Program (ASAP). Other tools under earlier stages of development in the past year include: 6) Advanced Oxidation Process Software (AdOx); 7) Membrane Process Model Software (MPMS); 8) Multi-Phase Multi-Component Catalytic Reactor Software (CatReac); 9) Ion Exchange Process Model Software (IonEx).

A brief description of the scope and status of each tool is presented below.

(1) FaVOr

FaVOr was developed to aid design engineers in determining the fate of VOCs in conventional wastewater treatment facilities. In many industrial applications, conventional activated sludge waste treatment facilities are used to treat industrial waste streams containing VOCs. FaVOr enables design engineers to evaluate the impact of VOCs on a treatment system, identifying potential compliance issues and incentives for source reduction. FaVOr will also evaluate the feasibility of using these conventional waste treatment systems to remove volatile organic compounds from waste streams. FaVOr is in beta testing stage and will be completed in late Spring 1998. Pending satisfaction of tester comments, release is expected in early Summer 1998.

(2) FaMe

FaMe was developed to aid design engineers in determining the fate of metals in conventional wastewater treatment facilities. In many industrial applications, conventional activated sludge waste treatment facilities are used to treat industrial waste streams containing metals. FaMe enables design engineers to focus on minimizing waste metals that are difficult to treat.

FaMe's front-end software architecture and model code has been completed resulting in a functional prototype. Based on a prioritization of potential interest and impact and associated funding limitations, FaMe will not be developed further under the current project.

(3) AdDesignS
AdDesignS was developed to aid design engineers in performing adsorption design calculations. AdDesignS consists of equilibrium and mass transfer models which are used to provide gas and liquid phase multi-component adsorption design calculations for fixed-bed adsorbers. The AdDesignS equilibrium isotherm database currently contains 650 aqueous phase isotherms for more than 300 compounds on 15 adsorbents and 300 gas phase isotherms for 150 compounds on two adsorbents. In addition, isotherm parameter estimation algorithms are also provided.

AdDesignS has been completed and passed the alpha testing stage. The tool has been turned over to the CPAS core group for distribution to beta testers. Over 70 professionals from industry, academia and government have offered to beta test the software. It is anticipated that final beta testing will be completed in the Winter of 1997-98. Expected release date is in early Spring 1998.

(4) StEPP
StEPP has been primarily developed under the Physical Properties Management System project. The linkage of StEPP to individual treatment modules and other development has been supported under this project.

(5) ASAP
ASAP was developed to aid design engineers in performing air stripping design calculations for the removal of Volatile Organic Compounds (VOCs) from aqueous waste streams. ASAP consists of three models applicable to aeration systems: packed tower aeration, bubble aeration, and surface aeration. ASAP has two modes; design mode for sizing new systems and rating mode for evaluating existing systems.

ASAP has been completed and passed the alpha testing stage. The tool has been turned over to the CPAS core group for distribution to beta testers. It is anticipated that beta testing will be completed in early Winter of 1997-98. At this time, the CPAS core group will perform the final modifications followed by marketing and distribution in early Spring 1998.

(6) AdOx
AdOx is being developed to aid engineers in the design of advanced oxidation processes (AOPs). These technologies may have significant use in water-reuse applications. The present work in the development of AdOx focused on the fundamental model development, model code development, and model verification for an hydrogen peroxide in the presence of UV-light. The model was verified by predicting the decomposition rate of organic contaminants in water.

The dynamic kinetic model developed under this project can predict the parent organic compound destruction and hydrogen peroxide consumption in both completely mixed batch reactors and completely mixed flow reactors. The model's capability of including the effect of background organic matter on the process efficiency in laboratory scale studies has been successfully verified. In addition, the consideration of pH decrease during the process due to the formation of mineral acids and carbon dioxide further improves model performance. A model front end will be developed during the Spring of 1998 and alpha tested.

(7) MPMS
MPMS is being developed to predict the separation performance of microporous membranes for a variety of operating conditions. This tool is being developed under the project, "Predictive Tool for Ultrafiltration Performance" by Dr. Michael Semmens of the University of Minnesota.

(8) CatReac
A model to predict the performance of a Multi-phase Low Temperature Catalytic Reactor System (e.g. trickle bed reactor system) has been developed. The model incorporates the following assumptions and mechanisms: 1) plug-flow in the gas and aqueous phases, 2) by-product contaminant formation and destruction in the catalyst phase described by first-order kinetics, 3) gas and water partitioning described by Henry's law, 4) mass transport across the gas-water and water-solid interfaces described by film diffusion, and 5) mass transport in the catalyst phase described by pore diffusion.

CatReac has been tested against analytical solutions (when available) and experimental results, for the decomposition of some primary and secondary alcohol type compounds. The model has shown good agreement with both analytical and experimental results. Additional model development work will include the multi-component competitive interactions among competing solutes and further model verification with experimental data. CatReac development, testing and verification will be completed by the end of Winter 1998.

(9) IonEx
IonEx is being developed to aid design engineers in performing fixed-bed ion exchange design calculations. IonEx is an equilibrium multi-component fixed-bed model that can be used to predict the performance of several types of resin beds: strong acid cation exchange, strong base anion exchange, weak base anion exchange, and mixed bed strong anion and cation exchange. The model is presently in the development and testing stage. A model front end will be developed during the Spring of 1998 and alpha tested.

Environmental Fate and Risk Assessment Tool (EFRAT™) David R. Shonnard, Alex S. Mayer, Kurtis G. Paterson, and Martin T. Auer; Michigan Technological University

Goal: CenCITT is funding a process design software tool which will estimate environmental and health impacts of chemical process design options through a combination of screening-level fate and transport calculations and risk assessment indices. EFRAT will be a menu-based advisory system, which allows the conceptual process designer a number of options in assessing environmental and health risks. The software will require a minimum of user-supplied data input and expertise. The risk indices will be calculated relatively quickly on a personal computer.

Rationale: Within the framework of pollution prevention, a methodology is needed for choosing the most environmentally benign chemical process or product design from a number of design options. It is highly desirable that such a methodology be scientifically based on the risks imposed to both human health, and to the environment, stemming from the operation of a chemical process or the production and use of a consumer product. Risk evaluation to the environment should be comprehensive, including the effects of pollutant emissions on global warming potential, ozone depletion, acid rain formation, smog formation, and accumulation of pollutants in all environmental compartments.

EFRAT will provide the process design engineer with the required environmental impact information, so that environmental, safety, and economic factors may be considered simultaneously. Inherent in the software is the ability to incorporate toxicological properties of the pollutants released from the process. Therefore, EFRAT will aid in focusing on steps to reduce not only the total amount of pollution, but also its toxicity.

Approach: The approach taken in this project is to develop a user-friendly software package that requires minimal user input. The software will consist of 1) a graphical user interface (GUI), 2) a multi-media environmental partitioning model, 3) an environmental risk index calculator (ERIC), and 4) chemical process emission estimation algorithms.

The fate and transport characteristics are based on the potential for a compound to accumulate and persist in an environmental compartment, such as a compartmental reaction residence time coupled with a "Level I" (partitioning) multimedia compartment model prediction. The ERIC portion of the software calculates environmental and health risk indices which are based on a combination of parameters indicative of human health and environmental damage, and fate and transport characteristics. The health and environmental risk indices are made relative rather than absolute by computing ratios of the risk from the compound in question to the risk from a benchmark compound.

As an example, the index for global warming potential, I_{GW}, is based on the global warming potential (GWP) of a compound in the troposphere, and the fraction of the released chemical distributed to the atmospheric compartment (D_A) relative to the water and soil.

$$I_{GW} = GWP \frac{D_{A,i}}{D_{A,CO_2}}$$

In this example, the benchmark compound is CO_2. Other environmental (global warming, ozone depletion, smog formation, acid rain, and fish toxicity) and human health (carcinogenic and non-carcinogenic effects for both ingestion and inhalation routes) risk indices are also computed in a similar fashion. A total of 9 relative risk indices generated in EFRAT are listed in the Table 1.

***Table 1**. Relative Risk Indices for Human Health and Environmental Impacts.*

Index	Description	Parameters	Benchmark
Abiotic Environmental Effects			
I_{GW}	Global Warming Index	D_A, GWP, τ_A	Carbon Dioxide
I_{OD}	Ozone Depletion Index	D_A, ODP, τ_A, x	CFC-11
I_{SF}	Smog Formation Index	D_A, MIR	Ethene
I_{AR}	Acid Rain Index		SO_2
Human Health Effects			
I_{ING}	Ingestion Non-carcinogenic	D_W, LD_{50}, τ_W	Toluene
I_{CING}	Ingestion Carcinogenic Index	D_W, WOE, τ_W	Benzene
II_{INH}	Inhalation Non-carcinogenic	D_A, LC_{50}, τ_A	Toluene
I_{CINH}	Inhalation Carcinogenic Index	D_A WOE, τ_A	Benzene
Biotic Environmental Effects			
I_{FT}	Fish Toxicity Index	D_W, LC_{50}, τ_W	PCP

Parameter Definitions:
D_A, D_W, and D_S are fractions distributed to the atmosphere, water, and soil respectively.
GWP is the global warming potential of the chemical.
ODP is the stratospheric ozone depletion potential of the chemical.
τ_A and τ_W are reaction residence times in the troposphere and water, respectively (d).
MIR is the maximum incremental ozone reactivity for smog formation.
LD_{50} is the inhalation or ingestion non-carcinogenic 50% lethal doses (mg/kg/d).
WOE is the inhalation or ingestion carcinogenic weight of evidence.
LC_{50} - the 4-day rodent or fish lethal dose (mg/L) which causes 50% mortality in a test population.
PCP - pentachlorophenol
x - Number of chlorine atoms on organic molecule.

Status: A prototype version of the EFRAT software has been developed using a Visual Basic platform. All of the environmental partitioning parameters (Henry's constants and soil/water partition coefficients) and environmental/health impact parameters have been input within the software as resident databases for 75 of the most hazardous organic compounds appearing on the Toxics Release Inventory of industrial chemicals.

In addition, a complete database of "landscape" properties has also been included for one location representing an upper midwest industrial site (Midland County, MI). Landscape properties are properties related to the geographic location where the chemical process design is to be implemented, Quality checks for the environmental partitioning algorithm have shown excellent agreement (within a few tenths of a percent) compared to literature compartmental distribution predictions. Additional quality checks of the ERIC portion of the software have also shown excellent agreement with published impact potentials.

In addition to these accomplishments, improvements in estimating vent emissions from distillation columns have been undertaken and are being incorporated into the software. Funding for this effort has been discontinued under the CenCITT base grant, however continuing work is being funded through a cooperative agreement with EPA's National Risk Management Research Laboratory. This has enhanced the capabilities of the EFRAT software beyond that which was originally proposed for this CPAS project. If funding can be identified, future improvements to the software will include the incorporation of a more sophisticated fate and transport model, data exchange between other CPAS software modules and commercial process design simulators, as well as automated reporting capabilities.

Predictive Tool for Ultrafiltration Performance Michael J. Semmens and Brian C. Huff; University of Minnesota

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

Rationale: Membrane separation processes are becoming increasingly popular in a variety of industrial applications since they can be used to separate products for reuse or recovery. However, the performance of the process is difficult to predict apriori since many factors including membrane type, water quality and operating conditions influence process behavior. As a result engineers rely on the recommendations of manufacturers or experimental studies to design a process application.

The intent of this project is to develop a tool that will assist design engineers in selecting a membrane and the best operating conditions for a particular application. It is hoped that the model will improve the design process by providing the engineer with preliminary estimates of membrane performance and recommendations for experimental testing to refine the design.

Approach: Currently, we are analyzing existing software and articles that relate to aspects of membrane performance to determine how we might incorporate them into a structured tool. The tool will use empirical relationships extracted from existing data bases and different models as sub-programs and to provide information on expected membrane performance. In addition, the tool will provide feedback on data needs and the recommended approach for data collection.

Status: Work on this project is in the very early stages. This project was initiated in July 1997 and the literature review and model assessment stage are currently underway.

Design Tools for Chemical Process Safety: Accident Probability Daniel A. Crowl; Michigan Technological University (References: Crowl, 1997)

Goal: To provide design tools for including process safety in the conceptual design of chemical processes. In particular, this part of the effort will be directed towards providing design tools to estimate the probability of an accident, and how this can be coupled to a cash flow analysis.

Rationale: Previous CenCITT project efforts have developed computer-based methods to estimate the relative hazard associated with a chemical process and to estimate the capital loss (financial consequence) associated with a process accident. Since risk is comprised of both consequence and probability, the addition of a tool to estimate accident probability would provide the user with a greater capability to estimate risk.

Approach: The work plan is to provide a number of interactive computer-based programs to assist the conceptual designer in estimating the risk due to episodic accidents from the processing of flammable and toxic chemicals Risk is comprised of both accident consequence and probability. To date, a program to estimate the hazards and financial consequence of an accident involving toxic and flammable chemicals has been completed (Dow Fire and Explosion Index, Dow Chemical Exposure Index). The work will also develop a database module to provide failure rate data to the designer and to describe the failure modes for various pieces of equipment. Finally, a method for coupling the accident probability to a complete cash flow analysis for the process will be developed, including the financial effects of an accident. This would provide an estimate of financial risk due to an accident.

Status: The implementation of the Dow Fire and Explosion Index and the Dow Chemical Exposure Index in an interactive Visual Basic environment has been completed. We have completed three evaluation cycles by Dow Chemical of this software and are completing changes to the programs for another evaluation by Dow. This is expected to be the final evaluation cycle, however, other cycles may be necessary depending on feedback by Dow. The indices provided by these tools are necessary to determine the relative hazard and financial consequence of an accident.

A beta version of a database to provide failure rate data for various pieces of process equipment has been completed. A beta version of a database to provide failure mode information for major process equipment, such as tanks, reactors, distillation columns, etc has also been completed in this period.

Both of these tools provide estimates of accident probability and are essential to estimate risk. Through the next year, we hope to couple these tools to a complete cash flow analysis, including the financial effects of an accident. This aspect of the work has just begun. Current, plans are to use a Monte-Carlo type method to examine all of the possible accident modes during the lifetime of a chemical plant.

Recovery of Organics from Fluid Streams Using Adsorption and Distillation John C. Crittenden, David W. Hand, Tony N. Rogers, Andrew A. Kline, and John L. Bulloch; Michigan Technological University (References: Bulloch, 1997; Bulloch et al., 1997a)

Goals: The primary goals of this project are to develop two software modules: 1) Adsorption for Recovery (AdRecover) of organics, and 2) Multi-Component Distillation (MC-Dist).

Rationale: There are many liquid and vapor streams that require enrichment or recovery of organic fractions in order to be reused or recycled. Adsorption and distillation are two technologies that may be used for this purpose. The AdRecover and MC-Dist software modules will broaden the base of the separation technologies modeling tools within CPAS. Moreover, commercial process simulators generally do not contain dynamic models for adsorption or databases including the latest adsorbents that may be used for enrichment of chemical process streams.

AdRecover and MC-Dist will utilize other software modules within CPAS, including Isotherm Parameter Estimation Software (IPES; a part of the Adsorption Design Software) and Software to Estimate Physical Properties (StEPP). The AdRecover activity will be closely linked to other CPAS development projects since the regeneration of adsorbents can generate liquid streams which need further enrichment by other technologies (e.g. membrane separations or distillation). The dynamic models and the databases included in the software will also be useful for interpreting data and selecting adsorbents for the separative reactor work within the Clean Reaction Technologies Focus Area.

Approach: AdRecover will focus on the removal of organic compounds from air and water streams and their recovery using novel adsorbents and activated carbon. Recovery methods being modeled are 1.) adsorption and steam regeneration with organic/water separation by condensation, phase separation and/or distillation, and 2.) adsorption and hot purge gas regeneration with organic separation by condensation and/or distillation.

Laboratory data is being provided by the Rohm and Haas Chemical Company (Philadelphia, PA) to calibrate and verify AdRecover. AdRecover will require adsorption equilibrium relationships covering a wide range of operating conditions. Therefore, methods of predicting adsorption equilibria based on the nature of the adsorbates and the fundamental forces of attraction are also being further developed for use in AdRecover and the Isotherm Parameter Estimation Software.

MC-Dist will consider the separation of multiple organic compounds from by-product streams such as steam condensate from adsorbent regeneration. MC-Dist can represent several important separation processes including: single-stage flashing, steam stripping, absorption, and conventional fractionation. MC-Dist will use the combined methods of Fenske/Underwood/Erbar-Maddox to solve the total reflux mass balance for a column. A fourth method, that of Kirkbride, will be used to locate the optimum feed tray location for design applications of the model.

Status: Several different thermal swing adsorption (TSA) models are at various stages of development. A Fortran model was developed for modeling multi-component adsorption/ regeneration cycles with externally heated hot purge gas regeneration. The model predicts the breakthrough of compounds from adsorption/regeneration cycles given input temperature cycles. The model includes both fluid phase and solid phase mass transfer and is useful for modeling TSA processes relying on external heat sources for regeneration.

A Fortran model was developed for modeling single component TSA processes employing hot inert purge gas regeneration. The model predicts effluent temperature and concentration profiles based on simultaneous solution of the mass and energy balances assuming local equilibrium between the solid and fluid phases. Preliminary modeling calculations have compared favorably to steam regeneration data from Rohm and Haas Co. on novel adsorbents.

Currently, a TSA model is in development that will rigorously account for steam regeneration. Several different chemical properties have been used to improve adsorption equilibria correlation and prediction methods. In recent meetings, Calgon Carbon Co. indicated a willingness to work together and supply thermal swing adsorption data for model verification.

Current upgrades to MC-Dist are aimed at linking it to StEPP (and its successor, the Physical Property Management System, or PPMS) to provide the thermodynamic properties (e.g., relative volatilities, bubble points, dew points, heats of vaporization, etc.) required for the distillation calculations. Both design and rating mode calculations are now being implemented by a student programmer.

MC-Dist will ultimately be used as a stand-alone tool with an optional link to a process simulator or other CPAS modules (e.g., DORT). MC-Dist's front-end software architecture is a Visual Basic graphical user interface designed for the Microsoft Windows environment, while the model code is developed in Fortran.

The basic MC-Dist calculations have passed the alpha testing stage, through intensive use by faculty and students in the chemical engineering undergraduate Plant Design series, but the overall module still requires some minor programming modifications and additions, which are underway at the present time (October 1997). After the upgrades are finished, MC-Dist will be turned over to the CPAS core group for distribution to beta testers.

Environmentally Conscious Design for Construction: Phase II Robert M. Patty; Michigan Technological University; Darryl W. Hertz and Jim Harper; The M.W. Kellogg Company (References: Patty and Hertz, 1997)

Goal: The goal of this project is to develop a CD-ROM based multimedia system for designers to infuse environmental considerations into the design process for constructed facilities, while simultaneously evaluating other facility performance criteria. This system will also serve as a resource database for manufacturers desiring to better understand field problems associated with installing their products.

Rationale: Choosing environmentally preferred options can produce beneficial effects to the entire construction or remodeling project. A well-known example of this is the use of citrus or other aqueous-based solvents to strip paint to avoid volatile organic compound (VOC) releases which are associated with chlorinated solvents. When employees are not distracted by health or safety hazards, they can be attentive to production. Modular designs, to reduce the cost of field assembly, are also likely to be safer to build. Modular considerations, beyond their initial construction, could make them easier to maintain, and hence, more reliable. This extends the life of the facility and reduces waste, which is of primary environmental concern. Further, modular prefabrication and assembly can allow large assemblies to be hoisted into place, reducing worker exposure to elevated work tasks. Included in the database are specific examples, pictures and video clips on how to successfully do these things at several facilities.

Incorporating safety and environmental issues routinely into design decisions requires improved availability of usable and applicable information for the work at hand. If information is unavailable or hard to reach, one must rely on one's own experience, plus that of others to make decisions. These other sources of advice or experience are not always available, so decisions are often made in rather isolated conditions. The new software being developed in this project is intended to fill this important void, and to improve constructability within the facility planning and engineering design stages, as well as during construction operations.

Advanced ergonomic and cognitive learning research in this area by the primary investigator and others has found constructability data to be diverse and interrelated, usually containing issues relating to more than one facility performance criteria. Further, use of a large constructability information base must be intuitive, matching the natural cognitive organization of other information used in the design process. By extracting and matching this natural organization, the interface becomes intuitive and easy to use. The search process actively draws existing knowledge into the engineer's working memory, preparatory to infusing it with the new environmental criteria.

Approach: The M.W. Kellogg Company and MTU are collaborating in this co-development project. The combined effort will create an interactive multimedia information database, containing constructability examples from environmental and safety perspectives, applicable to many of the tasks performed during design and construction. Advanced ergonomics are being incorporated into this tool.

The industrial quality product produced by this research will contain sufficient material to plant principles of pollution prevention and sustainable development at the forefront of constructability design tools. It will be usable on individual PCs from CD-ROM or from network servers. A team and track record has been established, which is attracting new data sources and funding to expand and update the database with environmental/ safety/constructability technology appropriate for use by practicing facilities planners and designers. Promising new or existing pollution prevention technologies, requiring additional research to enable and encourage reduction to practice, will be identified.

Status:
Project accomplishments to date include:

- Kellogg's VAX-Based Constructability Checklist has been translated to a PC format
- The Houston Business Roundtable Constructability manual and database has been combined with Kellogg's knowledge base
- 80 additional lessons learned have been added through secondary research
- Beta version has been developed and tested at the KELSAFE 97 conference.
- Beta version has been tested at sites inside and outside The M.W. Kellogg Company.
- Technical review of lessons learned generated is nearly complete for version 1 but will continue as development is ongoing.
- Confidentiality, non-disclosure, and copyright issues are currently being formalized.
- Current system includes: (~325 MBytes)
    - 1850+ Lessons Learned - mostly low density
    - 320+ Lessons Learned - high density
    - 650+ Construction Images, digitized & hyperlinked in database
    - 490+ Construction Images, digitized & organized to create a graphical front end
    - 25 Construction Process Digital Video Clips
    - 250+ environmental issues included
    - M.W. Kellogg Constructability Manual, modules 1, 2, 3 & 4
    - Houston Business Roundtable Model Plan for Constructability Complete
    - User Interface Beta and system setup programming is complete, version 1 programming is underway
    - Field data collection and database content development for version 1 ~95% complete
    - Industrial information provider review & permissions ~95% complete
    - Introduction Video Clip, developed
    - 4 Guided Tours for system use, developed

Clean Process Advisory System (CPAS) Core Activities Project James R. Baker, Bruce A. Barna, Tony N. Rogers, and Peter P. Radecki; Michigan Technological University (References: Baker, 1997a,e; Baker and Crittenden, 1997; Baker and Quigley, 1997)

Goal: The goals of the CPAS Core Project are to coordinate individual development projects in the CPAS Focus Area with industrial representatives and to facilitate the delivery of CPAS tools and concepts to the public and private sector in a timely fashion.

Rationale: Maintaining a central node for distribution and coordination of design tools developed under the CPAS Focus Area is the most effective way to supply them to industry. Quick distribution in a consistent fashion will provide the greatest opportunity to realize pollution prevention benefits from the collective efforts of all CPAS investigators. The CPAS Core Activities Project provides this central node, including staff and other resources for distribution and promotion of design tools and concepts.

Approach: The approach of the CPAS Core Project is to support and promote the accomplishments of the individual CPAS projects though the use of professional computer programmers and other full-time staff. This allows the project investigators on the individual projects to apply their intellectual talents most effectively in project development. Specific aspects of this work include:

- Outreach through sponsoring and attending regional and national meetings to familiarize the industrial sector with efforts within the CPAS Focus Area.
- Constructing and refining a single front-end interface that will allow all CPAS design tools (including tools developed by strategic alliance partners, National Center for Manufacturing Sciences (NCMS), Center for Waste Reduction Technologies (CWRT) and other outside parties) to be accessed once installed on a personal computer. This front end will also provide a mechanism for transfer of data between CPAS tools.
- Development of a CPAS business plan and framework for sustainable product distribution on a not-for-profit basis.
- Release of demonstration versions of CPAS and other promotional materials to provide information about current and future expected activities and software products.
- Management of testing by outside parties.
- Software release on a single set of media (floppy disks, or CD ROM) from a single source, as opposed to requiring users to request software from each individual investigator.
- Provide a consistent dedicated point of contact to coordinate with various parties interested in participating in CPAS development, scoping, or distribution.

Status: Achievements toward project deliverables include:

- Preliminary development of a one-day workshop and five-day short course on CPAS and pollution prevention.

- Continued development and maintenance of a CPAS marketing database with more than 500 individuals expressing interest in various tools upon release.
- Maintaining communications with parties interested in CPAS developments.
- Continued Beta testing of Adsorption Design Software (AdDesignS), Aeration Systems Analysis Program (ASAP), and Software to Estimate Physical Properties (StEPP).
- Continued development of a CPAS business and distribution plan. The plan is expected to be completed and implemented for the first release of CPAS in the Spring of 1998.
- Ongoing communication with the Center for Waste Reduction Technologies (CWRT), the National Center for Manufacturing Sciences (NCMS), and several individual companies and organizations including the National Pollution Prevention Roundtable, the Chemical Manufacturers Association, Dow Corning, Boeing, and others.
- Continued Participation with the CWRT CPAS Task Force to provide industry review of CPAS tools.
- Consultation in support of graduate student developers on programming conventions including the continued development and implementation of a software engineering plan that will educate developers on software engineering fundamentals.
- Implementation and management of a Revision Control System for source code management, backup and security.
- Presentation of CPAS tools and concepts at various national meetings including the National Pollution Prevention Roundtable Technology Transfer Workgroup and Research and Technology Transfer Workgroup, the Chemical Manufacturers Association, among others. Participation in venues such as this allow us to review ongoing pollution prevention activities, identify potential areas of collaboration, benchmark and promote CPAS activities.

Efficient Materials Utilization (EMU)

Means for Producing 100% Kraft Lignin-Based Biodegradable Plastics Simo Sarkanen; University of Minnesota (References: Li, Y. et al., 1997)

Goal: The research project is dedicated to developing the basic technology necessary for establishing a plant where the first biodegradable plastics that are truly lignin-based can be manufactured. The industrial byproduct lignin for producing these plastics is to be 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 that 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. It is difficult to envisage a more compelling way of responding to the problem than by 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.

More recently, through CenCITT funded work, alkylated 100% kraft lignin-based plastics with comparable tensile properties have been produced in the principal investigator's research group. Thus the proposed work seeks to develop feedstocks suitable for injection-molding biodegradable plastic components that are composed entirely of simple industrial kraft lignin derivatives.

Approach: Ultrafiltration is being employed to purify and fractionate industrial kraft lignin samples that, after simple derivatization, can be extrusion-molded into strong plastic components. The compositions of the resulting preparations are being monitored through chromatographic analysis and molecular weight determinations.

The plasticizers being sought for use with the new alkylated kraft lignin-based plastics are themselves ultimately expected to be kraft lignin-based also. It is intended that these will be made from narrow fractions of kraft lignin component derivatives carrying substituents that enhance their tendency to associate selectively with high molecular weight kraft lignin species. The development of effective kraft lignin-based plasticizers relies heavily upon testing with low molecular weight aromatic compounds possessing substitution patterns deemed likely to create this critical aspect of their function.

The final step in making these new biodegradable plastics involves spray-drying aqueous suspensions of the kraft lignin derivatives to produce powders that will 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 of 95-100% alkylated kraft lignin has been amply confirmed. From the perspective of all previous accomplishments, this is remarkable.

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

It has recently been found that removal of low molecular weight kraft lignin components by ultrafiltration yields improved preparations for successful plastic formulations. This was readily evident with the ethylated higher molecular weight kraft lignin fraction obtained by ultrafiltration through a 10,000 nominal molecular weight cutoff membrane, which exhibited better plastic tensile behavior than the parent preparation.

Numerous trials have been performed in searching for signs of plastic deformation and attempting to understand the basis of plasticizing activity in alkylated kraft lignin-based plastics. Polymeric materials containing 95% (w/w) of the ethylated methylated high molecular weight kraft lignin fraction blended with appropriately substituted plasticizers have indeed exhibited plastic behavior. Under tensile stress, the materials approach a region of plastic deformation before fracture.

Since the strong non-bonded orbital interactions between the aromatic moieties of the kraft lignin components lead to brittleness in these polymeric materials, plasticizers will play a decisive role in achieving successful plastic formulations. Without explicitly disclosing information with potential proprietary value, it can be said that effective plasticizers have now been established to be compounds which *preferentially* interact with the kraft lignin components in such a way as to increase their chain segmental mobility. After the substituents which efficiently impart plasticizing activity have been completely or largely documented, the low molecular weight kraft lignin components themselves are destined to be derivatized accordingly into compounds that effectively fulfill this function.

In-Line Copper Recovery Technology Michael J. Semmens, and Carla Dillon; University of Minnesota

Goal: The objective of this project is 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 will be performed:

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. Interim Report Preparation - Prepare a summary of Tasks 1 and 2.
4. Pilot-scale Testing - Run experiments using a larger CDI unit and operating for longer time periods.
5. Final Report Preparation - Prepare a detailed report of the technical and economic feasibility of CDI for in-line copper recovery.

Status: To date, a process review has been completed including determination of operating parameters and treatment objectives. Bench-scale experiments have been conducted operating under both batch and single-pass flow regimes. Bench-scale testing is continuing, and the preparation of an interim report is in progress.

Oil Recovery From Cutting Fluids Michael J. Semmens; University of Minnesota (References: Semmens, 1997)

Goal: To determine whether membranes can be used effectively for the recovery of the oil content of spent cutting fluids. To characterize the factors that affect oil separation, and provide the information needed to determine whether membrane technology can be an effective pollution prevention and source reduction technology for the metal machining industry.

Rationale: The recovery and reuse of the oil content of the cutting fluids generated in machining shops will have several benefits: 1) the life-cycle of the oil used in the machining processes will be extended, 2) the amount of waste generated by a machining facility will be reduced, and 3) the oil content of wastewaters will be reduced.

Approach: Cutting fluids are designed to be very stable. High concentrations of surfactants are added to the oil and water so that a stable emulsion is formed. This fluid is used to lubricate and cool the parts being machined. Spent cutting fluids can be treated with acids and coagulants to crack the emulsion and separate the oil and water phases. Most oily wastewaters contain only a small concentration of oil (typically less than 5%), so this treatment results in an oily sludge and a large volume of strongly acidic water, both of which require further treatment before they can be disposed of safely. This conventional approach does not lend itself to oil recovery.

Recently, the use of ultrafiltration has been used to remove trap oil and solids from cutting fluids, however, they are prone to fouling by the free oils. In addition, the oil concentrate still needs to be disposed of and a large volume of water must be treated to separate a small (<5%) amount of oil.

In this study, we use a different approach. The hollow fiber membranes are treated to make them selectively transport oil and reject water. They are then used to separate the small concentration of oil from the spent cutting fluid. The approach is based on earlier work, conducted at UM, that showed oil saturated membranes reject water, but transport oil.

Status: This project is now complete and a final report is on file at CenCITT. Samples of new and spent cutting fluids obtained from local machine shops were characterized using droplet size distribution analysis, titration curves and zeta potential measurements. Oil separation tests were conducted for two spent cutting fluids using an experimental membrane testing apparatus. These tests were used to determine flux permeation rates and permeate character under different operating conditions.

Selective oil filtration of the spent cutting fluid with the bench scale membrane module was not achieved. The results show that the module functioned primarily as an ultrafiltration membrane unit allowing water as the permeate under all conditions tested. However, destabilization of the initial solution with acid produced an unstable “creamy” oil phase in the permeate which phase separated within 12 hours. This is thought to result from emulsion inversion in the membrane pores. Results indicate that the effect of the emulsifying agent and the degree of membrane wetting it causes must be neutralized to achieve selective recovery of emulsified oils from solution.

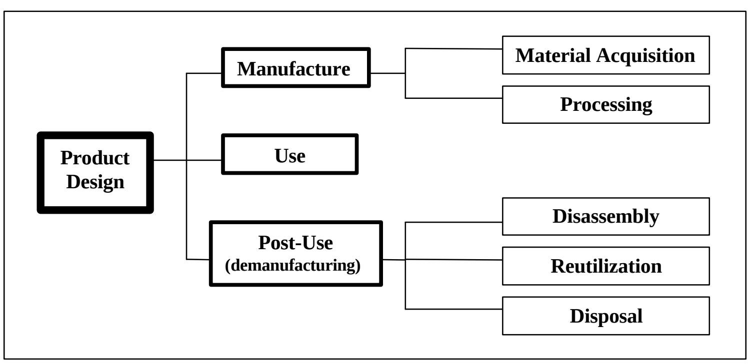
<u>**Environmentally Conscious Manufacturing (ECM)**</u>

Environmentally Conscious Manufacturing: Prediction of Processing Waste Streams for Discrete Products John W. Sutherland and Walter W. Olson; Michigan Technological University (References: Batzer et al., 1998; Bergstrom, 1997; Cozzens et al., 1998; Gowaikar, 1997; Huang et al., 1996; Li, H., 1997; Rao, 1997; Soni, 1997; Sutherland, 1997a,b,c,d,e,f,g)

Goal: The aim of the project is to characterize the waste streams produced during product manufacture. Waste stream characteristics of various manufacturing processes are to be predicted with the objective of developing a decision making tool which will enable manufacturing process modification so as to minimize waste.

Rationale: Product manufacture often produces undesirable environmental, health, and safety impacts. The long term cost associated with manufacturing processes need to take these environmental factors into consideration. Therefore, it is desirable to identify processes and processing conditions that minimize waste streams. This economic aspect provides the motivation for developing tools and enhancing knowledge related to reducing waste. This contributes to a central mission of CenCITT, pollution prevention.

Approach: The ECM focus area is being jointly undertaken by Michigan Technological University and the University of Wisconsin-Madison. The ultimate goal of the focus area is to produce an Environmental Advisory System that can be used to evaluate product concepts early in the design process. The following figure illustrates the structure of the product evaluation tool.



Product Evaluation Tool Structure

The research work at MTU is focused on the development of a manufacturing process waste stream evaluation software tool based on appropriate theoretical underpinnings. Initial efforts have been directed at identifying appropriate process models for waste streams. The other part of the product design tool is being developed at the University of Wisconsin-Madison under the supervision of Dr. Rajit Gadh and is focused on the post-use processing of a product.

Status: Efforts over the past year have focused on characterizing one class of manufacturing processes: machining operations. Waste streams associated with machining operations may be classified into the following areas (relative performance measures given in parentheses): material (chip geometry), energy (power, heat source strength, and temperature distribution), cutting fluid (mist formation, and heat transfer coefficient), and cutting tools (tool life). Characterization of these streams and their sources is currently underway.

Design for Disassembly to Support Demanufacturing Rajit Gadh; University of Wisconsin (References: Gadh et al., 1997; Shyamsundar and Gadh, 1997a,b,c,d,e; Sonthi et al., 1997; Srinivasan and Gadh, 1997a,b,c; Srinivasan et al., 1997a,b, 1998)

Goal: The goal of this research is to establish a systematic framework for investigating disassembly as relevant to designing environmentally conscious products through demanufacturing analysis. This framework allows designs to be classified for applications such as recycling, refurbishing, or reuse. These classifications enable the development of algorithms and software programs for their analysis.

Rationale: The current research analyzes Design-for-Disassembly of assemblies as it relates to Design-for-Environment and hence for pollution prevention/reduction. The disassembly analysis determines the ease/difficulty of disassembling each component in a product. It also determines the cost of disassembly (a portion of the cost of recycling) and therefore decides the economics of recycling products. This will result in a reduction of the amount of disposable products such as molded plastics, aluminum engine blocks, steel components, cables, etc. Disassembly makes separation possible, resulting in reuse/recycling and thus reduction of raw material usage.

Approach: The Environmentally Conscious Manufacturing project is directed at developing tools and methods that can 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. The methodology involves: (i) assessment of the product design for demanufacturing via disassembly analysis, and (ii) prediction of manufacturing waste stream for discrete products based on manufacturing feature determination (manufacturing feature determination being researched at UW-Madison, and waste stream generation being researched at MTU through a separate project in the ECM Focus Area).

Status: Building on last year's work, in relation to demanufacturing via disassembly, the disassembly framework and supporting software for Design for the Environment was developed further in the following areas: 1) de-manufacturing framework, 2) methodology and, 3) software.

Although no single disassembly strategy works for all products, we have found that generally the most effective method is to employ non-destructive disassembly until it is no longer effective. After non-destructive disassembly reaches the point of diminishing environmental returns then destructive disassembly becomes a viable option. This general use of a non-destructive method minimizes the destruction of the product and maximizes the potential of not only material resources but also sub-component reuse.

For assemblies whose components are made of different materials, it is necessary to disassemble the product prior to recycling or reuse. Existing methods primarily address the problem of disassembly planning without regard to recycling or solid waste recovery. In addition, existing research does not provide a quantitative assessment of disassembly. The current research work specifically addresses the difficulty or ease of disassembly and provides a quantitative assessment to that effect. In the current research, algorithms to perform disassembly of virtual prototypes are investigated.

In order to arrive at an acceptable disassembly sequence, it is necessary to determine methods or metrics for comparing different disassembly sequences. Two metrics have been formulated: (i) the range of disassembly directions, and (ii) the volume/weight of the components belonging to the assembly. These serve as a basis for identifying the optimal disassembly sequence.

The first metric, the range of disassembly directions indicates the ease with which a component can be disassembled. Therefore, if there are two components and one of them only has a single axis direction and one has three or four axis directions, then the latter is easier to disassemble and therefore the latter component is the preferred one for disassembly. In general, we found through studying the automotive industry that components with larger range of disassembly directions generally need less disassembly time and are easier to disassemble.

The second metric, volume/weight of a component, also plays important role in disassembly cost. For example, removing a screw is generally easier than removing an electric motor. Therefore, when there is a choice of either removing a screw and having the electric motor fall down by itself versus removing the electric motor, the screw removal is the preferred choice. The metrics developed in effect try to provide an estimate for the cost of disassembly. In the given duration of the project we have been able to investigate these two metrics. However, further research needs to be done before a software tool can be made available to industry.

To further our computational models of disassembly, an experimental investigation into the practical disassembly of an instrument panel of a Ford Taurus was performed utilizing the various metrics developed in the theory, this product was disassembled. The results of these disassembly tests revealed that by appropriately sequencing the disassembly, the disassembly cost could be reduced, thereby resulting in more economically beneficial recycling. Further investigation into other automotive subassemblies and assemblies will be performed. A technical report is being developed for this research which will be available for public dissemination in the near future.

Integrating this research, a virtual disassembly tool to assess products for de-manufacturing at the design stage is being developed. The disassembly software tool evaluates: (i) disassembly sequence for the selected set of components to be recycled/reused, (ii) cost for disassembly, recycling/reuse and disposal, and (iii) net profit/loss in product de-manufacturing. Based on the de-manufacturing evaluations, the product design is further analyzed to determine: (i) the maximum net de-manufacturing profit and an optimal disassembly sequence, and (ii) disassembly and design change recommendations to increase the overall de-manufacturing profit of the product. Also, the methodology presented in this project based on the analysis of physical and virtual prototype of products can serve as a basis for identifying an efficient product design for de-manufacturing.

In the area of manufacturing waste stream generation, research involves determining automatically from CAD models of machined parts, machining features and their dimensions. This work is performed at the University of Wisconsin-Madison, and utilizes a previously known CAD construct called C-Loop. The features are subsequently inputted via the Internet to the waste stream determination software program at MTU which determines the waste stream generated from the machined part. A technical report is being developed and will be submitted for publication.

A number of software programs have been developed to perform non-destructive and destructive disassembly. Non-destructive disassembly allows for disassembling components without the destruction of any of the components within the disassembly. In contrast, destructive disassembly allows the destruction of one or more components to facilitate the disassembly of the rest of the components. The non-destructive disassembly software utilizes information such as constraints in physical space to obtain steps for the entire past.

The second software developed incorporates the destructive disassembly evaluation of computer models of solid assemblies. The objective of the destructive disassembly approach is to minimize the amount of destruction required of the product, subject to the constraints and requirements provided by the user as discussed in the previous section.

A preliminary version of the waste stream from discrete products software has been prototyped. A feature decomposition software module has been developed at UW-Madison, with the waste stream assessment based on the manufacturing/machining features was developed at MTU. Initial results prove this to be a promising future collaborative project as part of the CenCITT program.

KEY PERSONNEL

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Program Manager
James R. Baker - MTU

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Dr. Michael J. Semmens - UM
Dr. C. Robert Baillod - MTU

University of Minnesota - Twin Cities

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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

Dr. Douglas C. Cameron	Chemical Engineering
Dr. Randy D. Cortright	Chemical Engineering
Dr. James A. Dumesic	Chemical Engineering
Dr. Rajit Gadh	Mechanical Engineering
Dr. John T. Quigley	Engineering Professional Development
Dr. Dale F. Rudd	Chemical Engineering (retired)

Michigan Technological University

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Mr. John L. Bulloch	Civil and Environmental Engineering
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Dr. Alex S. Mayer	Geological Engineering and Sciences
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Dr. Walter W. Olson	Mechanical Engineering
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Dr. David R. Shonnard	Chemical 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

A.E. Staley Manufacturing Co.
Air Products & Chemicals, Inc.
ALCOA
American Energy Technologies, Inc.
Amoco
Arizona State University
Ashland Chemical Limited
AT&T
Barneby-Sutcliffe
Boeing - McDonnell Douglas Helicopter Systems
Boise Cascade Corporation
Borden Corporation
Calgon Carbon Co.
Cargill Corporation
Center for Dairy Research
Central Illinois Light Company
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Deluxe Corporation
Department of Energy, Office of Industrial Technology
Design Institute for Physical Property Research Consortium of AIChE
Dow Chemical Company
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The M.W. Kellogg Company
Machine Tool - Agile Manuf. Research Institute (NSF/ARPA)
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NASA - Ames Research Center
NASA - Johnson Space Center
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Osmonics, Inc.
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Thermatrix Corporation
3M Corporation
Trojan Industries
Upper Peninsula Power Co.
U.S. Air Force
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Research Laboratory
USCAR Vehicle Recycling
Partnership
USDA Forest Products Laboratory
U.S.EPA National Risk
Management Research Lab.
U.S. Filter Recovery Services, Inc.
Universal Oil Products, Inc.
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University of Karlsruhe, Germany
University of Nebraska
University of Sonora, Mexico
Versar, Inc.
Water Environment Research
Foundation
Whirlpool Corporation
W.R. Grace Company

SCIENCE ADVISORY COMMITTEE

Member	**Affiliation**	**Expertise**
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James E. Alleman, PhD Vice Chair	Purdue University	Biological Treatment and Solids Residuals

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Hugh J. Campbell, Jr., PhD	E.I. Du Pont de Nemours & Company	Physical and Chemical Treatment Processes
Dennis A. Clifford, PhD (Former member)	University of Houston	Water and Hazardous Waste Treatment
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Michael C. Kavanaugh, PhD	Malcolm Pirnie, Inc.	Remediation of Wastewater
Barbara Karn, PhD (non-voting member)	U.S. EPA Office of Research and Development	Acting EPA/CenCITT Project Officer
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Edward A. Weinbrecht	Sandia National Laboratories	Environmentally Conscious Manufacturing

CENTER FUNDING AND STUDENT SUPPORT

CENTER FUNDING *	Program Funds FY 1997	Total Funding 6/1/92 through 9/30/97 FY 1992 - FY 1997
EPA core funding	$ 1,000,000	$ 5,915,000
EPA, other	$ 0	$ 175,000

Other federal	$ 0	$ 0
State/local	$ 22,550	$ 235,952
University Cost Share	$ 223,009	$ 1,357,819
Private Sector	$ 50,480	$ 292,589
Total Funds Received through 9/30/97		$ 7,976,360
Total Funds Expended through 9/30/97		$ 7,319,109

STUDENT SUPPORT **	Students Funded FY 1997	Students Funded to Date	Funds Expended FY 1997	Funds Expended to Date
Graduate	22	162	$171,403	$ 1,248,373
Post Doctoral	0	11	$ 0 -	$ 117,937
Undergraduate	13	100	$ 31,320	$ 152,257
Total	35	273	$202,723	$ 1,518,567

* 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 are not shown in the figures above; CenCITT estimates this level of effort to be in excess of $880,000. 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 28% 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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Sutherland, J.W., "An Overview of Environmentally Conscious Machining at Michigan Technological University", presented to the Ford Motor Company, Livonia, MI, March, 1997a.

Sutherland, J.W., "Characterizing the Role of Cutting Fluids in Machining Processes", invited presentation at the SME - Advances in Metal Working Fluids Workshop, Fort Mitchell, KY, April, 1997b.

Sutherland, J.W., "Environmentally Conscious Machining: Recent Developments Relating to Cutting Fluids and Dry Machining", invited presentation at Cooper Industries (Crouse-Hinds), Syracuse, NY, June, 1997c.

Sutherland, J.W., MT-AMRI Workshop on Environmentally Conscious Machining, Ford QMP Facility, Dearborn, MI, September 19, 1997d.

Sutherland, J.W., "Overview of the Programs and Activities of the Machine Tool Agile Manufacturing Research Institute," invited presentation at the DARPA/NSF Agile Manufacturing Initiative Principal Investigators Meeting, Alexandria, VA, September 23, 1997e.

Sutherland, J.W., "Research on Environmentally Conscious Machining-Dry Machining", presented to GM, Pontiac, MI, February, 1997f.

Sutherland, J.W., "The Role of Cutting Fluids in Machining Process Performance", presented to Monsanto Chemical Company, Urbana, IL, February, 1997g.

TECHNOLOGY TRANSFER MEETINGS AND PRESENTATIONS:

(See also research presentations made)

Allegier, Peter, Diplome Arbeit, University of Karlsruhe, Karlsruhe, Germany, Chemistry Department, Visiting Scholar, Michigan Technological University, Summer and Fall 1997.

Baker, J.R., workgroup participant, "Research and Technology Transfer Workgroup and Information Workgroup", National Pollution Prevention Roundtable, Annual Conference, Denver, CO, April, 1997b.

Baker, J.R., workgroup participant, "The Role of Simulation and Modeling in Environmental Management", U.S. Department of Energy, Albuquerque, NM, September, 1997c.

Baker, J.R., "Chemical Industry Compliance Assistance Center, Center Introduction and Collaborative Opportunities Discussion", Association of Small Business Development Centers Fall Confernce, Keystone, CO, October, 1997d.

Baker, J.R., "Pollution Prevention in Design Through the Clean Process Advisory System", CAREline - The International Responsible Care Newsletter, October, 1997e.

Cameron, D.C., Session Chair - Biosynthesis, Green Chemistry and Engineering Conference - Implementing Vision 2020 for the Environment, Washington, DC, June, 1997.

Crittenden, J.C., “The Activities of the Center for Clean Industrial and Treatment Technologies”, Department of Urban Engineering, The University of Tokyo, Tokyo, Japan, June, 1996.

Crittenden, J.C., participated in session development, “Adsorption in Water Environment and Treatment Processes”, IAWQ, Shirahama, Wakayama, Japan, November, 1996.

Crittenden, J.C., collaborative opportunities discussion, NASA Marshall Flight Space Center, Huntsville, AL January, 1997.

Crittenden, J.C., collaborative opportunities discussion, NASA Johnson Space Center, Houston, TX, March, 1997.

Crittenden, J.C., Session Chair - Chemical Processing & Modeling, Green Chemistry and Engineering Conference - Implementing Vision 2020 for the Environment, Washington, DC, June, 1997.

Crittenden, J.C., Panel Member - Synthesis and Processing Environmental Priorities for Vision 2020, Green Chemistry and Engineering Conference: Implementing Vision 2020 for the Environment, Washington, D.C., June, 1997.

Crittenden, J.C., workshop participant “EPA's Pollution Prevention Assessment Framework”, U.S. EPA, Santa Clara, CA, October, 1997.

Crittenden, J.C., collaborative discussions with Professor Eckhard Worch, Director of Institute of Water Chemistry and Technology, Chair of Hydrochemistry Department, Technische Universitat Dresden, Houghton, MI, October, 1997.

Crittenden, J.C., D.W. Hand, J.R. Baker, and P.P. Radecki, discussion of potential collaborative projects in software development with OLI Systems, Inc., Houghton, MI, March, 1997.

Hertz, D.W. and P.P. Radecki, “Research Progress Update on CWRT/CenCITT Collaborative Projects in the Clean Process Advisory System, Emerging Separation Technologies and Separative Reactors for Industry Pollution Prevention and Pollution Prevention and Assessment Software for Chemical Industry Process Simulators”, Center for Waste Reduction Technologies meeting, Richland, WA, July, 1997.

Radecki, P.P., overview of CenCITT EH&S design decision support software, Boeing Commercial Airplane Group, Seattle, WA, January, 1997.

Radecki, P.P., collaborative proposal development discussion, 3M, Minneapolis, MN, January, 1997.

Radecki, P.P., J.R. Baker, and J.C. Crittenden, collaborative projects opportunities discussion, Air Products and Chemicals, Inc., Houghton, MI, February, 1997.

Radecki, P.P., A.L. Tonkovich, D. Ruthven, and K. Knaebel, “Early Results of CWRT Separation Technologies Roadmapping Project”, March, 1997.

Radecki, P.P., J.R. Baker, and J.C. Crittenden, collaborative proposal development discussion, Dow Corning Corporation, Houghton, MI, April, 1997.

Radecki, P.P., participant in Organizing for R&D in the 21st Century conference and American Association for the Advancement of Science Colloquium on Science and Technology Policy, Washington, DC, April, 1997.

Radecki, P.P., session co-chair, “Computer-Based Methods for Design of Clean Products and Processes”, Engineering Foundation Conference on Clean Products and Processes, San Diego, CA, May, 1997.

Radecki, P.P. Overview of CenCITT program, Dow Corning Corporation, Midland, MI, September, 1997.

Salman, Salman R., Professor, Chemistry Department, Yarmouk University Irbid, Jordan, Fulbright Fellow Visiting Researcher Sponsorship, Michigan Technological University, Summer 1996.

Ulmer, Marcus, Ph.D. Student, University of Karlsruhe, Karlsruhe, Germany, Chemistry Engineering Department, Visiting Scholar, Michigan Technological University, January, 1997.

CONFERENCES/MEETINGS HELD:

CenCITT Science Advisory Committee Meeting, Center Review and Update, by Teleconference, May, 1997.

CenCITT Science Advisory Committee Meeting, Project Review and Poster Session, Houghton, MI, September, 1997.

Pollution Prevention and Assessment Software for Chemical Industry Process Simulators (P2SCIPS), Industry and Simulation Company Advisory Group Meeting, Richland, WA, July, 1997.