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A REVIEW OF COMPUTER PROCESS SIMULATION IN INDUSTRIAL POLLUTION PREVENTION

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FOREWORD

Today's rapidly developing and changing technologies and industrial products and practices frequently carry with them the increased generation of materials that, if improperly dealt with, can threaten both public health and the environment. The U.S. Environmental Protection Agency is charged by Congress with protecting the Nation's land, air and water resources. Under a mandate of national environmental laws, the agency strives to formulate and implement actions leading to a compatible balance between human activities and the ability of natural systems to support and nurture life. These laws direct the EPA to perform research to define our environmental problems, measure the impacts, and search for solutions.

The Risk Reduction Engineering Laboratory is responsible for planning, implementing, and managing research, development and demonstration programs to provide an authoritative, defensible engineering basis in support of the policies, programs, and regulations of the EPA with respect to drinking water, wastewater, pesticides, toxic substances, solid and hazardous wastes, and Superfund-related activities. This publication is one of the products of that research and provides a vital communication link between the researcher and the user community.

Pollution prevention (P2) is the use of materials, processes, or practices that reduce or eliminate the creation of pollutants or wastes at the source. Once limited to easy practices such as good housekeeping, P2 is currently evolving to include new methods of process design and new process technologies. Process simulation, a process design tool once used only by experts but now developed for a broader user community, has great potential to contribute to these new P2 efforts. The intent of this document is to foster the use of process simulation for P2 by environmental professionals by discussing and demonstrating the user-friendliness and capabilities of state-of-the-art simulation software.

ABSTRACT

The objective of this report is to provide environmental professionals with an understanding of the power and utility of state-of-the-art process simulation software for industrial pollution prevention (P2) analysis. Process simulators are process design tools that were once used only by experts in the chemical process industries (CPI), but are now sufficiently user-friendly to be used by a wider range of people. These tools are important for P2 efforts because of the potential for application to processes outside the CPI.

To better understand the issues that are discussed, background information is first provided on process simulation, including historical development, current applications, and current research. Also, to better understand the features of state-of-the-art process simulators, a review is provided on several commercially-available simulation software packages. A case study is then performed using one of the simulators reviewed, in order to demonstrate the P2 analysis capabilities of existing process simulators.

State-of-the-art process simulators are shown to have the ability to do rapid and convenient analysis of process design options leading to P2. Powerful analytical features and enhanced user environments make this possible. Existing process simulators can also contribute to U.S. industrial P2 efforts by their ability to model waste water systems, and to measure P2 progress. However, despite these strengths, existing simulators have some important weaknesses that must be addressed for P2, such as in modeling fugitive/trace emissions and dynamic/batch process operation.

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SECTION I

INTRODUCTION

Report Objective

The objective of this report is provide environmental professionals with an understanding of the power and utility of state-of-the-art process simulation software for industrial pollution prevention analysis. Most environmental professionals have very little knowledge of these process analysis tools. Until the past few years, process simulation has been used primarily by a relatively small number of process design experts in the chemical process industries (CPI). The intent of this document is to foster the use of these tools for pollution prevention by non-experts by discussing and demonstrating the capabilities and user-friendliness of the software.

The document does not promote process simulation as a pollution prevention tool applicable to all industrial processes and problems. Within the CPI, the software has been available mostly for continuous rather than batch process design, and therefore this report explores the use of process simulation for general manufacturing processes that are continuous or quasi-continuous only. Further, the current software has some other important needs that must be addressed for pollution prevention purposes. This report presents some of these needs.

The Definition of Pollution Prevention

The U.S. Environmental Protection Agency (EPA) defines pollution prevention (P2) as the use of materials, processes, or practices that reduce or eliminate the creation of pollutants or wastes at the source. A strict interpretation of this definition has been adopted in this report by equating P2 to "source reduction" only, and therefore recycling is included in the realm of P2 only when it occurs *before* the subject waste is discharged from a process or facility to the environment. This is not to imply that end-of-pipe techniques such as off-site recycling are not desirable; it does, however, indicate that while these methods can help, there are often better approaches.

Report Motivation

A prime motivation for promoting the application of process simulation to industrial P2 is the technological evolution of P2. Initial P2 efforts, which have focused on the easiest practices such as good housekeeping, are approaching a limit, and a second phase is underway in which existing processes will be modified by the use of separation technology. This second phase will also inevitably reach a limit, and a third phase will be necessary in which new methods of process design and new process technologies will be used specifically for P2 [1]. Process simulation is a process design tool with great potential to contribute to these second and third phase P2 efforts.

Report Organization

Section II of this report provides background information on process simulation, including a basic system description, and discussions on historical development, current applications, and current research. Section III presents a review of some of the leading, state-of-the-art commercial process simulation software packages. Section IV provides a case study demonstrating some of the P2 analysis capabilities of state-of-the-art process simulators. Process simulation needs for P2 design and analysis are discussed in Section V. Finally, some conclusions are offered in Section VI.

SECTION II

BACKGROUND ON PROCESS SIMULATION

Process Simulator Description

A process simulator, or flowsheeting system, is a large computer program that aids in engineering analysis. It can be defined further as a computer system that accepts, as input, information about a process at the flowsheet level of detail and performs analyses useful in process development, design, or operation [2]. All flowsheeting systems are comprised of the basic building blocks of models, algorithms, software, and a user interface, as shown in Figure 1.

The models are the foundation of a process flowsheeting system. The models mathematically describe the key process unit operations by relating the inlet and outlet stream variables, model parameters (i.e., unit operation performance parameters), sizing and performance requirements (e.g., heat duty for a heat exchanger), and internal variables (e.g., internal stage temperatures for a distillation column). A schematic diagram of a unit operation model is provided in Figure 2. The mathematical relations are all in the form of algebraic and differential equations that are based on the applicable laws of chemistry and physics [2].

The algorithms solve the mathematical equations provided by the models. The two leading types of algorithms used in current commercial process simulators are a sequential-modular algorithm and an equation-oriented algorithm. In a sequential-modular algorithm, the unit operation models are implemented sequentially as computer subroutines that calculate the outlet stream variables as functions of the inlet stream variables and model parameters. A computation sequence is initially determined, either automatically or by the user, and the output from one unit serves as input to the next unit. In an equation-oriented algorithm, all of the flowsheet equations are collected and solved simultaneously as a large system of nonlinear algebraic equations [2].

The software consists of everything needed to implement the algorithms on a particular computer and operating system. Included within the category of software are: the program and system architecture, database structures, file-system interface, programming language, computer code, and system documentation [2].

The user interface is the window by which the user views and operates the flowsheeting system. This includes the input language, or other means, whereby the user describes his or her problem to the system; the reports that contain the results; user documentation that explains how to use the system; and protocols to interface with other computer programs or systems [2].

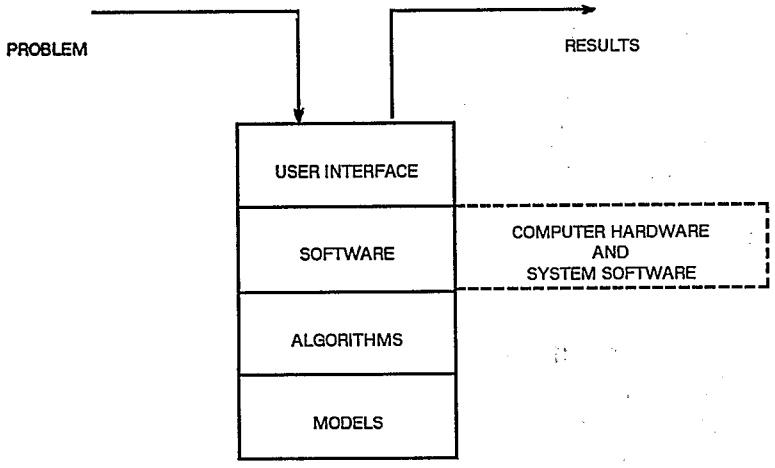

Figure 1: Building Blocks of a Computer System to Aid in Engineering Analysis (Reprinted from Foundations of Computer-Aided Chemical Process Design, 1981, by U.S. EPA with permission of Engineering Foundation.)

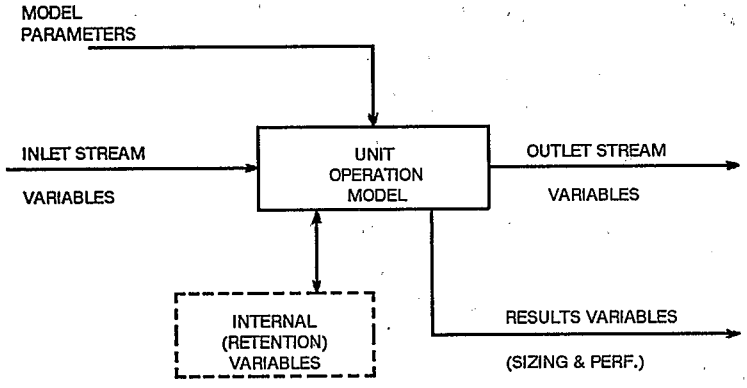

Figure 2: Schematic Diagram of a Unit Operation Model (Reprinted from Foundations of Computer-Aided Chemical Process Design, 1981, by U.S. EPA with permission of Engineering Foundation.)

Historical Development

Current flowsheeting systems have their roots in flowsheet simulators developed in the 1960's [3]. Computer processing and thermodynamic data limitations in these earlier systems did not permit the simulation of a wide variety of plant equipment, and as a result systems were only available for a small number of components, such as distillation columns. Computer processing limitations also restricted flowsheeting systems initially to large mainframe computers, and to steady-state and continuous process operation. In steady-state operation temperatures, pressures, and flowrates are fixed over time, while in continuous operation startups and shutdowns are infrequent and intermediate process interruptions such as handling, sampling or storage are minimal. Steady-state programs use sequential-modular modular algorithms, and thus have lower computer power requirements.

Over time, significant increases in computer processing and thermodynamic data availability have led to many improvements in flowsheeting systems. For one, they can now model a wide variety of plant equipment, allowing one system to simulate many processes. These systems are often referred to as general process simulators. General process simulators such as the ones reviewed in the following section of this report usually have a unit operation library, which provides the user with a large selection of unit operation models for flowsheet construction, and a large data bank of physical property data for user selection of pure chemical components.

Increased computer processing power, as seen in the development of the personal computer (PC), has also enabled the simulation of dynamic and batch processes, although to a limited degree. Some dynamic simulation can now even be done on PC's, while steady-state programs are now widely available for both mainframe computers and PC's. In dynamic operation, the process temperatures, pressures, and flowrates are not fixed over time, while in batch process operation startups and shutdowns are frequent and intermediate process interruptions often occur. Dynamic simulators use equation-oriented algorithms, and since as many as 30,000 differential equations may need to be solved when simulating an entire process plant, these systems often require massive amounts of computer power and are more time-consuming [4].

Process optimization is also now possible in some commercial process simulators. Optimization allows the user to determine plant operating conditions that will maximize or minimize any objective that is specified by the user. In some simulators, these objectives can be either technical or economic. Economic evaluation capabilities built into some simulators allow the performance of equipment sizing calculations, and capital and operating cost estimation. A design specification feature, used in conjunction with optimization, can allow the user to set a target value, or design constraint, on any flowsheet variable or function of a combination of flowsheet variables. In some simulators, a target value can be set for any unit operation result, stream flow or property, or component flow or purity, and there is no limit to the number of specifications or constraints that can be established.

Last but not least, a number of user interface developments have resulted in new features that have significantly increased the utility of some commercial process simulators. One feature is expert guidance, which can help the user to build a flowsheet model and also prevent errors. On-line help, prompts, and tutorials are often available to assist the user. Another feature is interactive simulation, which depending upon the flowsheeting system, will allow the user to stop a simulation at any point, examine the results, change any of the specifications, and then repeat or continue the simulation. A third feature is graphic interfacing, which again depending upon the system, will allow the user to build a flowsheet graphically, using block symbols or pictorial icons to represent unit operations. Also known as process flow diagrams (PFD), these graphic flowsheets can often be printed as output from the computer.

Current Applications

As a result of the development of commercial process simulators as described above, these flowsheeting systems have rapidly emerged as process design and analysis tools that are increasingly applied by engineers and scientists in many different fields. In fact, an extensive review of the published technical literature revealed a wide range of recent applications of flowsheeting systems for process design and analysis [5]. Many of these applications had an environmental focus, although the vast majority were for treatment purposes and did not involve P2. A list highlighting the various fields in which process simulation has been applied includes:

- power generation/energy distribution
- nuclear fuel production
- chemical processing/production
- mining
- transportation systems
- petroleum/reservoir engineering
- incineration/combustion
- groundwater contamination/remediation
- wastewater treatment
- biotechnology/bioengineering

Of all of these applications, chemical plant processing/production represents the largest use of process simulation, primarily because it was developed by and for this field. In the CPI, process simulation is typically used for:

- process design and economic evaluation of a new plant
- evaluation of different design configurations for a new plant
- optimization of operating conditions for a new plant
- simulation of the operation of an existing plant
- optimization of the operation of an existing plant
- retrofit studies for an existing plant [6].

Current Research

Despite the varied and growing application of flowsheeting tools in process design and analysis, these tools have yet to be sufficiently employed for industrial P2. This conclusion is based on the small number of published documents in the literature on this topic, as mentioned above, and on the results of a December 1992 process simulation research workshop jointly sponsored by EPA, the U.S. Department of Energy (DOE), and the American Institute of Chemical Engineers (AIChE). The workshop report states that "currently ... process simulators do not effectively integrate the technical and economic considerations of environmental needs." [7].

Attendance at the EPA/DOE/AIChE workshop consisted of 50 leading practitioners in the fields of process design and simulation, including university professors, simulation software developers, process designers, and federal research and development (R&D) managers. The overall objective of the workshop was to identify process simulation R&D areas addressing environmental needs in the CPI. The workshop results - the R&D needs with some perspective on priorities and development time periods - are included in the workshop report. A number of critical areas for R&D emerged from the results of the workshop, and these are presented and discussed in Section V. It was also noted in the workshop report that many of the areas identified for R&D have already been the subject of some level of research to date.

One R&D area identified by the workshop, and in fact the leading area of R&D activity in process simulation over the past several years, is known as process synthesis. Process synthesis has also been the leading area of simulation R&D activity for P2 purposes, as evident by the literature. Process synthesis can be defined as "determining the optimal interconnection of processing units as well as the optimal type and design of the units within a process" [8]. One of the most significant P2 activities in this area in recent years is a concept developed at the University of California at Los Angeles known as mass exchange network (MEN) synthesis.

MEN synthesis involves "the systematic generation of a cost-effective network of mass exchangers (i.e., separation units) with the purpose of preferentially transferring certain species from a set of rich streams to a set of lean streams" [9]. Limiting the amount transferred are mass balance and equilibrium constraints. A simplified example of an MEN problem is shown in Figure 3, in which phenol in petroleum refinery waste water is transferred from rich streams (R_i) to lean streams (L_i), with the goal of identifying the process configuration that minimizes the amount of phenol that appears as a pollutant. MEN synthesis is somewhat analogous to the well-studied process synthesis topics of heat exchange networks, and optimal distillation column trains.

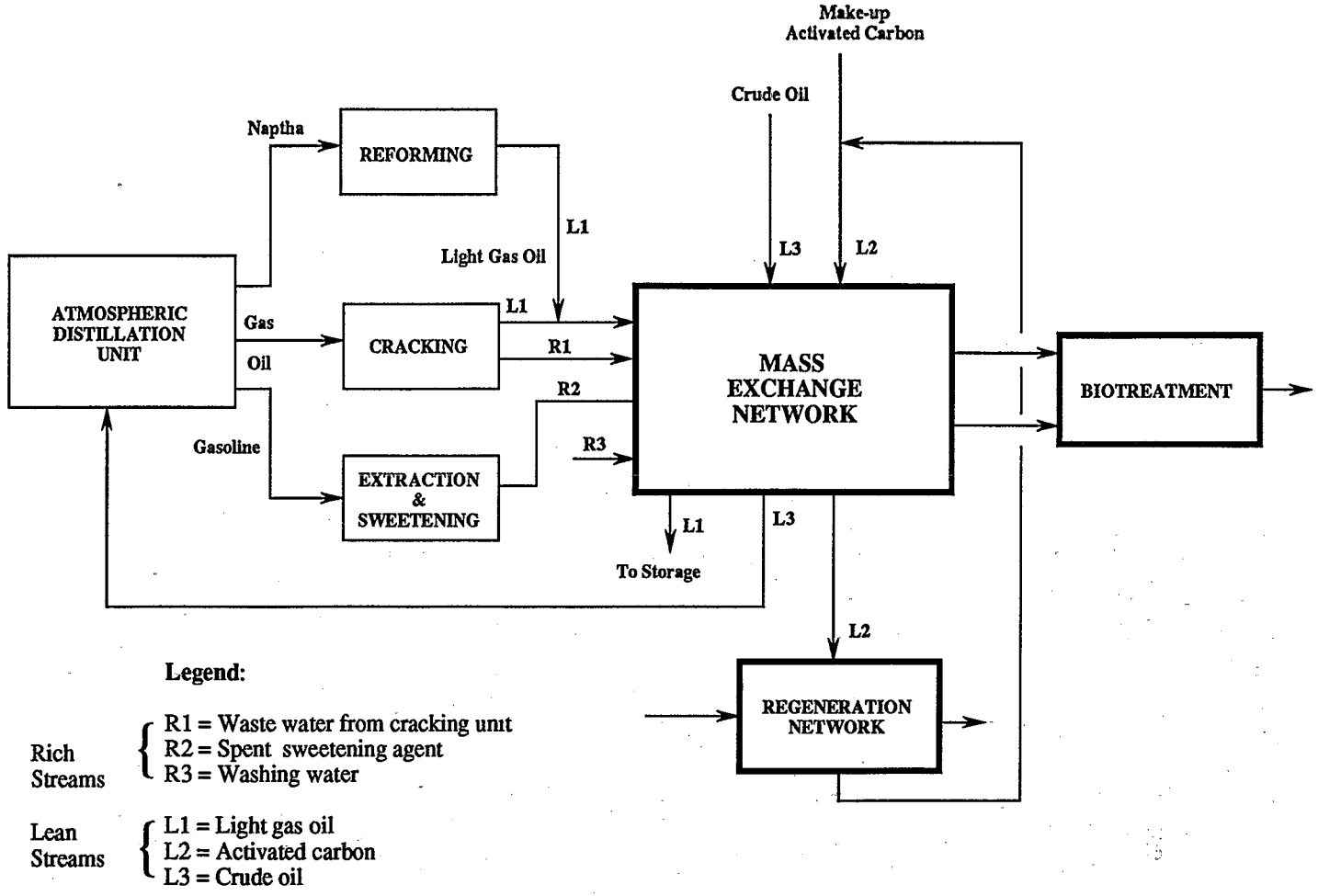

Figure 3: Simplified Example of a Mass Exchange Network (MEN) Problem for Phenol in a Petroleum Refinery

SECTION III

PROCESS SIMULATION SOFTWARE REVIEW

The objectives of this review are to: (1) present a sample of the state-of-the-art process simulation software that is commercially-available; and (2) highlight the specific features of these process simulators that can be used for P2. The review focuses on process simulators that can be used to model a wide variety of chemical and petrochemical processes (i.e., general process simulators), since this software is the most applicable to achieving widespread P2. It includes some dynamic and batch process simulators, although the majority are for steady-state and continuous operation since these simulators are still much more prevalent. Exclusion of similar commercial process simulators is not meant to imply that they have limited P2 capabilities; rather, those included are ones for which sufficient information was available.

The process simulators that are reviewed are listed in Table I, along with each supplier's name, address, and phone number. The important features of each process simulator are summarized in Table II, and discussed in the following section. All of the information provided for these software packages was obtained from suppliers' marketing literature, phone calls to suppliers, and journal literature [10, 11, 12]. However, it is recommended that a supplier be contacted directly for the most up-to-date information.

Commercial Software Packages

1. ASPEN PLUS

ASPEN PLUS is a steady-state process simulator that is used for numerous industrial processes involving complex chemistry. This is due to having comprehensive libraries of unit operation and physical property models than can handle all media, including solids and electrolytes. There is also a physical property data bank of over 4000 chemical components, as well as a data regression system to determine property parameters using laboratory data, and a property constant estimation system to estimate missing property parameters. The user can also incorporate their own unit operation models, physical property models and data, and in-line FORTRAN into the program without flowsheet size limitations.

Design specifications can be used to specify a target value for a unit operation output, stream flow or property, or component flow or purity. An optimization capability can determine process operating conditions for any type of objective function, such as technical or economic, with no limit on the number of constraints. ASPEN PLUS costing methodologies can then perform a full process economic evaluation, including capital and operating costs, using equipment size and operating data as input.

TABLE 1			
Sample of Commercial Process Simulation Software Packages			
Name	Supplier	Address	Phone #
ASPEN PLUS	Aspen Technology Inc.	10 Canal Park Cambridge, MA 02141	617-577-0100
BATCHES	Batch Process Technology	1291E Cumberland Ave. W. Lafayette, IN 47906	317-463-6473
ChemCAD III	Chemstations Inc.	10375 Richmond Ave. Houston, TX 77042	713-954-4100
DESIGN II	ChemShare Corp.	P.O. Box 1885 Houston, TX 77251-1885	713-267-5600
ESP	OLI Systems Inc.	108 American Rd. Morris Plains, NJ 07950	201-539-4996
HYSIM	Hyprotech Ltd.	10333 Richmond Ave. Houston, TX 77042	713-780-7087
MAX	Aspen Technology Inc.	10 Canal Park Cambridge, MA 02141	617-577-0100
PD-PLUS	Deerhaven Software	7 Shady Lane Dr. Burlington, MA 01803	617-229-2541
PRO/II	Simulation Sciences Inc.	1051 W. Bastanchury Rd. Fullerton, CA 92633	800-854-3198
PROSIM	Bryan Research & Engineering	P.O. Box 3403 Bryan, TX 77805	409-846-8771
SPAN	Kesler Engineering Inc.	1200 Tices Ln. E. Brunswick, NJ 08816	908-249-4100
SPEEDUP	Aspen Technology Inc.	10 Canal Park Cambridge, MA 02141	617-577-0100

Table 2

Summary of Features Available in Commercial Process Simulation Software Packages

Package	Simulation			Unit Operation Library	Physical Property Data	Process Optimi-zation	Electro-lytes Modeling	Solids Modeling	Expert Guidance System	Graphic Inter-facing	Economic Analysis	Models/ Data Importing	Data Regression
	Steady State	Dynamic	Inter-Active										
ASPEN PLUS	X		X	X	X	X	X	X	X	X	X	X	X
BATCHES		X		X	X	X				X		X	
ChemCAD II	X		X	X	X	X	X	X		X		X	X
DESIGN II	X		X	X	X	X	X			X		X	
ESP	X	X		X	X		X	X				X	X
HYSIM	X		X	X	X			X		X		X	X
MAX	X		X	X	X				X	X		X	X
PD-PLUS	X		X	X	X							X	
PRO/II	X		X	X	X	X	X	X	X	X		X	X
PROSIM	X		X	X	X				X	X			
SPAN	X		X	X	X				X	X	X	X	
SPEEDUP	X	X	X	X	X	X	X	X				X	X

A user interface system, ModelManager, provides interactive building of flowsheets with the help of an expert guidance system. Graphics are available to build a process flow diagram (PFD) with either block symbols or pictorial icons. Interactive simulations can then be performed, with the user free to stop at any point to examine the results or to change a specification, and then either continue or repeat the process. Sensitivity analyses can also be performed. ASPEN PLUS can be run on mainframes, workstations, and personal computers (PCs).

2. BATCHES

BATCHES is a process simulator for managing multiple product, recipe-driven batch and semicontinuous flow processes in the biochemical, food, pharmaceutical, and specialty chemical industries. It enables optimization of process configurations and operating procedures, sizing of process equipment, and process scheduling. A graphical user interface facilitates data entry and analysis through case comparison and animation. It is available for workstations and mainframes.

3. ChemCAD III

ChemCAD III is a steady-state process simulator with large unit operation and physical property model libraries, including models for solids and electrolytes processing. A chemical components data bank contains physical property data for approximately 1450 components, while a data regression system permits the use of laboratory data. There is also a facility for the user to supply their own unit operation models, physical property data, and in-line FORTRAN.

TALK, an interactive program within ChemCAD III, handles all input, calculations, and output for a simulation. TALK allows the user to stop the simulation at any point, review the results, edit the data, and rerun the program. The user may perform calculations for the entire flowsheet, or for individual unit operations within the flowsheet, permitting sensitivity analyses. Graphics enables the drawing of PFDs, while an interface to spreadsheet software enables supplemental analysis, such as for an economic evaluation. ChemCAD III is for use only on PCs.

4. DESIGN II

DESIGN II is a steady-state process simulator that is used for oil/gas production, petroleum refining, petrochemicals, and other chemical processing systems. The software includes a unit operation library that contains over 20 process equipment models, a chemical component data bank with over 850 pure components, and a petroleum crude library with over 150 published crudes. The user may also add proprietary unit operation models, physical property data, and in-line FORTRAN subroutines with no limits on flowsheet size, components, feeds, and products.

An optional Windows user interface allows process flowsheets to be created graphically using pictorial icons, and the user can then perform the flowsheet simulations interactively by stopping the calculations in progress and reviewing interim results. Also available are features for sensitivity analyses and optimization. Spreadsheet interfacing is permitted. DESIGN II is for use on PCs, workstations, and mainframes.

5. Environmental Simulation Program (ESP)

ESP is both a steady-state and dynamic flowsheet simulator that can be applied for a variety of processes involving complex chemistry, although it was developed primarily for environmental treatment and remediation processes. It has a unit operation model library, and a chemical component data bank of approximately 2,000 components. ESP has the ability to model aqueous and non-aqueous reactive systems. A data estimation and regression system allows users to add new components to the data bank.

Dynamic simulations, which are run through ESP by a program component known as DynaChem, may be conducted interactively. And ESP simulation output files may be exported to other software to do supplemental analyses. ESP runs on PCs and workstations.

6. HYSIM

HYSIM is a steady-state process simulator that is used for design and evaluation in the gas processing, petroleum refining, petrochemical, and chemical industries. There are comprehensive unit operation and physical property model libraries, as well as a component data bank that contains approximately 1,500 components. There are models for solid processing, but not for electrolytes. A data regression and estimation system is available for using experimental data, and proprietary unit operation models, data, and in-line programming ("C" language) may be used.

Simulations can be performed interactively with the help of built-in intelligence in order to perform process sensitivity and case study analyses. Graphic interfacing allows for PFD display and output, and software interfacing provides access to spreadsheet software. HYSIM runs on PCs, workstations, and mainframes.

7. MAX

MAX is a steady-state flowsheet simulator that is built on core ASPEN PLUS modeling technology, and is designed so that engineers new to simulation can get fast and meaningful results. It has full upward compatibility with ASPEN PLUS. MAX has large unit operations and physical property model libraries, and a pure component data bank of over 1,300 components. There are also data regression and property constant estimation systems. Proprietary models and data, and in-line FORTRAN, can be used with no limits on the number of components, blocks, or size of the flowsheet.

Aspen's ModelManager user interface system provides icons for problem specification and PFD-style diagram generation, as well as a patented expert guidance system. Interactive control of process calculations permits sensitivity analyses for any process variable. Simulation results may be exported to a spreadsheet for additional analysis. MAX is run only on PCs.

8. PD-PLUS

PD-PLUS is a steady-state process simulator for chemical processes including refinery systems and non-ideal chemicals. It has a large unit operation library, in which all operations allow multiple feed streams and in general can produce multiple product streams, with some exceptions. There are two pure component data banks, one small and one large. The small data bank contains 59 components (mostly hydrocarbons and water) and is standard, while the large data bank contains 1,284 components and is optional.

PD-PLUS has an interactive ability that allows the user to stop the program as the next calculation step is about to begin. At this point the user can display unit operation and streamflow conditions, change unit operation and streamflow specifications, and rerun the simulation at any point in the flowsheet. It also interfaces to other software, such as spreadsheets, enabling the ability to run economic analyses, if desired. The software may be run on PCs.

9. PRO/II

PRO/II is a steady-state flowsheet simulator that is used for gas processing, petroleum refining, and many other chemical and petrochemical processes. It has comprehensive unit operation and physical property model libraries, and a component data bank that has over 1,450 pure components, including physical property data for solids and electrolytes. In addition, the program has a data estimation and regression system, as well as the ability to handle mixture data. Proprietary models, data, and in-line FORTRAN can also be used, and any number of components, unit operations, and streams can be simulated.

PRO/II has the ability to set process design specifications and operating constraints, and to then optimize the flowsheet. Simulations can be performed interactively, with the ability to view any stream or unit operation, change any unit operation or design specification, and then automatically do case comparisons. Graphics interfacing, an expert system, and links to third party software such as spreadsheets are part of the user environment. PRO/II runs on PCs, workstations, and mainframes.

10. PROSIM

PROSIM is a steady-state flowsheet simulator for designing and optimizing plants in the gas, oil, and petroleum industries. It has multiple unit operation models, two physical property models, and a pure component data bank with approximately 100 components.

Graphic interfacing enables the user to build a flowsheet PFD on the screen and enter operating data on forms with the help of an expert system. Interactive simulations may then be performed, allowing for interruption and recalculation. Simulation results may be exported to third party software. PROSIM software runs on PCs, workstations, and mainframes.

11. SPAN

SPAN is a steady-state process simulator for use in the gas processing, petroleum, and petrochemical industries. It has a large unit operation library, and can accept user-supplied models. There is a comprehensive physical property data bank, as well as several physical property models, with facilities for blending of petroleum streams. Simulations can handle up to 100 streams, 50 components, and 50 unit operations in one flowsheet.

Process flowsheeting is interactive, with diagnostics and expert guidance. The user can selectively execute any portion of the flowsheet, and there are automated facilities for economic analysis and parametric studies of the effect of changing process variables on profitability. The user can also create files that can be interfaced with CAD packages in order to generate process flow diagrams including the simulation results. SPAN runs on PCs.

12. SPEEDUP

SPEEDUP is an equation-based process modeling system that offers facilities for both steady-state and dynamic simulation and optimization of chemical processes. The program allows the user a great deal of flexibility in the way he or she defines a model for their process, since it will deal with an arbitrary mixture of equations and procedures (subroutines) relating the variables in the process.

There is a unit operations library and a physical property data bank, and the user can import unit operation models and physical property data into the program. It is available for use on workstations and mainframes.

Software Summary

Several state-of-the-art process simulators are now available that enable the simulation of a wide range of industrial processes. These simulators have extensive libraries of unit operation models and physical property data, and also allow for the importation of user-supplied models and data. Most existing state-of-the-art process simulators also have good user interfacing capacity through interactive simulation and graphic display/output features, and can do sensitivity analyses and set design specifications using any process variable. All of these features make process simulation very useful for P2 analysis of many industrial processes, as will be demonstrated in Section IV.

Despite possessing the abilities stated above, however, many state-of-the-art process simulators lack certain features that place a limit on the application of process simulation to P2. For one, most existing process simulators can only model steady-state and continuous process operation, as opposed to dynamic and batch process operation. For another, most of these simulators can not model either electrolytes (i.e., ionic species) or solids. And two other critical limitations of most current process simulators is the inability to do optimization and economical analysis. These and several other critical process simulation needs will be discussed further in Section V.

SECTION IV

CASE STUDY: METHYLENE CHLORIDE SOLVENT RECOVERY

In order to demonstrate the power and utility of state-of-the-art process simulation for industrial P2, a case study was performed using the process simulator MAX. The case study illustrates how some of the important features of existing process simulators can be used to do rapid and convenient process analysis leading to P2. MAX was chosen because it possesses most of the features reviewed in Section III, and because it is marketed as user-friendly. No prior experience or training with process simulation software was held by the author before this case study analysis was attempted.

The case study is based on one of ten examples provided in an Environmental Casebook written by Aspen Technology Inc. (AspenTech) to illustrate the use of process simulation to solve environmental problems [13]. The examples, listed in Table III, use the process simulator ASPEN PLUS to solve these problems. Three important points need to be made about the AspenTech examples in order to understand their value for P2. First, most of the examples illustrate waste treatment, although the first two examples can be considered cases of in-process recycling and therefore P2. Second, half of the examples involve waste water, which is beneficial since over 90% of U.S. hazardous waste generated is in this form [14]. And third, the Zero Discharge Waste Water Treatment System example involves the simulation of zero water discharge; not zero pollution discharge.

Problem Statement

The problem in the case study was to examine one of the AspenTech example processes for possible P2 opportunities or improvements. This was done using the process simulator MAX to analyze process design alternatives.

The AspenTech simulation example that was examined in this case study is Methylene Chloride Solvent Recovery. A flowsheet is shown in Figure 5. Two steam-injection flash towers (TOWER1 and TOWER2) remove methylene chloride solvent (1.4%) from a combined waste water stream (FEED) before discharge to the sewer (BOT2). In the AspenTech example, the minimum total steam flow (STEAM1 + STEAM2) required to meet a solvent concentration limit in BOT2 of 150 parts per million (ppm) was determined. Some P2 is achieved in the example, since approximately 99% of the solvent is recovered in stream MECL with minimum steam flow, but there is opportunity for more P2 because stream WATER becomes a waste stream with a higher solvent concentration than waste stream FEED (.019 vs. 014).

The process simulator MAX was used to study two possible P2 opportunities for the recovery process: (1) recycling of stream WATER into stream FEED; and (2) increasing steam flow. A simulation model of a modified methylene chloride solvent recovery process

TABLE 3	
Example Problems in the Aspen Technology Inc. Environmental Casebook [13]	
Case Study	Subject Media
Methylene Chloride Solvent Recovery	water
Acetone Solvent Recovery	water
Water Absorber for Hydrogen Chloride	gas
Sour Water Stripping System	water
Flue Gas Desulfurization	gas
Sweetening Natural Gas by Diglycolamine Absorption	gas
Nitric Acid Absorption	gas
Waste Water Treatment	water
Mobile Incineration of Heavy Oil-Laden Soil	soil
Zero Discharge Waste Water Treatment System	water

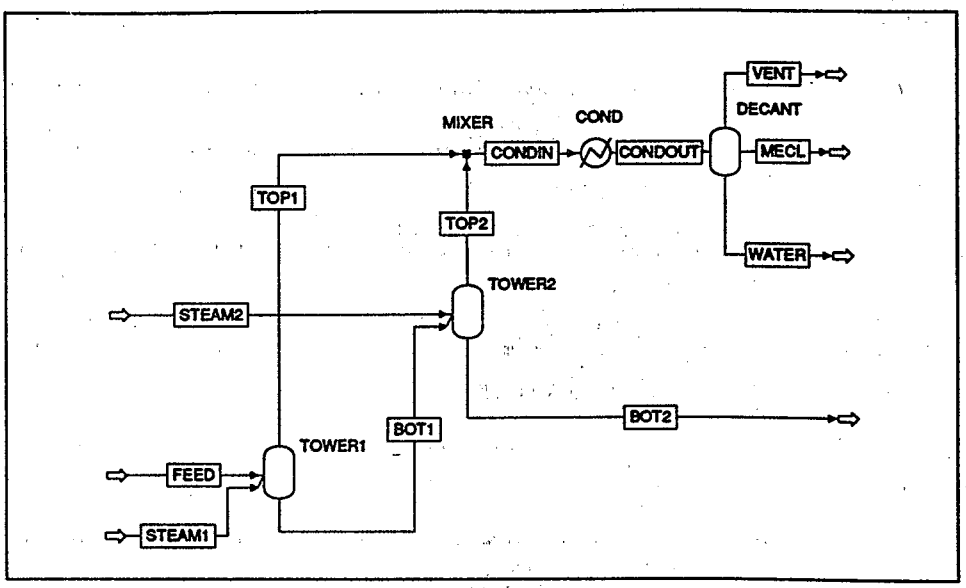

Figure 4: Methylene Chloride Solvent Recovery Flowsheet (Reprinted from ASPEN PLUS APPLICATIONS: Environmental Casebook by U.S. EPA with permission of Aspen Technology, Inc.)

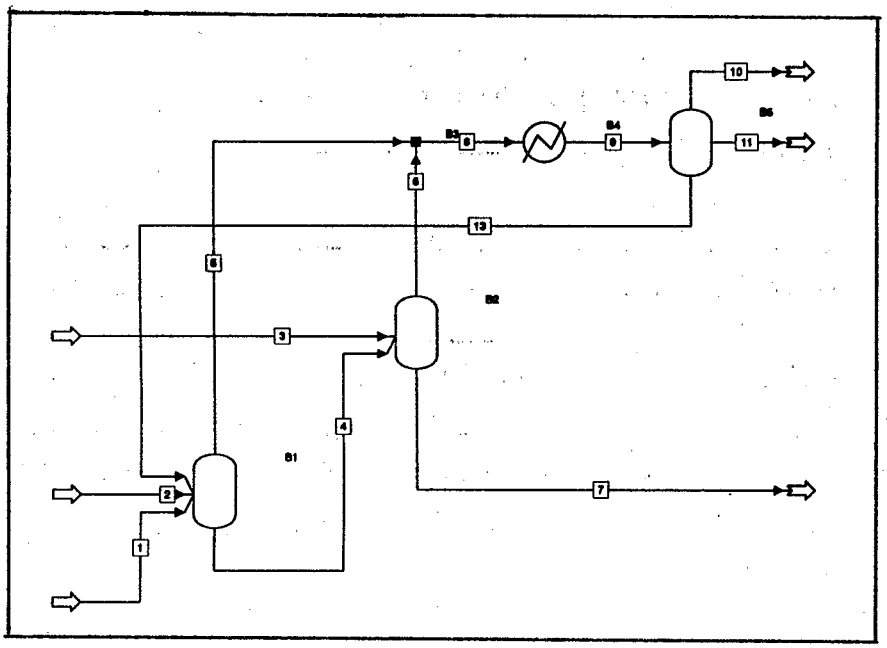

Figure 5: Methylene Chloride Solvent Recovery Flowsheet Modified for Water Recycling (created with MAX)

with water recycling was built with MAX, as seen in Figure 6. Several design specificationruns were then performed with this modified model to determine: (1) the effect of recycling WATER on process performance (e.g., steam required, solvent recovery, and solvent purity) at the 150 ppm solvent discharge limit; and (2) process performance at 1 ppm and 1 ppb (part per billion) discharge levels. Sensitivity runs were also performed to characterize the impact of the steam flows on the solvent discharge concentration.

Computed Results

A summary of the results from four design specification runs completed with the methylene chloride solvent recovery flowsheet models is provided in Table IV. In the first row of the table are results of a specification run with the original process flowsheet (i.e., no water recycling) to determine process performance at the 150 ppm solvent discharge limit. In the second row are the process performance results at the 150 ppm limit, with the modified process flowsheet (i.e., water recycling). The third and fourth rows are the computed results, with the modified flowsheet, of the process performance at 1 ppm and 1 ppb solvent discharge limits.

The performance results in Table IV include both technical and economic process parameters, and a benchmarking parameter for the purpose of comparison. The technical parameters include: the minimum total steam flow required; the percentage of the solvent recovered in methylene chloride-rich stream MECL; and the purity of the recovered solvent. The economic parameter is the steam generation cost per gallon of waste water treated in stream FEED, assuming fuel oil at $1/gallon or $6/MMBTU. The benchmarking parameter, dilution water, is the amount of water that would need to be added to stream FEED to reach the design specification discharge concentration if dilution was used as the treatment instead of flash stripping.

A summary of the results of six sensitivity runs completed with the modified flowsheet model is provided in Table V. The table is a six-by-six array of solvent discharge concentrations at various combinations of flash tower steam flows. In the first column are the steam flows to the first flash tower, STEAM1. In the remaining columns are the solvent discharge concentrations at the corresponding steam flows to the second flash tower, STEAM2. For instance, when there is no flow to either flash tower the solvent discharge concentration is 14,000 ppm. These data are also presented in the form of surface and contour maps in Figures 7 and 8, respectively. These results help to illustrate the impact of the combined flash tower steam flows on the solvent discharge concentration.

Discussion

The design specification and sensitivity runs performed in the case study demonstrated the capabilities of the process simulator MAX to do rapid and convenient analysis of process design options. These capabilities enabled the examination of the impacts of waste water recycling and flash tower steam flow on process performance.

TABLE 4					
Results from Case Study Design Specification Runs: Process Performance at Various Solvent Discharge Concentrations					
Design Spec. Solvent Discharge Concentration	Minimum Steam Required (lb/hr)	Solvent Recovery (%)	Solvent Purity (%)	Steam Cost (¢/gal waste)	Dilution Water (lb/hr)
150 ppm[1]	12,892	97.3	99.8	0.98	9.3 E+6
150 ppm[2]	13,080	98.8	99.8	0.99	9.3 E+6
1 ppm[2]	33,170	99.99	99.8	2.52	1.4 E+9
1 ppb[2]	456,000	-	-	34.67	1.4 E+12

[1] No water recycling.
[2] Water recycling.

TABLE 5						
Results from Case Study Sensitivity Runs: Solvent Discharge Concentration (ppm) at Various Flash Tower Steam Flow Combinations						
STEAM1 (lb/hr)	STEAM2 (lb/hr)					
	0	10,000	20,000	30,000	40,000	50,000
0	14,000	1,530	129	65.6	46.8	37.9
10,000	1,500	23.4	14.4	12.2	11.5	11.2
20,000	45.2	1.43	1.08	1.11	1.29	1.59
30,000	16.3	.668	.44	.382	.372	.387
40,000	10.5	.484	.304	.251	.23	.225
50,000	8.07	.404	.248	.199	.178	.168

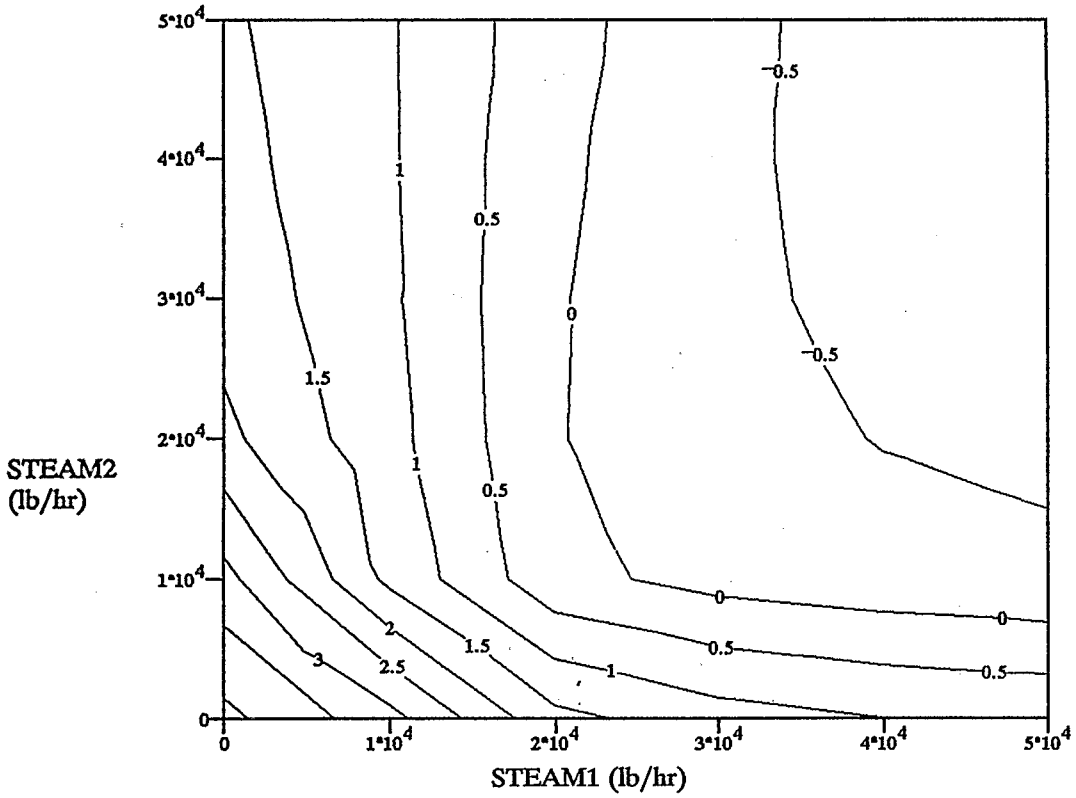

Figure 6: Surface Plot of Methylene Chloride Discharge Concentrations (base 10) Over a Range of Steam Flow Combinations

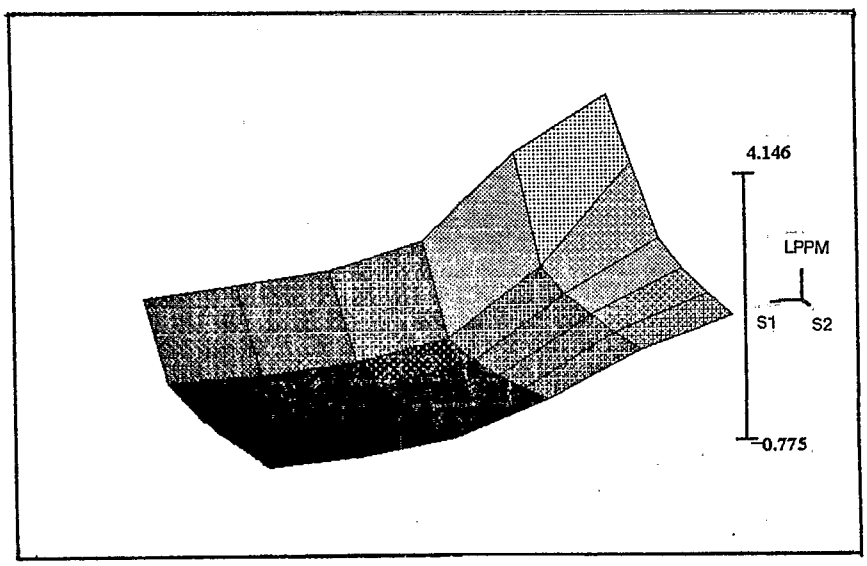

Figure 7: Contour Plot of Methylene Chloride Discharge Concentrations (base 10) Over a Range of Steam Flow Combinations

Comparision of the first two specification runs in Table IV indicates that approximately 1.4% more steam is needed to meet the 150 ppm methylene chloride discharge limit with the change to water recycling. This is due to the higher solvent concentration in the recycled water stream than in the influent waste water stream. It can also be seen that 1.5% more solvent is recovered, while solvent purity is maintained. The comparison of the two design specification runs indicates that P2 can be achieved with recycling of stream WATER, because of the higher level of solvent recovery and the elimination of one waste stream.

Other ways of assessing the P2 impact of the process change include examining the treatment cost and dilution water values in Table IV. For the case of the first two runs, the dilution water parameter does not change because the solvent discharge limit is the same. However, the value indicates that more than 9 million lb/hr of water would be required if dilution were used, rather than steam stripping, and also serves as a benchmark for the other runs. The dilution water parameter indicates that steam stripping is the better choice from a water usage standpoint. The treatment cost increases a very small amount because of the small increase in the steam flow required.

The third specification run in Table IV gives the results for a 1 ppm methylene chloride discharge. For this level of discharge, the steam required is much higher, approximately 33,000 lb/hr, but the solvent recovery is 99.99%. The purity of the methylene chloride-rich stream recovered, MECL, does not increase above 98.8% because the water in this stream is below it's solubility limit in methylene chloride and therefore can not be separated out. This is essentially the purity limit for the recovered solvent.

The dilution water required in the third specification run is 1.4 billion lb/hr, which again shows why steam stripping is the preferred treatment method. The treatment cost increases by a factor of 2.5, however, because of the similar increase in the steam flow. These results all help to show the cost-benefit trade-off involved in decreasing the solvent discharge to 1 ppm.

The surface plot, Figure 7, contains curves of constant solvent discharge concentrations (in the logarithm of ppm), for a range of steam flow combinations from: no flow to either flash tower (i.e., the origin point in the plot); to a flow of 50,000 lb/hr of steam to each tower (i.e., the point [$5x10^4$,$5x10^4$]). From this plot, the optimum steam flow combination (i.e., the one for which the total steam flow is the minimum) for each concentration level can be estimated by constructing a 45 degree line tangent to the curve of interest, as seen in Figure 7. The tangency point is the optimum. This is true because a 45 degree line is a line of constant total steam flow, and the tangency point will give the smallest steam total. For instance, the optimum steam flow combination for a 1 ppm solvent discharge is at approximately STEAM1 = 23,000 lb/hr and STEAM2 = 10,000 lb/hr, as seen in Figure 7.

The contour plot, Figure 8, shows the solvent discharge level contour (again in the logarithm of ppm) over the same steam flow range as the surface plot. The contour plot shows how the concentration level changes (increases or decreases) along the vertical axis with a varying steam flow combination. The darker the shade of the contour plot, the smaller the discharge concentration. Both the contour plot and the surface plot indicate that STEAM1 has a greater impact on solvent discharge concentration than STEAM2, which is seen by a greater decrease in concentration level along the STEAM1 axis. Both plots also show that as both STEAM1 and STEAM2 are increased, the solvent discharge concentration is minimized.

The fourth design specification run in Table IV provides the results for a 1 ppb, or "nominal zero," solvent discharge level. Much discussion has transpired in recent years concerning the technical and economic feasibility of achieving near-zero or zero waste discharge for many industrial processes. These results indicate that to reduce the solvent concentration to this level would require 456,000 lb/hr of combined steam flow. The steam cost and dilution water values for this level are also very high, at approximately 35 cents per gallon and one trillion gallons, respectively. Solvent recovery and purity values are not given in the table because at the steam flow required, the solvent is below it's solubility limit in water for the stream entering the decanter, and therefore can not be separated out.

The results indicate that for the process analyzed "nominal zero" solvent discharge is neither technically nor economically feasible. Both the level of steam flow required and the cost to generate this steam would be enormous. One must also consider the atmospheric emissions and other life cycle impacts associated with the high steam generation. These impacts may present an even greater health risk than simply discharging the waste water to the sewer.

The solvent discharge concentrations provided in the results of both the design specification and the sensitivity runs are waste generation data that can be used to measure the P2 potential of the hypothetical process changes. These are relatively accurate and reliable data that would otherwise need to be either collected from pilot or actual facility testing, or estimated using engineering judgement. The data are generated using process material balances, although some emissions, such as fugitive and trace emissions, are not included in the material balances because they are several orders of magnitude smaller than the main process flow streams.

Summary

The case study demonstrated the ability of MAX to do rapid and convenient analysis of process design alternatives leading to P2. With no prior training or experience by the author in using process simulation software, a process simulation model of the solvent recovery example was easily constructed, and process design alternatives for P2 were analyzed.

The design specification and sensitivity analysis features, along with user interface features such as graphic display/output and an expert guidance system, all facilitated easy and reliable process analysis. Design specifications were used to determine the process operation required to meet a desired waste discharge level. Sensitivity analyses provided a means to determine the impact of key process variables on system waste generation. And the user interface features allowed the powerful process analysis capabilities to be used rapidly with no training or experience.

The case study analysis also demonstrated the ability of MAX to model aqueous systems, and to generate waste generation data that can be used for P2 measurement. Both of these capabilities are critical to existing industrial P2 efforts. Modeling aqueous systems is critical because industrial aqueous waste represents the largest volume of hazardous waste in the U.S. [14]. And P2 measurement is important in order to meet existing regulatory and practical requirements that justify continued P2 efforts.

SECTION V

PROCESS SIMULATION NEEDS

Despite possessing many features that make them powerful and convenient tools for process design and analysis, as discussed in the previous two sections, current process simulators still lack many critical aspects required to be widely effective for P2. A number of these aspects were pointed out already during the process simulation software review of Section III, such as shortfalls in dynamic and batch process simulation, process optimization, and economic analysis. Also, several critical needs were identified in the December 1992 EPA/DOE/AIChE process simulation research workshop discussed in Section II. The purpose of this section is to discuss these and other needs important for P2 design and analysis in the CPI.

General P2 Needs

Possibly the best source of information on process simulation needs for P2 is the report from the EPA/DOE/AIChE workshop discussed in Section II. The objective of this workshop was to identify the critical areas for R&D needed in order to incorporate environmental factors into process simulation and design tools for the CPI. With this in mind, several areas were identified and they are summarized here in a table reproduced from the report as Figure 8. These areas represent common themes that were agreed upon by most participants in the workshop, and are neither specific in nature nor inclusive of all ideas presented by the attendees. Specific ideas from workshop participants are included in the breakout group results found in the Appendix.

It is important to note that this list essentially reflects the R&D interests of the process simulation community, and therefore includes mostly complex and long-term goals, such as process synthesis, rather than more immediate and practical needs such as fugitive emissions estimation. For instance, process synthesis is at the top of the list in Figure 8 because it received the highest number of "top" priority votes from the workshop attendees. This high vote count for process synthesis is not surprising since it has been the leading area of interest in process simulation research for several years. Also, there may have been a disproportionate number of workshop attendees who had this topic as their primary research interest.

Despite the probable bias towards process synthesis at the workshop, there is no disputing it's potential value for P2. Process synthesis could possibly help to determine alternative chemical reaction pathways and catalysts, determine alternative chemical separation sequences, and efficiently incorporate waste treatment units into a process design. The objective in developing process synthesis according to the workshop report would be to incorporate P2 concepts into chemical process design, but there would undoubtedly be many applications beyond those in the environmental field.

Topic	Findings	Identified Needs
Process Synthesis	Developing new and improved methods for synthesizing chemical processes that meet environmental objectives is one of the most important needs for incorporating pollution prevention concepts into process design. This will enable alternative process flow sheets and has applications beyond process simulators.	• Develop expert systems for synthesis. • Develop tools to identify alternative reaction pathways and catalysts. • Pursue non-conventional technology alternatives. • Develop methods for defining "ultimate" limiting process efficiencies. • Determine if barriers lie in models or heuristics. • Couple synthesis and simulation. • Use mathematical programming to synthesize processes.
Dilute Streams	Improving characterization and the ability to separate dilute components of streams through acquisition of data and enhanced modeling is critical for developing cost-effective process designs.	• Improve simulation models and tools to better handle dilute components of process streams. • Determine reaction equilibrium partitioning constants. • Determine reaction rates and byproducts. • Improve measurement capability to meet process control, regulatory, and other needs. • Determine data needs for modeling in the dilute region. • Use computational chemistry to estimate properties and behaviors of mixtures in the dilute region.
Optimization Methodologies	Development of new optimization strategies will allow users to identify process designs that best satisfy a range of environmental, cost, and operating requirements.	• Develop large-scale optimization methodologies. • Develop non-linear optimization strategies. • Develop methods for dynamic optimization of processes. • Enhance stochastic modeling and optimization. • Optimize agregate process models. • Develop on-line optimization methods.
Modeling Techniques	Better modeling is needed to accommodate process synthesis and optimization methodologies. The probabilistic nature of much environmentally-based data makes stochastic modeling essential in developing effective design tools and simulators. Greater flexibility in modeling is needed to accommodate different levels of detail, data, and rigor.	• Develop large-scale modeling methodologies (larger than unit operations.) • Improve probabilistic and stochastic modeling techniques. • Develop better hierarchical models. • Develop dynamic simulation models with process control. • Develop heuristic modeling capabilities to accommodate uncertainties and provide flexibility. • Take advantage of parallel computing techniques.

Figure 8: Summary of Results from the EPA/DOE/AIChE Process Simulation Research Workshop Report [7].

Topic	Findings	Identified Needs
Rate-Based (Non-Equilibrium) Processes	Data and research are needed to characterize rate-based processes that are not adequately modeled in current simulators.	• Characterize non-equilibrium phenomena. • Improve interfacing and sequencing of rate-based processes.
Environmental Costs	The lack of environmentally-related cost information in current simulators is a key barrier in identifying cost-effective process designs. Until process simulators accurately account for waste treatment costs and intangible costs on a process-by-process basis, pollution prevention approaches may not appear cost competitive with designs based on end-of-pipe treatment.	• Define and quantify intangible costs. • Develop methods to allocate costs to specific processes and products. • Develop a flexible cost estimating system. • Define cost of various end-of-pipe treatments and associate residuals. • Develop a library of cost models. • Develop environmental cost factors/integrate environmental considerations with cost.
Environmental Impact Assessment	Better methods are needed to determine the environmental impact of alternative process designs. Tools to quickly determine whether processes will meet environmental standards are needed.	• Develop an environmental impact index. • Develop quick risk assessment techniques. • Include environmental regulations in process simulators. • Quantify or weigh competing environmental, cost, and energy concerns. • Link ecological and process models.
Process Characterization	Better characterization and modeling of unit operations and process streams is needed to understand the environmental implications of alternative process configurations.	• Improve characterization and simulation of trace components (of environmental concern) in process streams. • Integrate property data into models and simulators. • Characterize and define benefits of hybrid units. • Predict environmentally-troublesome byproducts. • Characterize and simulate alternative waste treatment and recycling technologies.

Figure 8 (cont.): Summary of Results from the EPA/DOE/AIChE Process Simulation Research Workshop Report [7].

The high priority given to the areas of dilute streams and process characterization reflects the fact that in most instances, the hazardous components in chemical process streams are present in very small (i.e, trace) concentrations that are difficult to predict, quantify, and separate. Process simulation tools could potentially be very helpful in this area, especially in evaluating alternative reaction pathways to prevent these troublesome byproducts. According to the workshop report, however, current process simulators can not adequately handle dilute components of process streams primarily because of existing data gaps for many of these species, and also because of the lack of byproduct tracking models. In order to strengthen the ability of process simulators to handle dilute components, there is a need for good measured data in the dilute region, and for reliable data estimation techniques using computational chemistry.

The areas of optimization methodologies, modeling techniques, and rate-based processes all relate to the need for improved mathematical methodologies. Optimization methodologies such as sequential quadratic programming (SQP) are already available in some current process simulators, as seen in Section III, but according to the workshop report there is a need to develop new strategies, especially for large-scale or dynamic optimization. Under modeling techniques, improvements are needed for: dynamic simulation of process transients such as start-ups and shut-downs; stochastic modeling to deal with non-routine events such as accidents, upsets, and spills; and large-scale modeling to understand the environmental conditions that result from interactions among unit operations. And for rate-based processes, process simulators need to improve upon their ability to handle the various non-equilibrium phenomena (e.g., reaction kinetics, sorption, and transport) impacting waste generation.

The emphasis on the areas of environmental costing and environmental impact assessment is due to the inability of current process simulators to determine the true (i.e., total) impact, both environmental and economic, of a chemical process design. Both of these are often key barriers to incorporating P2 approaches because if these true impacts are not known, then a design incorporating P2 may not seem as attractive (e.g., as cost competitive) as one incorporating end-of-pipe treatment. For environmental costing, high priority was given by the workshop to developing and incorporating total cost accounting models and factors that help to quantify and allocate intangible costs such as liability and public relations. For environmental impact assessment, priority was given to developing the ability of process simulators to quickly determine the risk or impact of alternative process designs.

As previously stated, the areas discussed above and presented in Figure 8 are common themes that were ageed upon by most participants in the workshop. Because of the size of the workshop and the breadth of interests, the topics agreed upon are not very specific, and in fact most of them, such as process synthesis and optimization, have widespread application beyond P2. Many specific ideas were offered by individual workshop participants, however, and these can be found in the breakout group results in the Appendix. Some of these specific ideas are discussed in the following subsection.

Specific P2 Needs

The following list contains some more specific capabilities that would be desirable in process simulators for P2 purposes:

1. Fugitive emissions estimation. These emissions have become increasingly important for industrial P2 in recent years because of regulations requiring their reporting and reductions. Current fugitive emissions estimation methods are frequently criticized as inadequate and costly. Current process simulators do not have the ability to estimate these emissions, but possible simulation methodologies do exist, such as incorporating emissions factors into simulation architecture; application of deterministic emissions correlations; and application of equipment failure analysis [15].

2. P2 technology databases. A large number of P2 case studies have revealed a series of effective equipment and process modifications. These technologies can be organized by chemical, process, or unit operation, and can be made available in the form of an expert system to the industrial designer using a process simulator.

3. Access to public domain data. The Toxic Release Inventory, the Resource Conservation and Recovery Act (RCRA) biennial survey, the Chemical Manufacturers Association waste data bank, and a number of other sources of data could be useful to an industrial designer in benchmarking process configurations. Process simulators should have the ability to query these data banks.

4. Life cycle and ancillary operation analysis. Simulation tools could be useful in evaluating the upstream and downstream impacts of alternative process designs and modifications, as well as the impacts of process ancillary operations such as maintenance, cleaning, and storage.

5. Combustion byproduct estimation. Stack air emissions from hazardous waste incinerators and combustors typically contain trace quantities of products of incomplete combustion (PICs), such as chlorinated dioxins and furans, and unburned principal organic hazardous constituents (POHCs). These emissions are difficult to both predict and measure. Process simulators do not currently offer sufficient data support to model these trace species, but they have the potential to do so.

6. Biological process modeling. Biological processes are increasingly being applied for the treatment, remediation, and separation of hazardous wastes in air emissions, waste waters, sludges, soils, and sediments. Very few process simulators currently contain unit operation models for these processes.

SECTION VI

CONCLUSIONS

1. Most existing state-of-the-art process simulators provide many features that make them powerful tools for the analysis of P2 design alternatives in a wide range of industrial processes. These features include: extensive libraries of unit operation models and physical property data; the ability to incorporate user-supplied models and data; and the ability to perform sensitivity analyses and set design specifications using any process variable. Other important features that are available in only some of the existing simulators include: process optimization; electrolytes modeling; and solids modeling.

2. Most existing state-of-the-art process simulators are now sufficiently user-friendly that they can be used with little or no training or experience to do rapid process P2 analysis. Features such as an expert guidance system and graphic display/output have greatly enhanced the user environment of current process simulators compared to the earlier versions that were used only by people with specialized training or experience.

3. Existing process simulators can significantly contribute to U.S. industrial P2 efforts because of the capability to easily model and analyze waste water systems. This is important because industrial waste water is the largest volume of hazardous waste in the U.S. Waste water treatment is probably the largest application of process simulation currently.

4. Existing process simulators can significantly contribute to U.S. efforts to measure progress in P2. Current measurement obstacles of data collection and data quality are overcome by the accurate and reliable waste generation data provided by simulation models. The obstacle of material balance closure is also overcome with the material balances done by these simulators.

5. Despite possessing many features that make them powerful and convenient tools for process design and analysis, current process simulators still lack many critical aspects required to be widely effective for P2. Some of these shortcomings are general in that they have potentially widespread applications other than the environment, while some of these are specific to P2. Specific needs include, but are not limited to:

- Fugitive emissions estimation
- P2 technology databases
- Access to public domain data
- Life cycle and ancillary operation analysis
- Combustion byproduct estimation
- Biological process modeling

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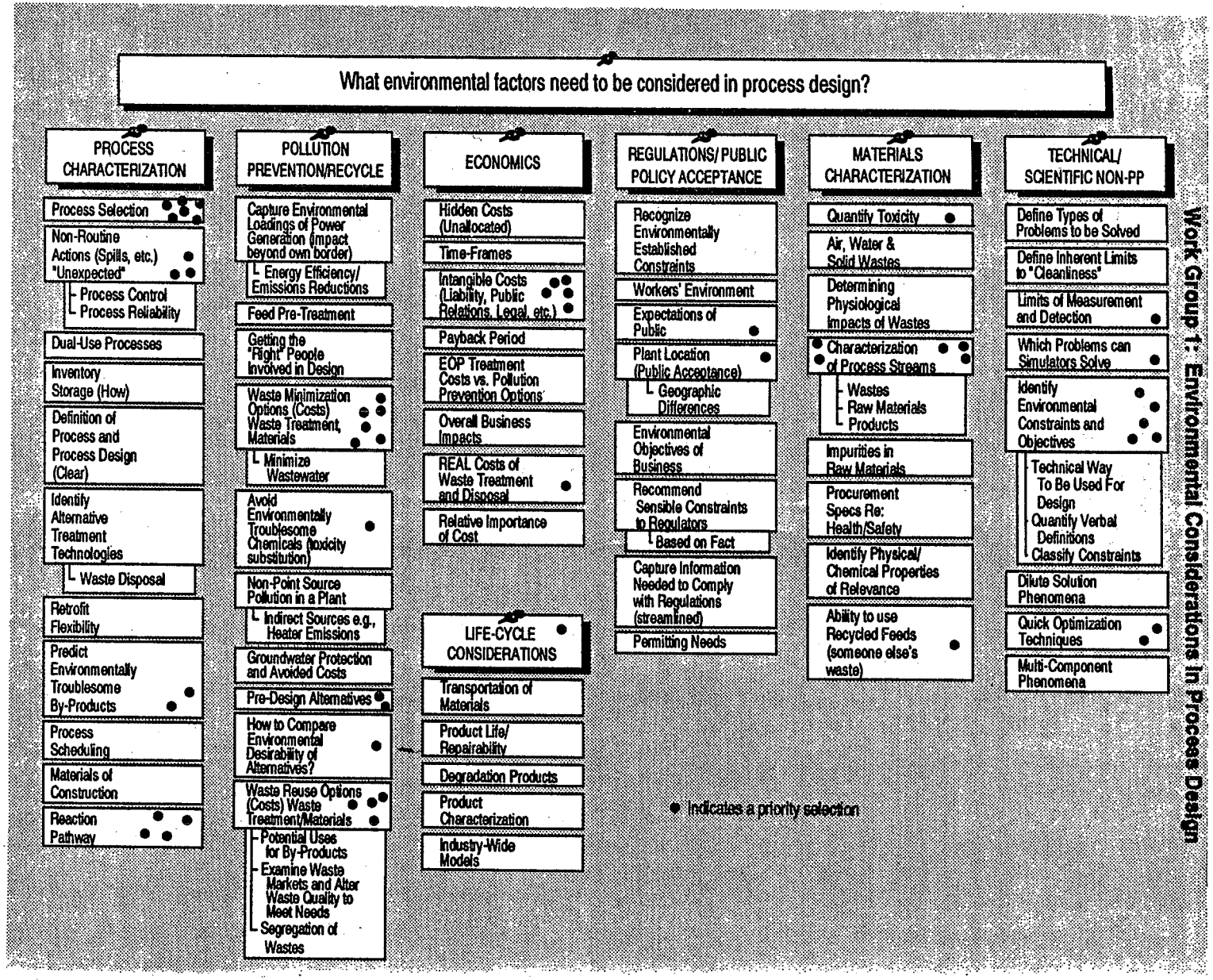
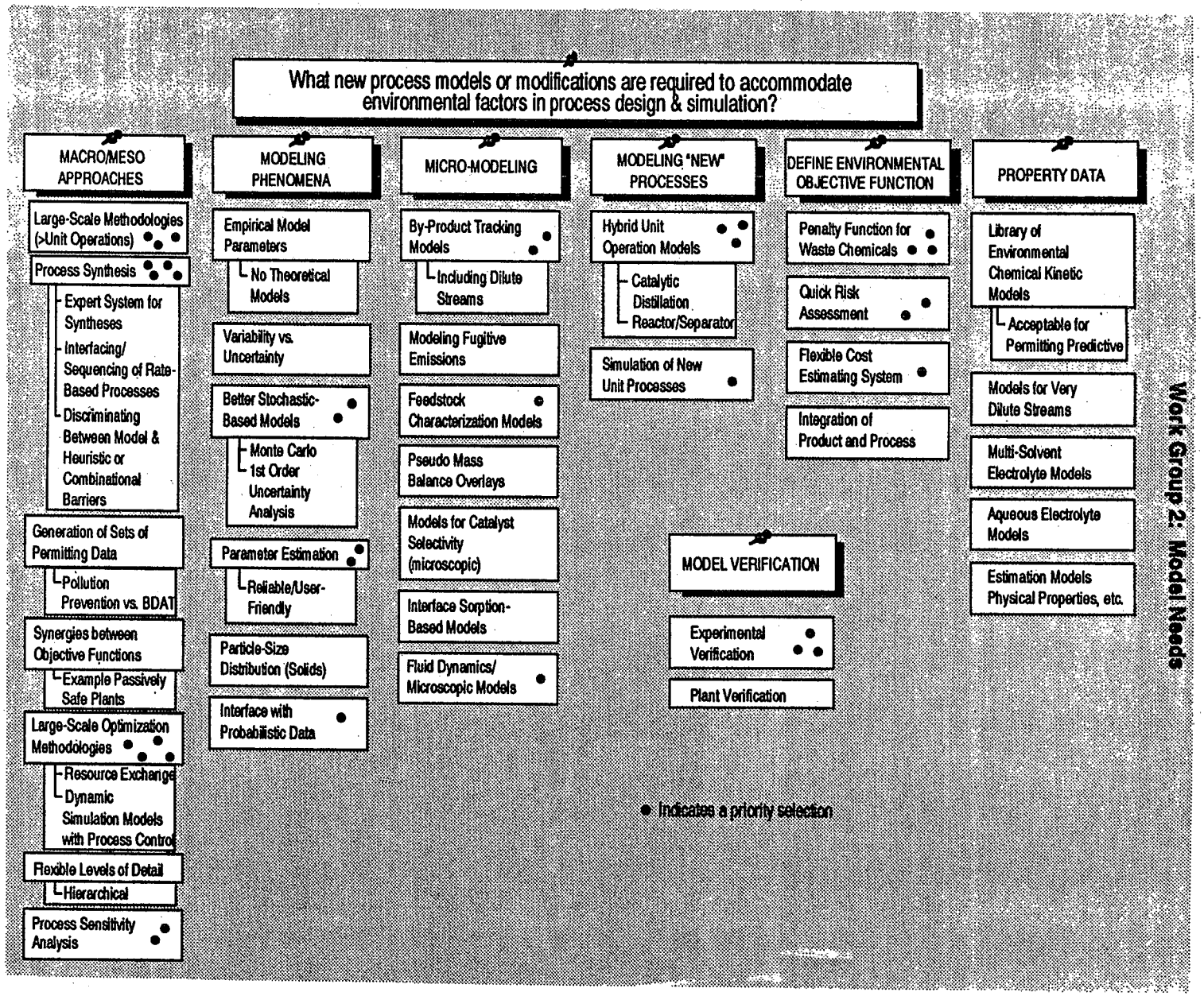
APPENDIX:

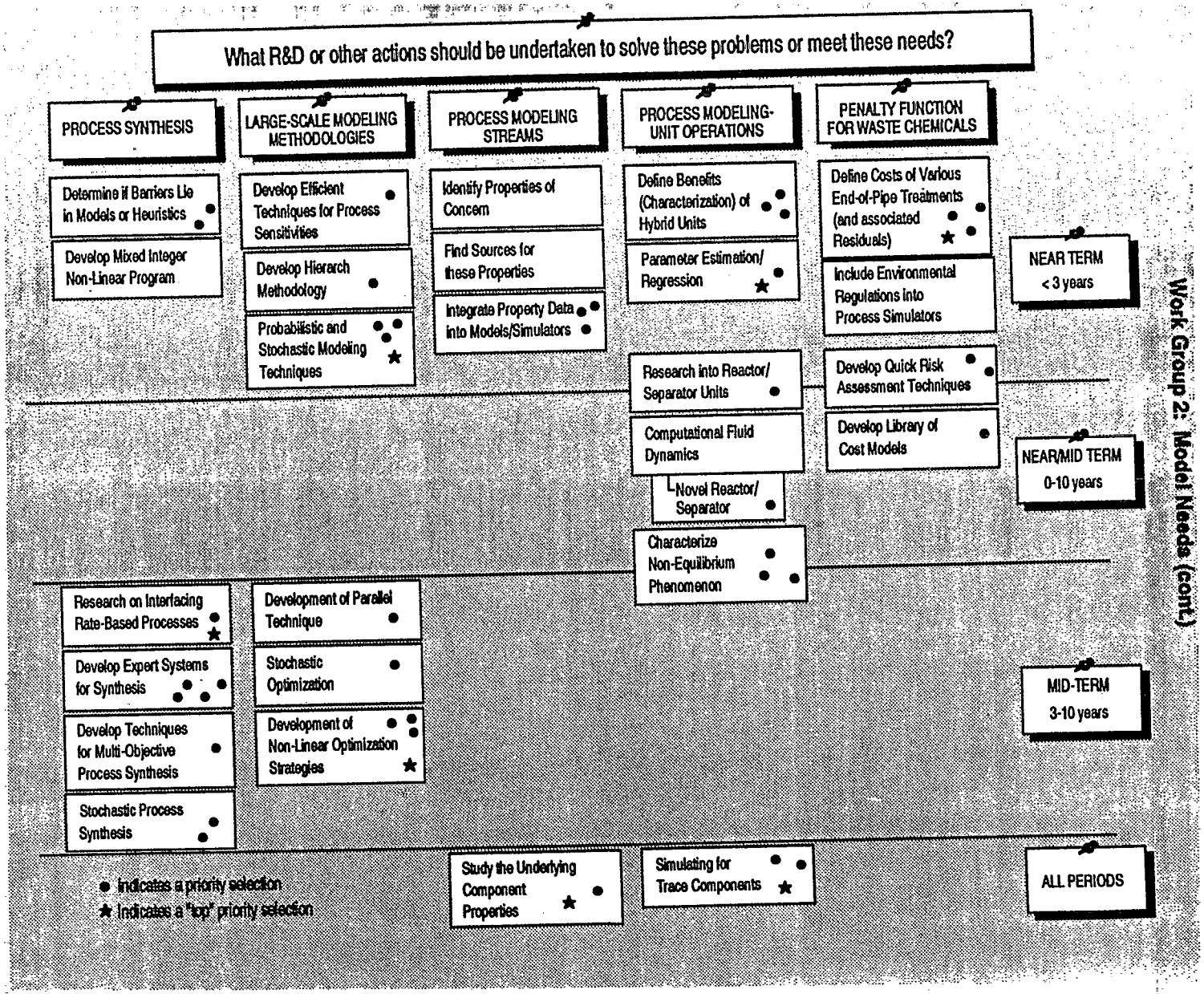
BREAKOUT GROUP RESULTS FROM EPA/DOE/AIChE

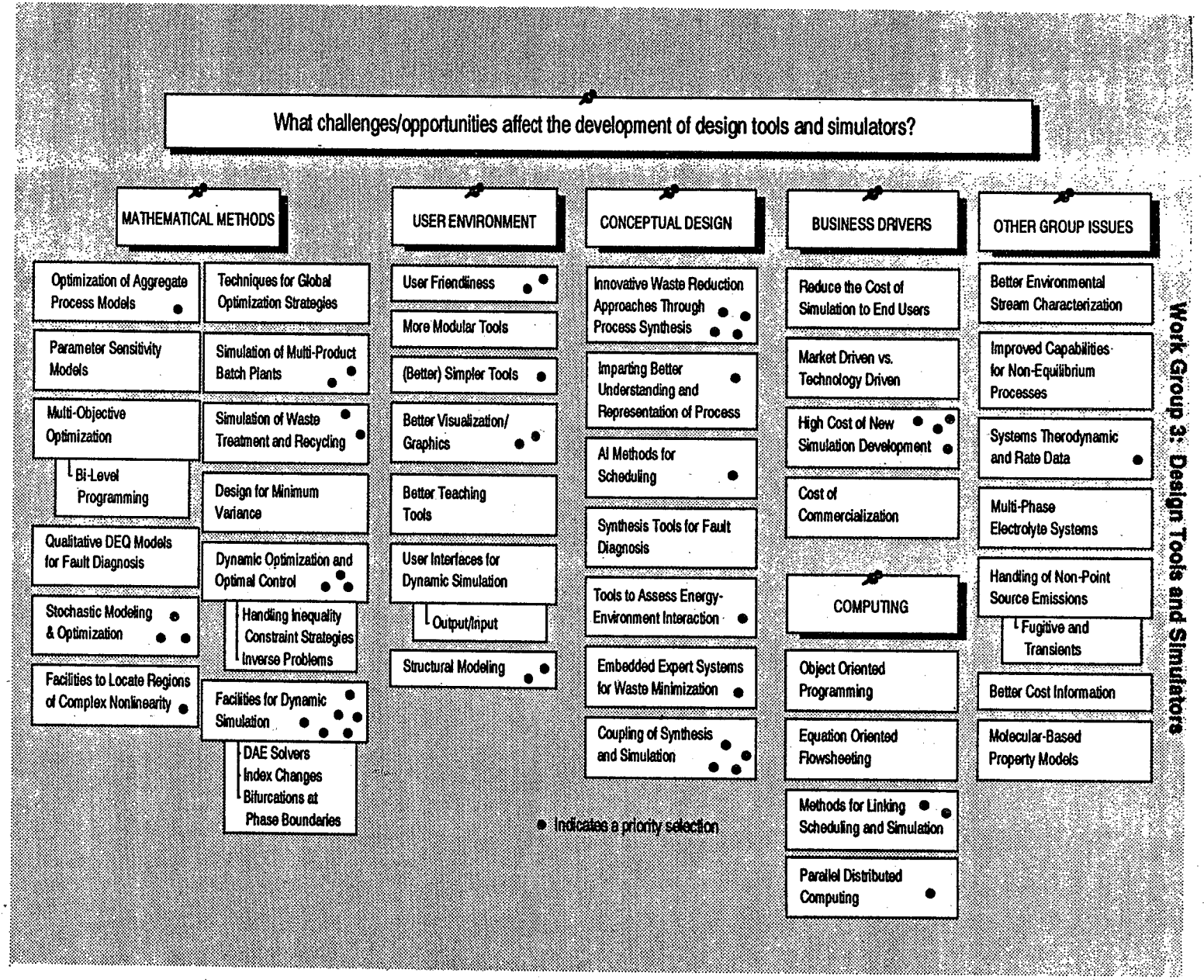
PROCESS SIMULATION RESEARCH WORKSHOP


What environmental factors need to be considered in process design?
PROCESS CHARACTERIZATION
Process Selection
Non-Routine Actions (Spills, etc.) "Unexpected"
Process Control
Process Reliability
Dual-Use Processes
Inventory Storage (How)
Definition of Process and Process Design (Clear)
Identify Alternative Treatment Technologies
Waste Disposal
Retrofit Flexibility
Predict Environmentally Troublesome By-Products
Process Scheduling
Materials of Construction
Reaction Pathway
POLLUTION PREVENTION/RECYCLE
Capture Environmental Loadings of Power Generation (impact beyond own border)
Energy Efficiency/ Emissions Reductions
Feed Pre-Treatment
Getting the "Right" People Involved in Design
Waste Minimization Options (Costs) Waste Treatment, Materials
Minimize Wastewater
Avoid Environmentally Troublesome Chemicals (toxicity substitution)
Non-Point Source Pollution in a Plant
Indirect Sources e.g., Heater Emissions
Groundwater Protection and Avoided Costs
Pre-Design Alternatives
How to Compare Environmental Desirability of Alternatives?
Waste Reuse Options (Costs) Waste Treatment/Materials
Potential Uses for By-Products
Examine Waste Markets and Alter Waste Quality to Meet Needs
Segregation of Wastes
ECONOMICS
Hidden Costs (Unallocated)
Time-Frames
Intangible Costs (Liability, Public Relations, Legal, etc.)
Payback Period
EOP Treatment Costs vs. Pollution Prevention Options
Overall Business Impacts
REAL Costs of Waste Treatment and Disposal
Relative Importance of Cost
LIFE-CYCLE CONSIDERATIONS
Transportation of Materials
Product Life/ Repairability
Degradation Products
Product Characterization
Industry-Wide Models
REGULATIONS/ PUBLIC POLICY ACCEPTANCE
Recognize Environmentally Established Constraints
Workers' Environment
Expectations of Public
Plant Location (Public Acceptance)
Geographic Differences
Environmental Objectives of Business
Recommend Sensible Constraints to Regulators
Based on Fact
Capture Information Needed to Comply with Regulations (streamlined)
Permitting Needs
MATERIALS CHARACTERIZATION
Quantify Toxicity
Air, Water & Solid Wastes
Determining Physiological Impacts of Wastes
Characterization of Process Streams
Wastes
Raw Materials
Products
Impurities in Raw Materials
Procurement Specs Re: Health/Safety
Identify Physical/ Chemical Properties of Relevance
Ability to use Recycled Feeds (someone else's waste)
TECHNICAL/ SCIENTIFIC NON-PP
Define Types of Problems to be Solved
Define Inherent Limits to "Cleanliness"
Limits of Measurement and Detection
Which Problems can Simulators Solve
Identify Environmental Constraints and Objectives
Technical Way To Be Used For Design
Quantify Verbal Definitions
Classify Constraints
Dilute Solution Phenomena
Quick Optimization Techniques
Multi-Component Phenomena
● Indicates a priority selection

Work Group 1: Environmental Considerations in Process Design (cont.)


What new process models or modifications are required to accommodate environmental factors in process design & simulation?
MACRO/MESO APPROACHES
Large-Scale Methodologies (>Unit Operations)
Process Synthesis
Expert System for Syntheses
Interfacing/ Sequencing of Rate-Based Processes
Discriminating Between Model & Heuristic or Combinational Barriers
Generation of Sets of Permitting Data
Pollution Prevention vs. BDAT
Synergies between Objective Functions
Example Passively Safe Plants
Large-Scale Optimization Methodologies
Resource Exchange
Dynamic Simulation Models with Process Control
Flexible Levels of Detail
Hierarchical
Process Sensitivity Analysis
MODELING PHENOMENA
Empirical Model Parameters
No Theoretical Models
Variability vs. Uncertainty
Better Stochastic-Based Models
Monte Carlo
1st Order Uncertainty Analysis
Parameter Estimation
Reliable/User-Friendly
Particle-Size Distribution (Solids)
Interface with Probabilistic Data
MICRO-MODELING
By-Product Tracking Models
Including Dilute Streams
Modeling Fugitive Emissions
Feedstock Characterization Models
Pseudo Mass Balance Overlays
Models for Catalyst Selectivity (microscopic)
Interface Sorption-Based Models
Fluid Dynamics/ Microscopic Models
MODELING "NEW" PROCESSES
Hybrid Unit Operation Models
Catalytic Distillation
Reactor/Separator
Simulation of New Unit Processes
MODEL VERIFICATION
Experimental Verification
Plant Verification
DEFINE ENVIRONMENTAL OBJECTIVE FUNCTION
Penalty Function for Waste Chemicals
Quick Risk Assessment
Flexible Cost Estimating System
Integration of Product and Process
PROPERTY DATA
Library of Environmental Chemical Kinetic Models
Acceptable for Permitting Predictive
Models for Very Dilute Streams
Multi-Solvent Electrolyte Models
Aqueous Electrolyte Models
Estimation Models Physical Properties, etc.
● Indicates a priority selection
Work Group 2: Model Needs


Work Group 2: Model Needs (Cont.)
What R&D or other actions should be undertaken to solve these problems or meet these needs?
PROCESS SYNTHESIS
LARGE-SCALE MODELING METHODOLOGIES
PROCESS MODELING STREAMS
PROCESS MODELING-UNIT OPERATIONS
PENALTY FUNCTION FOR WASTE CHEMICALS
Determine if Barriers Lie in Models or Heuristics
Develop Mixed Integer Non-Linear Program
Develop Efficient Techniques for Process Sensitivities
Develop Hierarch Methodology
Probabilistic and Stochastic Modeling Techniques
Identify Properties of Concern
Find Sources for these Properties
Integrate Property Data into Models/Simulators
Define Benefits (Characterization) of Hybrid Units
Parameter Estimation/ Regression
Define Costs of Various End-of-Pipe Treatments (and associated Residuals)
Include Environmental Regulations into Process Simulators
NEAR TERM < 3 years
Research into Reactor/ Separator Units
Computational Fluid Dynamics
Novel Reactor/ Separator
Characterize Non-Equilibrium Phenomenon
Develop Quick Risk Assessment Techniques
Develop Library of Cost Models
NEAR/MID TERM 0-10 years
Research on Interfacing Rate-Based Processes
Develop Expert Systems for Synthesis
Develop Techniques for Multi-Objective Process Synthesis
Stochastic Process Synthesis
Development of Parallel Technique
Stochastic Optimization
Development of Non-Linear Optimization Strategies
MID-TERM 3-10 years
● Indicates a priority selection
★ Indicates a "top" priority selection
Study the Underlying Component Properties
Simulating for Trace Components
ALL PERIODS


What challenges/opportunities affect the development of design tools and simulators?
MATHEMATICAL METHODS
Optimization of Aggregate Process Models
Techniques for Global Optimization Strategies
Parameter Sensitivity Models
Simulation of Multi-Product Batch Plants
Multi-Objective Optimization
Simulation of Waste Treatment and Recycling
Bi-Level Programming
Design for Minimum Variance
Qualitative DEQ Models for Fault Diagnosis
Dynamic Optimization and Optimal Control
Stochastic Modeling & Optimization
Handling Inequality Constraint Strategies
Inverse Problems
Facilities to Locate Regions of Complex Nonlinearity
Facilities for Dynamic Simulation
DAE Solvers
Index Changes
Bifurcations at Phase Boundaries
USER ENVIRONMENT
User Friendliness
More Modular Tools
(Better) Simpler Tools
Better Visualization/ Graphics
Better Teaching Tools
User Interfaces for Dynamic Simulation
Output/Input
Structural Modeling
CONCEPTUAL DESIGN
Innovative Waste Reduction Approaches Through Process Synthesis
Imparting Better Understanding and Representation of Process
AI Methods for Scheduling
Synthesis Tools for Fault Diagnosis
Tools to Assess Energy-Environment Interaction
Embedded Expert Systems for Waste Minimization
Coupling of Synthesis and Simulation
BUSINESS DRIVERS
Reduce the Cost of Simulation to End Users
Market Driven vs. Technology Driven
High Cost of New Simulation Development
Cost of Commercialization
COMPUTING
Object Oriented Programming
Equation Oriented Flowsheeting
Methods for Linking Scheduling and Simulation
Parallel Distributed Computing
OTHER GROUP ISSUES
Better Environmental Stream Characterization
Improved Capabilities for Non-Equilibrium Processes
Systems Therodynamic and Rate Data
Multi-Phase Electrolyte Systems
Handling of Non-Point Source Emissions
Fugitive and Transients
Better Cost Information
Molecular-Based Property Models
● Indicates a priority selection
Work Group 3: Design Tools and Simulators

Work Group 3: Design Tools and Simulators (cont.)

Work Group 4: Data Needs
What are the major data needs required to support process simulation and design with environmental factors?
ACQUISITION
DATA SETS
PROCESS MODELS
DATA QUALITY
STRATEGIES
COST
PROPERTY MODELS
Good Measured Data in Dilute Regions
Mass Transfer Data
Electrolytes in Complex Mixtures
Reaction By-Products
Automated Instrumentation
Good Separation Efficiency Data in Very Dilute Regions
Kinetics Versus Equilibrium
Good Modeling Set of Data
Good Data In Air Side/Odors
Soil Water Partitioning
Regulatory Information
Baseline Identification
Condensing Data
Treatability Database
Sensitivity on Process
Match Model with Data
Critical Components Rate vs. Equilibrium
Event Probability
Mixed Media Process Models
Protocols
Sampling/ Measuring
Range of Data
Unnecessary Accuracy
Orders of Magnitude
User Requirement
Environmental Impact Index
Linking of Models for Process and Impacts
Two Sets of Priorities Short/Long Term
Conflicting Objectives
Clustering Approach
Environmental Cost Factors
Handle on Cost of Data
Integration of Environmental Considerations/ Costs
Correlation of Group/QSAR
Computational Chemistry
Models to Handle Mixture in Dilute Region
Mixed Media Property Models
Electrolytes in Complex Mixtures
● Indicates a priority selection

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