Computer-Aided Process Design and U. of South Florida

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ABSTRACT

Computer-Aided Process Design outside the petrochemical industry is no longer uncommon and a systems approach to data gathering, control, and optimization is a major philosophical change in industry. At the design stage, process synthesis is coming out of infancy and finding its way into practice. In academic circles, languages such as Fortran are being challenged by symbolic languages.

The engineering school at USF aspires to be one of the leaders in computer aided design and education. The Pr1me 850s and 750, VAX 11-750s, Cyber 170-730, and IBM 3081 mainframes coupled with a rich variety of personal computers gives the institution a unique flexibility with computing power. The Computer-Aided Process Design laboratory enjoys a similar richness in software and expertise. Examples drawn from various application areas and projects would illustrate the depth and breadth in computer-aided chemical engineering at USF.

INTRODUCTION

Computerization of the whole business of process development and plant operations is not a pipe dream of the future, but is here and now with todays technology. Several activities such as feasibility studies, process synthesis, process design, equipment design, plant layout and pipework, control system design and instrumentation, operability studies, reliability studies require a large collaborative from different disciplines and/or organizations. Each activity has a distinctive contribution. However, having multiple objectives and interdependence between activities require a "systems" approach.

At University of South Florida, the Computer-Aided-Process-Design program is fairly new- 28 months, though comprehensive and vigorous. The Engineering College's outstanding computer power is complemented by the software supported and developed by the Computer-Aided Process Design (CAPD) laboratory. (See Table I) The activities of the CAPD group could be broken down to following categories: Software development and support, continuing education, research, and consultancy. Our interests in CAPE are vast and varied, thus we will rather give excerpts of the some of the ongoing activities.

RESEARCH

The Computer-Aided Process Design research could be broken down to several broad categories as

a. Process Synthesis

b. Process Optimization
c. Flowsheet Simulation
d. Operability Studies
e. Economic Analysis

while the tools used are varied from simple analytical relations or rule-of-thumps to complex algorithms for optimization and numerical analysis. The present research needs for integration of the several activities are in application of Artificial Intelligence (AI) techniques, simulation techniques, and data base management techniques. Abstracts of some the thesis and dissertation work on Computer-Aided-Process-Design as follows.

Advanced Chemical Process Economics (ACPE)

Uncertainty and risk is present in virtually all engineering economic evaluations given that the data in the investment calculations is no more than an estimate of what might happen in the future. The future is never certain and so the known data --sales, costs, prices and inflation-- can all vary from the estimated values. Therefore, it is of critical importance to determine if the best alternative available at present --in an uncertain environment-- will contribute to the financial success of the company.

The Advanced Chemical Process Economics software package has been developed to perform economic feasibility analyses of chemical projects [1]. Several methods --implemented individually or in conjunction-- for taking uncertainty in engineering economy studies into account, are made available in ACPE: the deterministic estimation of factors is used to establish a range of extreme values for the economic measure of merit; sensitivity analysis is employed to isolate the relative importance of individual components; and probability functions for uncertain elements are estimated and directly incorporated into the analysis by use of Monte Carlo simulation. Once the necessary data --sales volume and sales price per year, plant capacity, investment cost, plant salvage value, etc.-- is available and the options for the study --extent of analysis, cost estimation method, feasibility and termination criteria, etc.-- are selected, the economic analysis can be performed.

The present version of ACPE is very user friendly due to the interactive ("conversational"), stepwise nature of its input instructions. A command procedure language program controls the software flow and establishes communication between the two major --Fortran based-- code blocks: data acquisition and execution. There are two aspects to the procurement portion. That is to say, the actual gathering of information, and the creation of a permanent --strictly formatted-- input file. The former is accomplished by posing a series of questions and selections to the user --which permit him/her to "talk" with the computer--, while the latter is to serve as the direct entry to the executing phase. At present, there are 14 subroutines and 10 functions interacting in this second block to carry out the economic feasibility calculations.

The diagram shown in Figure I aims to illustrate ACPE's flow scheme.

At execution completion, output follows an echo of the input. Capital requirements, financing, annual raw material and utility requirements, detailed annual cash flows, and a summary of cash flows are typical outputs for each deterministic --most likely, optimistic, pessimistic-- estimate. These in turn are followed by sensitivity analysis results and Monte Carlo simulation results. The user is provided with options to control the extent of the output and means for printing a hard copy of the same.

ACPE may thus be used as a tool in handling one of the problems in capital budgeting --namely, the uncertainty of future investment opportunities.

Applications of Artificial Intelligence

Applications of Artificial Intelligence have made their way into Chemical Inference, Medical Diagnosis, Geology and CAD/CAM.[2] The conventional approach was

DATA + ALGORITHMS = PROGRAM.

However not all knowledge is algorithmic or amenable to representation in conventional languages. For example :

IF The feed is in the liquid phase.

AND The feed contains large molecules or colloids.

AND High product purity is required.

AND Product phases are 2 liquids.

AND Feed is non-corrosive.

THEN Recommend Ultrafiltration with a certainity factor (c.f.) = 0.8

While one can conventionally code 1-20 rules like this it is a tough proposition to code 50-500 maybe up to 1000 rules. In the example above, the concept of "large" molecule, and "high product purity" are representative of the fragmentary or judgemental knowledge that exsists in Chemical Engineering. It would be absurd to try to establish numerical coefficients to define "largeness", then again one cannot establish sharp boundaries for largeness. Finally the judgement to recommend ultrafiltration has a subjective certainity associated with it. It would nightmare to tackle such a task with conventional tools.

Now, the alternative approach is:

KNOWLEDGE + INFERENCE = SYSTEM.

To implement this approach one has to resort to AI techniques and tools.

SYMBOL MANIPULATION LANGUAGES (LISP, PROLOG)

KNOWLEDGE REPRESENTATION (PRODUCTION RULES, FRAMES)

INFERENCE PARADIGMS (PATTERN MATCHING, BACKWARD CHAINING).

The applications of AI techniques in narrow domains of expertise have given us the so called EXPERT SYSTEMS.
An example (Figure II) of the same is DENDRAL, an expert system for chemical inference for the deduction of the molecular structure from physical and chemical data. It uses heuristics and facts to arrive at a final structure. It was written in LISP using production rules. Dendral far surpasses any human expertise in that field.
Another system is R1 which configures Digital Equipment Corporation's VAX systems. Savings are estimated at $ 10 million a year. [3]

With this introduction we see that we need to investigate applications of AI in Chemical Engg. Possible applications are :

FAULT DIAGNOSIS:	(Real time troble-shooting for a plant.)
CONSULTANCY:	(Selection of optimization algorithms, selection of equation of state etc.)
DESIGN:	(Process synthesis and design.)
CONTROL:	(Real time process control and monitoring.)

The CAPD group at USF is focusing mainly on the Design area

DESIGN : Separation Process Synthesis

Separation Process equipment and technology selection

Symbolic Optimization

Heat exchanger networks

An example of an expert system structure is shown in Figure III.

Design of Optimal Resilient Heat Exchanger Network Through Simulation

Ever escalating cost of energy has commpelled the process industry, a major consumer, to search for better and efficient ways of managing the use and recovery of energy. In the energy intensive industries integration of various process streams to recover thermodynamically useful energy, consequently reducing operating and capital cost through efficient network of heat exchangers has attracted much attention.

Simple and reliable methods to synthesize the most efficient nominal network of heat exchangers to heat and cool known process streams between stated temperature bounds have become available recently.

It is well comprehended that fixed flow rates and temperatures rarely occur, even under most sophisticated controlled environment, industrially. This necessiates the need for "Resilient heat exchanger network" that can cope with the uncertainties of industrial design and provide the ease of operation and control.

Some work has been done in this area in recent years, yet a lot remains to be understood and done. Most of the work done to-date towards design of resilient heat exchanger network has been based on the objective that the network should stand feasible under the most extreme conditions. This is an unrealistic approach given that it presumes that at some given instant of time all the streams shall be in their extreme state, thus leading to a feasible but non-optimal (uneconomical) network.

A more realistic approach to optimal design would be through simulation. A "Resilient Heat Exchanger Network (RESHEN)" software package has been developed to design, simulate and evaluate the cost of an optimal resilient heat exchanger network. RESHEN is coded in Fortran 77 and comprises of two main blocks, viz: synthesis of a nominal network, and optimization through Monte Carlo simulation of the stochastic nature of stream conditions. The synthesis problem is accomplished with the aid of thermoeconomic rules and heuristics. The optimization problem is accomplished through an objective cost function that include cost of failure associated with the probability of failure of the network to perform to a desired level, cost of flexibility in operation, capital cost and operating cost. The present version of RESHEN is very user friendly due to the interactive ("conversational"), nature of its input instructions. It is also very well structured, containing 21 subroutines and 4 functions.

The diagram shown in Figure IV illustrates RESHEN's flow scheme.

Applications of Game Theory and Input-Output Analysis in Chemical Process Design

The computerized Chemical Process Industry model shown in Figure IV require software to model chemical market and company behavior. At present work is underway for development of market models. The development of the market simulator is based on the micro-economic theory of the firm and game theory in order to simulate the oligopolistic market situation (5 to 10 firms producing a product, each of which can affect the price by changing production). A firm which partipates in an oligopoly must base its actions on some assessment of how its competitors will behave. Generally, any change in the output of one firm has a certain effect on the industry price to which, in turn, the other firms would respond. Cournot's analysis of oligopoly, the Stackelberg theory, and other market share theories would be used in the model. The demand/price/production relations are derived using regression and/or time-series analysis.

Input-Output Analysis is a macroeconomic tool used to account for interindustry interaction and to identify the value added contribution to Gross National Product (GNP) by industry. It is used to determine the extent of flexibility for chemical process design. A flexible plant should operate effectively despite variations that may occur in parameter values during operation. The research also investigates direct Input-Output coefficients to ascertain effects of technological improvements. The multi-period, dynamic Input-Output analysis is employed since responses of firms take place over several time periods.

SOFTWARE DEVELOPMENT AND SUPPORT

The software acquisition and development is part of a broad and ambitious endeveour- a computer model of chemical process industry (Summary in Figure IV). Its purpose is educational as well as research in interrelations between process engineering activities. Although the interface between programs is still to be developed, access to some of the individual programs is available through terminals or personal computers.

EDUCATION

The formal courses which include use of some of the computerized procedures are the senior Plant Design course and a graduate course on Computer-Aided-Process Design course. We do offer a short course through USF and McGraw-Hill Seminar Development Corporation. Various troubleshooting problems and business games provide a realistic and accelarated learning.

BIBLIOGRAPHY

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TABLE I

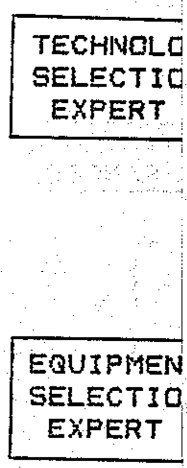
Software Purpose, Source, and Development Status

(All these programs are general, and have over 1000 executable statements)

NAME	SOURCE	DEVELOPMENT STATUS	PURPOSE
DESIGN	Chemshare Co.	Operating	Steady state flowsheet simulator with thermodynamic data bank
PROCESS	Simulation Sci.	Operating	Same as above
FLOWTRAN	Monsanto	Being Installed	same as above plus economic data bank
MULTI-BATCH	ETH, Switzerland	Operating	Batch process design package
RKPES	ETH, Switzerland	Operating	Parameter estimation from a set of stiff ODEs and algebraic equations
RKDESIGN	ETH, Switzerland	Operating	Experimental design package
RESHEN		Operating	Heat exchanger network synthesis
SEPARATION	in-house	Continuing	Process synthesis
MARKET	in-house	Continuing	Product market model
COMPANY	in-house	Continuing	Decision models
ACPE	in-house	Operating	Economic analysis under risk and uncertainty analysis

COLSYS	Lawerance Livermore Lab. (LLL)	Ready	Solution for mixed order of boundary value ODEs using collocation
PDECOL	LLL	Ready	Solution of PDEs using collocation
PDETWO	LLL	Ready	Solution for parabolic PDEs using finite differences
EFFECT	VPI&SU	Ready	Computes catalyst effectiveness factor
GAME	VPI&SU	Revised	Process design and economics game
DSS/2	Lehigh U.	Installed	ODE and PDE solver

Plans for purchase and installment of ASPEN (Flowsheet Simulator), MAPPS (Flowsheet simulator for pulp and paper processes), MACSYMA (Symbolic math package), Minos (An constrained optimization package) are underway.



Program Structure

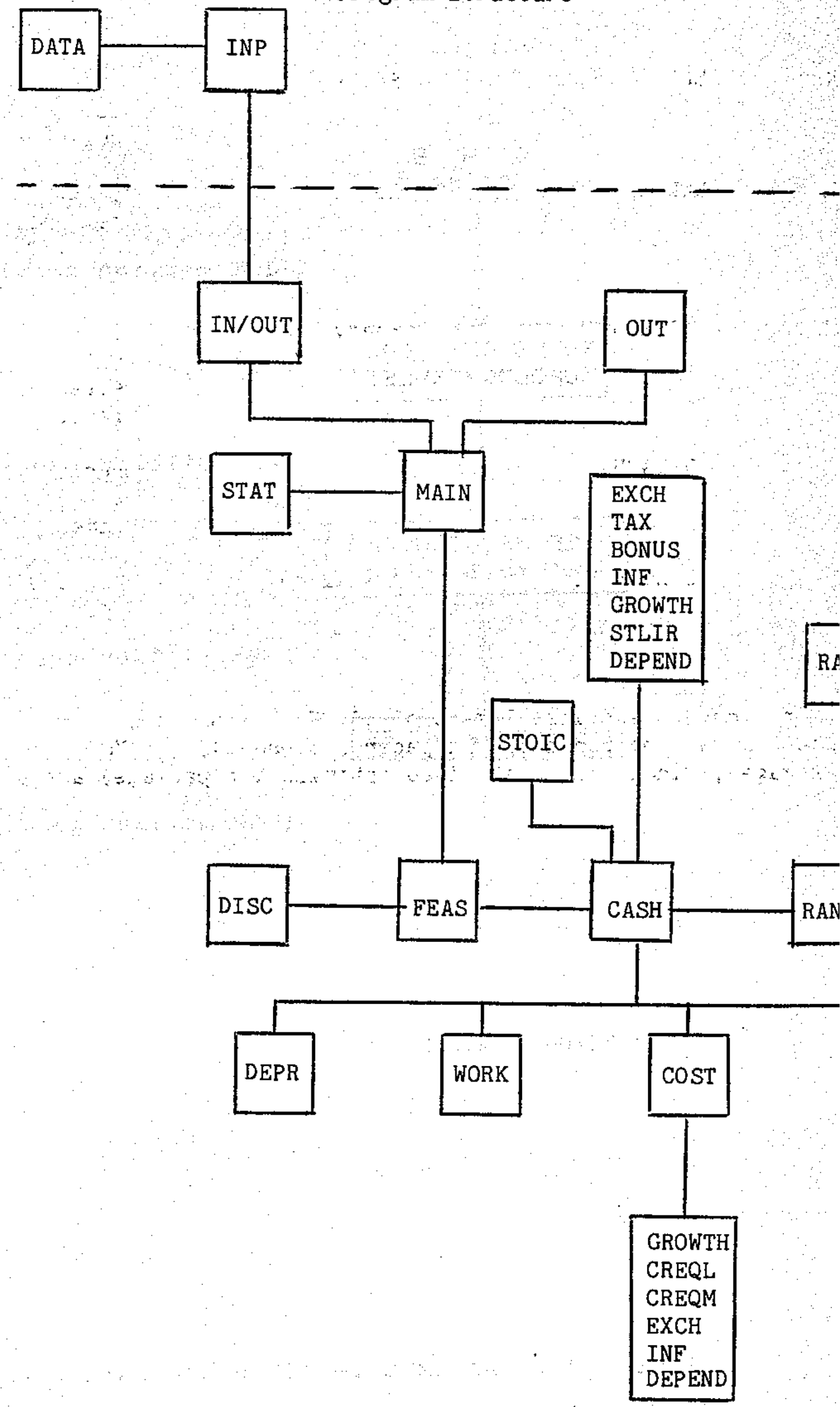


Figure I. Structure of ACPE