CACHE NEWS

NEWS ABOUT COMPUTERS IN CHEMICAL ENGINEERING EDUCATION.

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WHAT IS CACHE?

CACHE is a non-profit organization whose purpose is to promote cooperation among universities, industry, and government in the development and distribution of computer-related and/or technology-based educational aids for the chemical engineering profession.

CREATION OF THE CACHE CORPORATION

During the 1960's, the rapid growth of computer technology challenged educators to develop new methods of meshing the computer with the teaching of chemical engineering. In spite of many significant contributions to program development, the transferability of computer codes, even those written in FORTRAN, was minimal. Because of the disorganized state of university-developed codes for chemical engineering, 14 chemical engineering educators met in 1969 to form the CACHE (Computer Aids for Chemical Engineering) Committee. Initially, the CACHE Committee was sponsored by the Commission on Education of the National Academy of Engineering and funded by the National Science Foundation. In 1975, after several successful projects had been completed, CACHE was incorporated as a not-for-profit corporation in Massachusetts to serve as the administrative umbrella for the consortium activities.

CACHE ACTIVITIES

All CACHE activities are staffed by volunteers, including both educators and industrial members, and coordinated by the Board of Trustees through various Task Forces. CACHE actively solicits the participation of interested individuals in the work of its on-going projects. Information on CACHE activities is regularly disseminated through **CACHE NEWS**, which is published twice each year. Individual inquiries should be addressed to:

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CACHE TRUSTEES

CACHE NEWS

The CACHE News is published two times a year to report news of CACHE activities and other noteworthy developments of interest to chemical engineering educators. Persons who wish to be placed on the mailing list should notify CACHE at the aforementioned address. Contributions from CACHE representatives are welcome. This issue was edited by D.M. Himmelblau with contributions from a number of CACHE members and representatives.

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TABLE OF CONTENTS

FOCAPO UPDATE

CACHE is co-sponsor with the CAST Division of AICHE and the NSF of the Conference on Foundations of Computer Aided Process Operations to be held July 5-10 in Park City, Utah. The plans for this meeting are now being finalized, including the definition of the detailed schedule as given below as well as the selection and notification of the attendees.

The Proceedings of the conference, which will include the texts of the invited and contributed papers as well as summaries of the discussions and commentaries, will be generally available through Elsevier Science Publishers. For ordering information please contact the CACHE office or watch for an announcement in the next CACHE newsletter.

FOCAPO CONFERENCE PROGRAM

Sunday, July 5

5:30-7:00 pm	Reception
9:00-9:15	Opening Remarks: G.V. Reklaitis
9:15-10:00	Ralph P. Schlenker, Key Note Speaker
10:00-10:30	Discussion

Monday, July 6:

Process Data Acquisition & Interfaces

8:30-8:35 am	Opening Remarks: John Hale, Chairman
8:35-9:20	Lawrence DeHeer: Plant Scale Process Monitoring and Control Systems
9:20-10:05	Richard Mah: Data Screening
10:05-10:30	Coffee Break
10:30-12:00	Discussion: Patrick Kennedy, Commentator

Operations Planning

7:30-7:35 pm	Opening Remarks: David Rippin, Chairman
7:35-8:20	Charles White: Application of OR methodology to Process Operations
8:20-9:05	Eiji O'Shima: Automation of Plant Operating Procedures
9:05-9:30	Refreshment Break
9:30-11:00	Discussion: John A. Buzacott, Commentator

Tuesday, July 7

Process Safety

8:30-8:35 am	Opening Remarks: Gary Powers, Chairman
8:35-9:15	Malcolm L. Preston: The Process Systems Contribution to Process Safety
9:15-9:45	Harold Lindahl: Process Control for Safety
9:45-10:15	Gary Powers: Probabilistic Risk Assessment
10:15-10:35	Coffee Break
10:35-12:00	Discussion: (Commentator to be confirmed)

Maintenance Planning

7:30-7:35 pm	Opening Remarks: Tony Perris, Chairman
7:35-8:20	C.F.H. Van Rijn: A Systems Engineering Approach to Reliability, Availability, and Maintenance
8:20-9:05	Robert Wilson: Back to Basics: Redefining the Mission of Planning in an Automated World
9:05-9:30	Refreshment Break
9:30-11:00	Discussion: Frank Pierce, Commentator

Wednesday, July 8

Process Simulation

8:30-8:35 am	Opening Remarks: Rufus Baxley, Chairman
8:35-9:15	John D. Perkins: Modeling and Simulation in Process Operations
9:15-9:45	Toshi Shinohara: A Block Structured Approach to Dynamic Process Simulation
9:45-10:15	G. Boyd Gochenour: Equation Based Process Simulation
10:15-10:35	Coffee Break
10:35-12:00	Discussion: Jack Ponton, Edward M. Rosen, Commentators

Process Optimization

7:30-7:35 pm	Opening Remarks: Ignacio Grossmann, Chairman
7:35-8:20	David Hirshfeld: Large Scale Mathematical Programming Systems for Process Operations
8:20-9:05	Arthur Westerberg: Optimal Redesign and Modification of Existing Plants
9:05-9:30	Refreshment Break
9:30-11:00	Discussion: David R. Heltne, Jerry L. Robertson, Commentators

Thursday, July 9

Plant Networks and Databases

8:30-8:35 am	Opening Remarks: Norm Rawson, Chairman
8:35-9:20	R.J. Linn Jr.: Plant Information Networks
9:20-10:05	Wil Plouffe: Manufacturing Databases in Distributed Environments
10:05-10:30	Coffee Break
10:30-12:00	Discussion: D. Grant Fisher, Commentator

Contributed Papers: Innovative Research In Process Operations

2:15-2:20 pm	Opening Remarks: Jim Douglas, Chairman
2:20-3:00	Overview of Papers: Ernie Henley, Rapporteur
3:00-5:30	Poster Session
6:30-7:30	Cocktails
7:30-9:30	Banquet After Dinner Speakers: H. Steve Hamby, Rodney Falgout: Manufacturing Strategy: A Major Competitive Weapon

Friday, July 10

Intelligent Systems in Process Operations

8:30-8:35 am	Opening Remarks: George Stephanopoulos, Chairman
8:35-9:15	George Stephanopoulos: The Scope of Artificial Intelligence in Plant-Wide Operations
9:15-9:45	Mark Kramer: Expert Systems for Process Fault Diagnosis: A General Framework
9:45-10:15	P. Dhurjati: Evaluation of Experience with an Expert System for Fault Diagnosis in Commercial Scale Chemical Process
10:15-10:35	Coffee Break
10:35-12:00	Discussion: Brian Mathews, Commentator
12:00-12:15	Conference Closure: Dennis Spriggs

A TRANSPORT AND THERMODYNAMIC PROPERTIES PACKAGE FOR PERSONAL COMPUTERS

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INTRODUCTION

A transport and thermodynamic properties package for gases and liquids has been developed for personal computers. There were two incentives to do this work. First, (extensive) property-prediction packages were not available for personal computers at reasonably low costs. Second, the physical properties packages in current simulators (such as PROCESS and FLOWTRAN) had not employed the very best estimation techniques for transport properties. The proposed package can be applied to both mixtures and pure components over wide ranges of temperatures and pressures.

The transport and thermodynamic properties of pure components and mixtures are required in many chemical engineering calculations involving heat transfer, mass transfer, and fluid flow. The Transport and Thermodynamic Properties Package for Gases and Liquids (TTPGL) was set up for these purposes. The methods employed are believed to be among the best in the literature. In addition to those prediction techniques recommended by Reid et al. (1977) and Pan and Maddox (1981), new techniques developed in recent years such as the methods of Teja and Rice (1981a, 1981b) for the prediction of viscosity and thermal conductivity of liquid mixtures, the method of Lee and Thodos (1983) for the prediction of gas self-diffusivity, and the method of Hayduk and Minhas (1982) for the prediction of diffusivity of liquid mixtures were built into the package. The Peng and Robinson (1976) equation of state was used to estimate the vapor-liquid equilibrium ratio and other thermodynamic properties for mixtures. For pure component thermodynamic properties, however, the modified Benedict-Webb-Rubin (BWR) equation of state proposed by Lee and Kesler (1975) was employed.

Users are able to estimate diffusivity, thermal conductivity, viscosity, density, heat capacity, enthalpy, and K-value over wide ranges of temperatures and pressures. If some physical constants used as inputs are not available, the group-contribution subroutines can be invoked. The package TTPGL is intended to be interactive (with plenty of options) and user-friendly (with correction features) and is suitable for personal-computer-aided engineering or instruction. The package is now available for IBM PC's and TRS-80 models; the programming language is FORTRAN.

OUTLINE OF THE PREDICTIVE METHODS

The predictive methods for mixtures as well as the self-diffusivity estimation methods for pure components are presented in this section. Other physical properties prediction methods for pure components, which can be found in Pan and Maddox's (1981) paper, are not covered. This section contains a complete description of the methods used in the program, which will be presented in the following order: viscosity, thermal conductivity, diffusivity, density, K-value, enthalpy, and heat capacity. All the methods presented are for mixtures except in diffusivity where the methods for estimating self-diffusivity of pure components are discussed. Note that new predictive techniques have been included in order to give the best results.

A. Transport Properties

I. Gas Viscosity

The kinetic theory of Chapman-Enskog (1939) can be extended to determine the viscosity of a low pressure multicomponent gas mixture. The equation can be written as

$$\eta_m = \Sigma y_i \eta_i / (\Sigma y_i \phi_{ij}) \qquad (1)$$

where η_m = viscosity of mixture

η_i = viscosity of pure component i

y_i, y_j = mole fractions of component i and component j, respectively.

$$\phi_{ij} = [1 + (\eta_i / \eta_j)^{0.5} (M_j / M_i)^{0.25}]^2 / [8(1 + M_i / M_j)]^{0.5}$$

M_i, M_j = molecular weights of component i and component j, respectively.

The relation for ϕ_{ij}, proposed by Wilke (1950), was derived from Sutherland's kinetic theory model. Wilke (1950) compared calculated values with data (most of them were nonpolar mixtures) and reported an average deviation of less than 1%. For mixtures containing polar components, larger errors (up to 4%) may occur.

To estimate viscosities for dense-gas mixtures, the most accurate method at present appears to be that suggested by Dean and Stiel (1965),

$$(\eta_m - \eta_m^o)\xi_m = 1.08 [\exp(1.439 \rho_{rm}) - \exp(-1.111 \rho_{rm}^{1.858})] \qquad (2)$$

where η_m = high pressure viscosity, μ p

η_m^o = low pressure viscosity, μ p

$\xi_m = T_{cm}^{1/6} M_m^{-1/2} P_{cm}^{-2/3}$, T in ^oK, M in g/mol, and P in atm.

$T_{cm} = \Sigma y_i T_{ci}$

$M_m = \Sigma y_i M_i$

$P_{cm} = Z_{cm} T_{cm} R / V_{cm}$

$Z_{cm} = \Sigma y_i Z_{ci}$

$V_{cm} = \Sigma y_i V_{ci}$

$\rho_{rm} = V_{cm} / V_m$

$V_m = Z_m RT/P$

R = universal gas constant

The average error for Equation (2) was found to be 3.7% for nonpolar mixtures. When applied to polar mixtures, the expected error should be higher.

II. Liquid Viscosity

An extension of three-parameter corresponding-states principle using two real nonspherical reference fluids has recently been proposed by Teja and Rice (1981a). The Teja and Rice corresponding-states principle can be applied to the prediction of liquid viscosity for mixtures. The equation takes the form

$$\ln(\eta\xi) = \ln(\eta\xi)^{(rl)} + \frac{\omega - \omega^{(rl)}}{\omega^{(r2)} - \omega^{(r1)}} [\ln(\eta\xi)^{(r2)} - \ln(\eta\xi)^{(rl)}] \qquad (3)$$

where η = dynamic viscosity

$$\xi = V_{cm}^{2/3} T_{cm}^{-1/2} M_m^{-1/2}$$

$$V_{cm} = \Sigma \Sigma x_i x_j V_{cij}$$

$$M_m = \Sigma x_i M_i$$

$$T_{cm} V_{cm} = \Sigma \Sigma x_i x_j T_{cij} V_{cij}$$

$$V_{cij} = (V_{cii}^{1/3} + V_{cjj}^{1/3})^{3}/8$$

$$T_{cij} V_{cij} = \psi_{ij} (T_{cii} V_{cii} T_{cjj} V_{cjj})^{1/2}$$

$$\omega = \Sigma x_i \omega_i$$

$$V_{cii} = V_{ci}$$

(r1) and (r2) refer to two nonspherical reference fluids. They are usually designated in a way similar to the light key and heavy key concept for a multicomponent mixture in this work. In other words, the two most dominant components or the two with the most different accentric factors will be chosen. ψ_{ij} is set equal to 1.0 for nonpolar-nonpolar interaction. For polar-polar interaction, ψ_{ij} is designated as 1.05. Moreover, for polar-nonpolar interaction, ψ_{ij} is given as 0.955. The only exception to the above rules is that ψ_{ij} is set equal to 1.35 if either component i or component j is water. The ψ_{ij} values set above are based on a careful study of Teja and Rice's (1981a) data.

The average absolute deviations range from 1% for nonpolar mixtures to 3% for systems containing polar compounds and 9% for systems containing water.

III. Gas Thermal Conductivity

The Lindsay and Bromley (1950) method was chosen to estimate thermal conductivity of a gas mixture at low pressures. The equation is

$$\lambda_m = \Sigma y_i \lambda_i / (\Sigma y_i A_{ij}) \qquad (4)$$

λ_m = thermal conductivity of mixture

λ_i = thermal conductivity of pure component i

y_i, y_j = mole fractions of component i and component j, respectively.

$$A_{ij} = \tfrac{1}{4} \left[1 + \left[\frac{i}{j} \left(\frac{M_j}{M_i} \right)^{3/4} \frac{T + S_{ij}}{T + S_j} \right]^{1/2} \right]^2$$

η_i, η_j = pure gas viscosities

$S_i = 1.5 T_{bi}$, Sutherland constant

T_{bi} = normal boiling point

M_i, M_j = molecular weights

T = temperature, ^oK

$$S_{ij} = S_{ji} = C_s (S_i S_j)^{1/2}$$

C_s is set at unity unless one of the gases is very polar, when a value of 0.733 is used.

For gas mixtures at high pressures, the Stiel and Thodos (1964) relations were employed:

If $\rho_{rm} < 0.5$:

$$(\lambda_m - \lambda_m^o)\,\Gamma Z_{cm}^5 = 14.0 \times 10^{-8} (\exp(0.535\,\rho_{rm}) - 1) \qquad (5)$$

If $0.5 < \rho_{rm} < 2.0$:

$$(\lambda_m - \lambda_m^o)\,\Gamma Z_{cm}^5 = 13.1 \times 10^{-8} (\exp(0.67\,\rho_{rm}) - 1.069) \qquad (6)$$

If $2.0 < \rho_{rm} < 2.8$:

$$(\lambda_m - \lambda_m^o)\,\Gamma Z_{cm}^5 = 2.967 \times 10^{-8} (\exp(1.155\,\rho_{rm}) + 2.016) \qquad (7)$$

where λ_m = thermal conductivity at a high pressure, cal/ (cm s K)

λ_m^o = thermal conductivity at a low pressure, cal/ (cm s K)

$\Gamma = T_{cm}^{1/6} M_m^{1/2} P_{cm}^{-2/3}$, T_{cm} in °K, M_m in g/mol, and P_{cm} in atm.

Z_{cm} = critical compressibility factor

$\rho_{rm} = \rho_m / \rho_{cm}$, pseudo-reduced density

The Lindsay-Bromley method has an average error of 1.9%. Even for polar mixtures, errors rarely exceed 5%. The accuracy of the Stiel and Thodos relations is in doubt. However, the expected errors should be within 20% (Reid et al., 1977).

IV. Liquid Thermal Conductivity

A corresponding-states method for thermal conductivity of liquid mixtures was proposed by Teja and Rice (1981b),

$$\lambda\phi = \lambda\phi^{(rl)} + \frac{\omega - \omega^{(rl)}}{\omega^{(r2)} - \omega^{(rl)}} (\lambda\phi^{(r2)} - \lambda\phi^{(rl)}) \qquad (8)$$

where λ= thermal conductivity

$\phi = V_{cm}^{2/3} M_m^{1/2} T_{cm}^{-1/2}$

ω, V_{cm}, M_m, T_{cm} = as defined in Equation (3)

The average deviation between calculated and experimental values was found to be 3.11%. The ψ_{ij} used in this program is 0.85 for polar-nonpolar interaction; otherwise, ψ_{ij} is set equal to 1.0.

V. Gas Diffusivity

For self-diffusivity of dilute and dense gaseous states, Lee and Thodos (1983) presented the following equation:

$$D\,\delta\rho_r = 0.77 \times 10^{-5} T_r \qquad \rho_r \leq 1 \qquad (9)$$

In the supercritical region, where ρ_r may be greater than 1, the following equation proposed by Mathur and Thodos (1965) should be used,

$$D\beta\rho_r = 10.7 \times 10^{-5} T_r \qquad \rho_r > 1 \qquad (10)$$

where D = self-diffusivity, cm^2/s

$\beta = M^{1/2}P_c^{1/3}T_c^{-5/6}$

$\delta = M^{1/2}P_c^{-1/2}V_c^{-5/6}$

P_c = critical pressure, atm

V_c = critical volume, cm^3/g-mol

T_c = critical temperature, ^oK

ρ_r, T_r = reduced density and temperature, respectively.

The average error associated with Equation (9) is 0.51%. The deviations for Equation (10) were reported to be within 11% for $\rho_r \leq 1.5$. The expected error would be larger if ρ_r is greater than 1.5.

The widely used HBS equation derived by Hirschfelder, Bird, and Spotz (1954) is convenient for estimation of low pressure gas diffusivities. However, the modified version of the HBS equation proposed by Ramamurthy and Narsimhan (1970) was actually employed to predict binary diffusivity in the package. The equations are

If $T < 1.875 (T_{cA}T_{cB})^{1/2}$:

$$D_{AB}(1+\alpha)^2 M_r T_{cB}^{3/13} p_{cA}^{1/3} T_{cA}^{-107} = 3.65 \times 10^{-4} T_{rA} Z_{cA}^{-2/3} p_{rA}^{-1} \qquad (11)$$

If $T > 1.875 (T_{cA}T_{cB})^{1/2}$:

$$D_{AB}(1+\alpha)^2 M_r T_{cB}^{1/12} p_{cA}^{1/3} T_{cA}^{-0.92} = 6.45 \times 10^{-4} T_{rA}^{5/3} Z_{cA}^{5/3} p_{rA}^{-1} \qquad (12)$$

where D_{AB} = binary diffusivity, cm^2/s

A, B = species A, B

$\alpha = (V_B/V_A)^{1/3}$, cube root of molar volume ratio

$M_r = (M_A^{-1} + M_B^{-1})^{-1/2}$

Z_c = critical compressibility factor

r = subscript for reduced state

c = subscript for critical state

The prediction error of the Ramamurthy and Narsimhan method is about 5%.

Diffusivity in multicomponent mixtures is given by the following equation

$$D_{im} = \left(\sum_{\substack{j=1 \\ j\neq i}}^{n} \frac{x_j}{D_{ij}}\right)^{-1} \qquad (13)$$

for a dilute component i diffusing into a homogeneous mixture. D_{ij} is the binary diffusivity which can be estimated by the Ramamurthy and Narsimhan (1970) method. Errors should be around 5% or slightly higher.

The effect of pressure on binary and multicomponent diffusivities is not clear (Reid et al., 1977). Hence, one should expect even larger errors if estimating gas diffusivities at high pressures.

VI. Liquid Diffusivity

For self-diffusivity in liquids, the method of Riazi and Daubert (1980) was employed,

$$\mu^{2/3} D T^{-1} = 6.35 \times 10^{-8} (T/T_b)^{0.83} \qquad (14)$$

where D = self-diffusivity, m^2/s

μ = absolute viscosity, Ns/m^2

T = temperature, ^oK

T_b = normal boiling point, ^oK.

The average error associated with Equation (14) is 2 to 3% for liquids.

For a binary mixture of solute A in solvent B, the diffusivity D_{AB} implies that each A molecule is in an environment of essentially pure B. In engineering work, D_{AB} is assumed to be a reasonable estimation even for concentrations of A up to 5, perhaps 10, mole percent.

New correlations have been developed for liquid diffusivity at infinite dilution for polar and nonpolar solutions by Hayduk and Minhas (1982),

For water as solvent

$$D_{AB} = (1.25\, V_A^{-0.19} - 0.365) \times 10^{-8}\, \mu_B^{(9.58/V_A - 1.12)} T^{1.52} \qquad (15)$$

For systems containing normal paraffins only

$$D_{AB} = 13.3 \times 10^{-8} T^{1.47} \mu_B^{(10.2/V_A - 0.791)} V_A^{-0.71} \qquad (16)$$

For either polar or nonpolar solvent (except the above-mentioned two cases), if the parachor for solute and solvent are available,

$$D_{AB} = 1.55 \times 10^{-8} T^{1.29} \mu_B^{-0.92} V_B^{-0.23} p_A^{-0.42} p_B^{0.5} \qquad (17)$$

if not,

$$D_{AB} = 6.916 \times 10^{-10} T^{1.7} \mu_B^{-0.8} R_A^{-0.4} R_B^{-0.2} \qquad (18)$$

where D_{AB} = binary diffusivity, cm^2/s

V_A, V_B = molar volume at the normal boiling point of solute A and solvent B, cm^3/g-mol

P_A, P_B = parachor for solute A and solvent B

R_A, R_B = radius of gyration for solute A and solvent B

μ_B = viscosity of solvent B, cP

T = temperature, ^oK

The Wilke-Chang (1955) equation has been employed for estimating diffusivity in multicomponent liquid mixtures,

$$D_{Am} = 7.4 \times 10^{-8} \frac{(\phi M)^{0.5} T}{\eta_m V_A^{0.6}} \qquad (19)$$

where $\phi M = \sum_{\substack{j=1 \\ j \neq A}}^{n} x_j \phi_j M_j$

D_{Am} = diffusivity for dilute solute A into a homogeneous mixture, cm^2/s

η_m = mixture viscosity, cP

x_j = mole fraction of component j

T = temperature, ^oK

M_j = molecular weight of component j

V_A = molar volume at the normal boiling point of the solute, cm^3/g-mol

ϕ_j = Wilke-Chang association parameter

Wilke and Chang recommended that ϕ_j be chosen as 2.6 if the solvent is water, 1.9 for methanol, 1.5 for ethanol, and 1.0 for unassociated solvents.

The errors associated with the method of Hayduk and Minhas are as follows: The average error for normal paraffins is 3.4%, for water as solvent is 9.4%. The estimated errors for the Wilke-Chang method for the estimation of D_{Am} should be less than 20%.

B. Thermodynamic Properties

In this program, the modified Benedict-Webb-Rubin (BWR) equation of state is used to predict thermodynamic properties for pure components, while the Peng-Robinson (1976) equation of state is used to generate the mixture vapor pressure, equilibrium ratio, and other mixture thermodynamic properties. The reason for choosing the Peng-Robinson equation of state is the simplicity of its mixing rules and its capability to handle the liquid phase. When an equation of state for a mixture (such as the Peng-Robinson equation of state) represents the P-V-T-x behavior of the liquid as well as the vapor phase, the equation can be used to calculate thermodynamic properties for both phases. This calculation has the advantage of avoiding activity coefficients and their associated standard states, which in some cases are hypothetical. Equations of state that are cubic in volume are the simplest that can represent both liquid and vapor phase behavior.

I. Density

The density or molar volume can be calculated by the Peng-Robinson equation of state,

$$P = \frac{RT}{v-b} - \frac{a}{v(v+b) + b(v-b)} \qquad (20)$$

where P = pressure

v = molar volume

T = temperature

R = universal gas constant

$a_i = a_i (T_{ci})\, \alpha_i (T_{ri}, \omega_i)$

$a_i (T_{ci}) = 0.45724 R^2 T_{ci}^2 / P_{ci}$

$b_i = 0.0778 R T_{ci} / P_{ci}$

$\alpha_i = [1 + \kappa_i (1 - T_{ri}^{1/2})]^2$

$\kappa_i = 0.37464 + 1.54226\, \omega_i - 0.26992\, \omega_i^2$

ω_i = accentric factor for component i

$a = \Sigma\Sigma x_i x_j a_{ij}$

$b = \Sigma x_i b_i$

$a_{ij} = (1 - \delta_{ij})\, (a_i a_j)^{1/2}$

The density ρ can be obtained by 1/v. The anticipated errors for nonpolar systems should be within 5% for the vapor phase and 8% for the liquid phase except near the critical region where deviations as high as 15% may occur. For polar systems errors could be twice as large. The value of δ_{ij} has been set equal to zero for hydrocarbon mixtures. Otherwise, δ_{ij} is 0.130.

The option is available for the user to compute pure component liquid density by means of the Rackett equation or the Gunn and Yamada method (see Pan and Maddox, 1981), then apply Amagat's law,

$$V_m^L = \Sigma_j x_j V_j^L \qquad (21)$$

where V_j^L = molar volume of pure liquid j

V_m^L = molar volume of mixture

It is believed that this option gives better results for nonhydrocarbons at modest pressures. The errors should be less than 2% in most cases.

I. Density

II. Equilibrium Ration (K-value)

Vapor-liquid equilibrium requires that the fugacity is the same for each component in each phase. The K-value is defined as

$$K_i = x_i^V / x_i^L = \phi_i^L / \phi_i^V = [f_i^L/(x_i^L P)]/[f_i^V/(x_i^V P)] \qquad (22)$$

where P = system pressure

f_i^L, f_i^V = fugacity of component i in liquid and vapor phase, respectively

ϕ_i^L, ϕ_i^V = fugacity coefficients of component i in liquid and vapor phase, respectively

The fugacity coefficient of component i in a mixture predicted by the Peng-Robinson equation of state is,

$$\ln\phi_i = \ln \frac{f_i}{x_i p} = \frac{b_i}{b}(Z-1) - \frac{A}{2\sqrt{2}\,B}\left(\frac{2\Sigma x_k A_{ki}}{a} - \frac{b_i}{b}\right) \ln \frac{Z+2.414B}{Z-0.414B} \qquad (23)$$

where $A = aP/(RT)^2$

$B = bP/(RT)$

$Z = Pv/(RT)$

Equations (20) and (23) should be applied to both liquid and vapor phases. The converged compositions which satisfy the equilibrium requirement then give the K-values for the system.

The estimated errors for K_i should be within 5% in most cases. But deviations as high as 25% are possible.

III. Enthalpy

The enthalpy departure predicted by the Peng-Robinson equation of state is

$$H - H^* = RT(Z-1) + \frac{T\frac{da}{dT} - a}{2\sqrt{2b}} \ln \frac{Z + 2.414B}{Z - 0.414B} \qquad (24)$$

where H = enthalpy of mixture

$H^* = \Sigma x_i H_i^o$, enthalpy of mixture at ideal gas state

H_i^o = enthalpy for pure component i at ideal gas state

T, B, a, b, Z = as defined in Equations (20) and (23).

The expected errors should be within 7% for hydrocarbon mixtures.

IV. Heat Capacity

The constant pressure heat capacity is given by

$$C_p = \left(\frac{\partial H}{\partial T}\right)_p \qquad (25)$$

Where C_p = constant pressure heat capacity of mixture

H = enthalpy of mixture

The constant volume heat capacity is given by

$$C_v = \left(\frac{\partial U}{\partial T}\right)_v \tag{26}$$

where C_v =constant volume heat capacity of mixture

U = H - Pv, internal energy of mixture

The temperature derivatives can be evaluated numerically.

The accuracy of this procedure is still unknown, but the errors should be greater than the corresponding errors of enthalpy.

PROGRAM DESCRIPTION

The TTPGL package consists of a main program and 28 subroutines. It takes a total memory size of 98K (only 52K if overlay is used).

Figure 1 shows the flowchart of the main program. There are six subroutines in GROUP 1 (see Table I) using group-contribution techniques to calculate the critical properties (T_c, T_c, ρ_c), the normal boiling point, the parachor, the H factor (for liquid thermal conductivity), the correlation constants for ideal gas heat capacity, and the correlation constants for liquid viscosity.

There are thirteen subroutines in GROUP 2 to estimate the saturated thermodynamic and transport properties for pure components. Subroutines in GROUP 3 estimate superheated, subcooled, and supercritical properties for pure components. They are basically the same as those in GROUP 2 except that a subroutine which predicts self-diffusivity for gases and liquids has been added in. There is only one subroutine in GROUP 4, which calculates the true critical point of a mixture.

Subroutines is GROUP 5 use the Peng-Robinson equation of state to evaluate the equilibrium ratio, the enthalpy, the heat capacity, and the density for the equilibrium phases. Subroutines in GROUP 6 predict diffusivity, viscosity, and thermal conductivity of gaseous and liquid mixtures.

At the beginning of each run, the user has to enter whether the system is a pure component or a mixture. Once this information is in, the physical constants of each component are entered. If the physical constants needed as input are not available from data sources, the group-contribution subroutines will be invoked. During the data input procedure, if the user makes a mistake, correction features are available.

Particular groups and particular structural contributions are used in group-contribution techniques. The program asks a series of questions concerning groups and structures. To answer these questions, the user simply enters the number of a particular group for the compound of interest; enter 0 when no indicated group is present; and enter a negative integer when all groups or structures present in that compound have been asked.

For a given state (temperature, pressure, and composition) at which the properties are to be estimated, the phase must be known; if the phase is unknown, the subroutines in GROUP 4 and GROUP 5 will be called to determine the phase of the system.

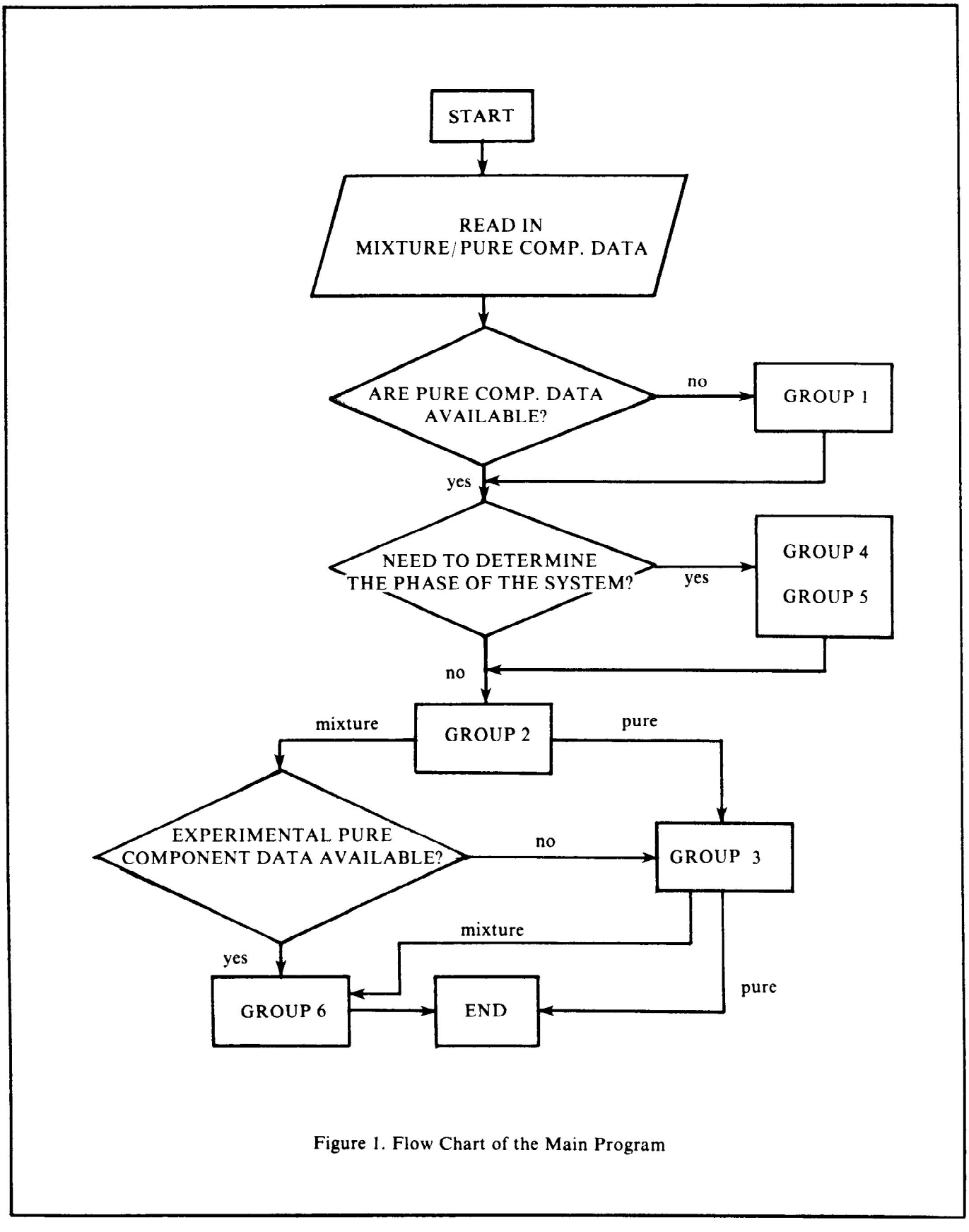

Figure 1. Flow Chart of the Main Program

TABLE I

GROUP 1 - SUBROUTINES USING GROUP CONTRIBUTION TECHNIQUES TO ESTIMATE PURE COMPONENT PHYSICAL CONSTANTS AND INPUT PARAMETERS

Subroutine	Methods	Estimated Constants/Parameters
BURNOP	Burnop	The Normal Boiling Point
LYDERS	Lydersen	The Critical Properties, P_C, T_C, ρ_C
ROBBIN	Robbins & Kingrea	The H Factor for Liquid Thermal Conductivity
RIHANI	Rihani & Doraiswamy	The Ideal Gas Heat Capacity
VANVEL	Van Velzen, Cardozo & Langenkamp	The Correlation Constants, VISB and VISTO, for Liquid Viscosity
PARA	Quale	The Parachor

EVALUATION OF THE PREDICTIVE METHODS

Methods for predicting the thermodynamic and transport properties in TTPGL are believed to be among the best in the literature. The errors claimed by the original authors or tested in this work have been summarized earlier. Generally, the errors obtained from our tests were close to those claimed by the original authors. Table II shows one of our comparisons where the calculated and experimental values for viscosity as well as the corresponding errors are listed.

The calculated results should be very good for nonpolar organic compounds and mixtures, while large errors may occur for systems containing highly polar or inorganic compounds.

Table III identifies the areas where new/improved predictive methods for transport properties of mixtures are needed. The predictive techniques for polar fluids and at high pressures are generally poor or even not available. Further investigation (experimental or theoretical) in these areas is recommended.

APPLICATION OF TTPGL IN MICROCOMPUTER-AIDED PROCESS DESIGN

When a design engineer selects the equipment of a process unit, he/she must determine the basic process design variables. The proposed program can be used if the user does not have experimental values of the needed thermodynamic and transport properties. An example is given in the case of calculating the heat transfer coefficient (modification of Peters and Timmerhaus's (1980) example) and the effect of physical properties estimation is evaluated.

Example: A shell-and-tube heat exchanger with one shell pass and one tube pass is being used as a cooler. The fluid is 0.75 mole% methanol and 0.25 mole% ethanol and the baffles are spaced equally 2 ft. apart. The safety factor F_s for use in evaluating the shell side film coefficient is 1.6. The inside diameter of the shell is 23 in. The OD of the tubes is 0.75 in. and the tubes are staggered. Clearance between tubes is 0.25 in. and the flow of fluid across the tubes is normal to this clearance. There is a total of 384 tubes in the exchanger, and the shell can be considered to be full-packed. The fluid temperature is 66° F, and the average temperature of the tube walls on the fluid side is 70° F. Estimate the film coefficient for the fluid.

TABLE II

COMPARISON OF CALCULATED AND EXPERIMENTAL VALUES FOR VISCOSITY (μ Pa s)

System	Phase	T,°K	P,atm	X_1[a]	Calc.	Exp.	Error
C_2H_4-C_2H_6	G	423.1	1	0.1865	13.51	12.81	5.5%
C_2H_4-C_2H_6	G	423.1	120	0.1865	19.52	18.82	3.7%
CCl_4-CH_3OH	L	313.2	1	0.5	632.1	600.0	4.2%
n-C_6H_{14}-C_6H_6	L	298.2	1	0.2	333.9	319.2	4.6%
H_2O-C_2H_5OH	L	298.2	1	0.89	227.2[d]	214.0	6.1%
$(CH_3)_2O$-CH_3Cl -SO_2	G	308.2	1	b	11.75	12.08	2.7%
$(CH_3)_2O$-CH_3Cl -SO_2	G	308.2	1	c	11.25	11.53	2.4%

a: The component indices 1, 2, 3 refer to the order of appearance in the description of the system

b: $X_1 = 0.263$, $X_2 = 0.256$, $X_3 = 0.481$

c: $X_1 = 0.357$, $X_2 = 0.335$, $X_3 = 0.329$

d: pure component experimental data are available.

TABLE III

IDENTIFICATION OF AREAS WHERE IMPROVED/ NEW PREDICTIVE METHODS ARE NEEDED

Mixture	Polar				Nonpolar			
State	gas		liquid		gas		liquid	
Pressure	high	low	high	low	high	low	high	low
Viscosity	X	X	X	X				
Thermal Conductivity	X	X	X	X				
Diffusivity	X		XX		X		XX	

X: Methods are available but need to be improved.

XX: No methods are available.

SOLUTION

Average fluid-film temperature = 68°F

From the program results

μ_f for fluid at 68°F = 0.6997 cP

k for fluid at 68°F = 0.067 Btu/ (h) (ft^2) (°F/ft)

C_p for fluid at 68°F = 0.414 Btu/ (lb) (°F)

D_o = 0.75/ 12 ft

Free area for evaluation of G_s occurs at the center plane of shell where the number of tube rows normal to flow direction = 23/ (0.75 + 0.25) = 23. Free area is based on the smallest flow area at the center plane. In this case, the transverse openings give the smallest free area.

Free area between baffles = 23 x 0.25 x 2/ 12 = 0.96 ft^2

a_o = 0.33, F_s = 1.6

G_s = 90,000/0.96 = 94,000 lb/ (h) (ft^2)

Calculation of Reynolds number = $D_o G_s / \mu_f$

= (0.75/ 12) x 94,000/ (0.6697 x 2.42) = 3625

$(C_p \mu / k)_f$ = 0.414 x 0.6697 x 2.42/0.067 = 10.01

The film coefficient

$$h_o = \frac{K_f a_o}{D_o F_s} \left(\frac{D_o G_s}{\mu_f}\right)^{0.6} \left(\frac{C_p \mu}{k}\right)^{1/3}$$

= 64.61 Btu/ (h) (ft^2) (°F)

The experimental data are as follows

μ_f for fluid at 68°F = 0.7132 centipoise

k for fluid at 68°F = 0.075 Btu/ (h) (ft^2) (°F)/ft)

C_p for fluid at 68°F = 0.383 Btu/ (1b) (°F)

Following the same calculations, the film coefficient is 66.78 Btu/ (h) (ft^2) (°F). The deviation is 3.24%.

CONCLUSIONS

The TTPGL package is fully updated in that it does include new prediction techniques for thermodynamic and tranport properties. The package is interactive, with correction features, and applicable for wide ranges of temperatures and pressures. Group-contribution subroutines are available in TTPGL to estimate input parameters when necessary. The Peng-Robinson equation of state has been employed to estimate thermodynamic properties for mixtures with considerable success. The calculated results should be very good for nonpolar organic fluids, although large errors may occur for mixtures containing highly polar or inorganic compounds.

ACKNOWLEDGEMENT

This work was presented to the 188th American Chemical Society Annual Meeting (Division of Industrial & Engineering Chemistry), Miami Beach, Florida, April 28 - May 3, 1985.

NOTE

A copy of the code described in this article can be obtained for $25.00 (prepaid) by writing to the Department of Chemical Engineering, Lamar University, P.O. Box 10053, Beaumont, TX 77710.

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MICROCOMPUTER CHEMICAL ENGINEERING PROGRAMS (developed by Professors)

Have you wondered what microcomputer programs are being used in other chemical engineering curricula? A new feature has been added to the CACHE newsletter. Bruce Finlayson will edit a column (titled above) that provides a mechanism for University professors to let others know about the programs they've developed and are willing to share on some basis.

There are two categories: 1. **Completed programs** and 2. **Programs for testing.** The **Completed programs** can be described by a 250 word description of the program, machine requirements, and ordering information. These programs should be ready to be shipped out the door, and should have been tested by students at more than one University. The **Programs for testing** are listed with title and 1-2 sentences. These are programs the author would like tested at other Universities. It would be helpful in both cases if the specific Chemical Engineering course were identified in which the program is useful. The programs will not be reviewed by Professor Finlayson, nor will they be certified by CACHE.

In order to edit the column efficiently, the submissions must be made to Finlayson via BITNET, using userid 27432 and node UWAV4. He will acknowledge receipt of the submission via BITNET, and will send the edited column to the CACHE office via BITNET. Letters will not be accepted or acknowledged. This requirement has two goals; to reduce the need for secretarial typing and to encourage academic chemical engineers to use electronic mail. Since anyone writing a computer code is computer literate, they can figure out how to use BITNET at their local installation when the incentive is exposure of their program. They can then share the protocols with their colleagues for other uses. Let us hear from you!

Here are the first announcements.

****

(1) Vapor Compression Refrigeration Cycle and (2) Compression of an Ideal Gas
Stanley Sandler, University of Delaware

This disk, for all IBM PC or compatible, contains two tutorial problems used in a first course in chemical or mechanical engineering thermodynamics. The first problem, RANKINE, begins with a short review of a vapor-compression refrigeration cycle. The student is asked to trace out the cycle on a pressure-enthalpy diagram for refrigerant-12, and then read the properties at each state from this diagram. Then, by using the data collected and the mass, energy and entropy balances, the student computes the rates which work needs to be supplied to the compressor and heat absorbed in the evaporator. Finally, the coefficient of performance is computed.

The second lesson, GAS, deals with the expansion of an ideal gas into cylinders which are partially or totally evacuated. This problem uses only the mass and energy balances, and the ideal gas equation of state.

To run these programs, an IBM compatible with DOS 2.0 or higher, 256 KB of memory and one disk drive is needed. A disk containing these programs and documentation may be purchased from Customer Services, Office of Instructional Technology, University of Delaware, Newark, DE 19716 for $29.

****

Computer Aided Analysis for Process Systems
Ted Cadman, University of Maryland

This is a series of PC-compatible programs for material and energy balances of chemical processes. The series is intended as the primary computational tool in the introductory course in chemical engineering. The series automates routine bookkeeping, organizational and computational tasks of analysis. The logical steps of analysis have purposely not been automated - rather a user-friendly environment is provided. A user's manual contains 25 chapters illustrating the use of the series with problems of increasing complexity.

The capabilities of the programs include 20 streams, 10 systems, including recycle. The material and energy balances use tools appropriate to the sophomore level - ideal mixing. The student can compute dew and bubble points, adiabatic flame temperatures, heats of reaction, and do simple heat exchanger calculations. The McCabe-Thiele method is used as an illustration of binary distillation. There is an automated degree-of-freedom analysis. The student can insert known data and then ask the program to do a degree-of-freedom analysis about a system. The computer then indicates which variables have been specified and which ones still need to be specified before the problem can be solved.

The programs come on two diskettes for the IBM PC. They work with high resolution graphics (the University of Maryland uses the IBM color graphics card). The code is compiled MS BASIC, so that no licenses are necessary. They have been used in class for three years. To obtain the diskettes, send a check for $20.00 made out to the Engineering Research Center. Send it to Chemical Engineering Program: Attn. Ted Cadman, Engineering Research Center, University of Maryland, Baltimore County, Catonville, Md. 21228.

****

Discounted Cash Flow Analysis (and Present Worth)
Bruce A. Finlayson, University of Washington

Program PROFIT does a discounted cash flow analysis of an investment. The information such as capital investment, revenue or expenses, can be different each year or be the same from year to year. The user must define the investments by specifying the capital investment, when it is made, when the service life begins and ends, what the working capital is and the salvage value. The revenue and expenses are also specified year by year. The tax rate is specified, and the method of depreciation is either straight-line, double-declining balance, or sum-of-years digits. The program then calculates the discounted cash flow rate of return. The present worth for a given interest rate can also be calculated. The capital investment, revenue and expenses, and discounted cumulative cash flow (for various interest rates) can be plotted using the program ENGNPLOT (included). The program runs on the Macintosh using pull-down menus.

This program has been used in the design course and runs on the Macintosh with 512K memory. The diskette with the system

and the program on it requires an 800K drive, but the program itself fits on a 400K drive. A disk containing this program and documentation may be purchased for $10, payable to the University of Washington. Send requests to Department of Chemical Engineering, BF-10, University of Washington, Seattle, WA 98195, Attn: Bruce Finlayson.

****

Short-cut Distillation and Flash Calculations
Bruce A. Finlayson, University of Washington

This program is designed to run in an interactive mode. It has the capability of doing both flash calculations and short cut distillation calculations, both with multi-component systems. The thermodynamics package is very general, with the vapor phase fugacity calculated by the Redlich-Kwong equation of state. The liquid phase is considered a non-ideal solution with activity coefficients based upon the Hildebrand solubility parameter. The short-cut distillation module uses the Fenske total reflux equation, Underwood's equation for minimum reflux, and Gilliland's correlation for the number of stages. Thermodynamic parameters are included for 98 different chemicals.

The short-cut distillation package requires the user to specify the ratio of reflux rate to minimum reflux rate, pressure of the column, and fraction of the light and heavy key. The output from the programs gives composition and physical properties (including K values) for the products, number of stages, feed stage and condenser and reboiler duties. The column is sized and the capital and operating costs are calculated. (The user can change the economic parameter if desired). The equivalent uniform annual cost (EUAC) is also calculated.

This program is a version of the same program that has been used in design applications for over 10 years. It has been ported to both the Macintosh and IBM PC. It uses no graphics. On the Macintosh it runs on a 512K machine with a 400K drive. On the IBM it runs on a machine with 256 KB memory. A disk containing this program and documentation may be purchased for $10, payable to the University of Washington. Send requests to Department of Chemical Engineering, BF-10, University of Washington, Seattle, WA 98195, Attn: Bruce Finlayson. The IBM version of this program will also be distributed at some future date by CACHE through their Curriculum Task Force.

****

BOOK ANNOUNCEMENT

The Art of Chemical Process Design

by **G.L. Wells,** *The University of Sheffield, Dept. of Chemical Engineering and Fuel Technology, Sheffield, UK, and* **L.M. Rose,** *Technisch-Chemisches Laboratorium, Eidgenossische Technische Hochschule, Zurich and CHEMENG Software and Services, Griefensee, Switzerland*

(Computer-Aided Chemical Engineering, 2)

1986 x + 704 pages
Price: US$88.00/ Dfl. 220.00
ISBN 0-444-42699-X

Illustrating all aspects of chemical process design, this book demonstrates process synthesis, material and heat balancing by manual and computerised methods, the use of flowsheeting programs and their construction, flowsheet development, plant safety, process economics and project engineering. The reader is introduced to each of the key areas and is given further information to follow these up. The process is developed as a whole entity with appropriate partitioning of certain tasks.

In recent years, there has been increased activity in process synthesis, particularly in the development of heat exchanger networks and distillation trains. Various chapters describe and develop these and other areas of interest. In particular, note is made of the need to select appropriate unit operations for given process tasks.

Traditional manual methods of material and heat balancing introduce the computerised methods used in flowsheeting programs. Plant safety continues to generate professional and public interest as catastrophes continue to occur. The recent developments in this area are described. Process economics, plant optimization and plant availability are introduced, as is the organization of projects. Particular emphasis is placed on these and on the development of process flow diagrams and piping instrument diagrams.

Although this is not the first book to tackle specific areas of process design and economics, it is the first to introduce and link all the relevant areas and will undoubtedly prove useful to practising chemical engineers and students alike.

Contents: 1. Process Design. 2. The Whole Project. 3. Process Economics. 4. Material and Heat Balances - Fundamentals. 5. Developing the Flowsheet. 6. Heat Exchanger Networks and Energy. 7. Distillation Trains. 8. Material and Heat Balances-Practice. 9. The Design Tool-The Flowsheet Program. 10. Data Banks and Data Bases. 11. Flowsheet Program Application. 12. Process Optimization. 13. Safety and Loss Prevention. 14. Storage Scheduling and Plant Availability. 15. Flow Diagrams and Control. Appendices: Notes on Hazardous Chemicals and Explosions. The International System (SI) of Units. Separation Methods. The Money Accounts. Program Manuals. Flowsheets and their Symbols. Subject Index.

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REVIEW OF GINO - PC SOFTWARE FOR NONLINEAR OPTIMIZATION AND EQUATION SOLVING

Ignacio E. Grossmann
Carnegie Mellon University

GINO is an interactive computer program for solving nonlinear programming problems with the GRG2 method by Professor Leon Lasdon and co-workers. The program runs on IBM compatible PC's (MS.DOS) and it requires 256K of memory. GINO can handle problems of up to 30 constraints and 50 variables, in addition to lower and upper bounds on the variables. There is also a larger version, SUPER-GINO, which can handle problems of up to 50 constraints, 100 variables, requiring 512K of memory.

GINO incorporates a user interface that is very similar to the computer program LINDO for linear and mixed-integer programming. With this interactive interface it is very easy to set up optimization problems as shown in the example below:

```
MODEL:
  1) MAX=0.75 * X-0.1 * X/(Y-X)-0.15 * Y-INV;
  2) Y>X+0.5;
  3) X=15-10 * EXP (-INV);
END

SUB    Y          15.000000
SLB    INV          .000000

: GO

SOLUTION STATUS: OPTIMAL TO TOLERANCES.
DUAL CONDITIONS: SATISFIED.

                OBJECTIVE FUNCTION VALUE
        1)    5.254271

VARIABLE          VALUE          REDUCED COST
   X           12.769861            .000000
   Y           15.000000           -.106759
  INV           1.500521            .000012

  ROW    SLACK OR SURPLUS          PRICE
   2)          1.730139            .000000
   3)           .000000            .448403
```

GINO can also be used as an equation solver, and in this regard we have found it to be more robust than TK! Solver since it is possible to specify bounds on the variables. This capability avoids the problem of converging to solutions that have no physical meaning (e.g. negative temperatures). Initial guesses on all or several of the variables can also be supplied.

We have been using GINO at Carnegie Mellon in several undergraduate and graduate courses in Chemical Engineering (e.g. Process Thermodynamics, Design, Economics and Optimization). We have found GINO to be a very valuable educational tool because it is much easier to use than other standard optimization and equation solving packages that are available in mainframes. Students can concentrate their attention on the modeling and formulation of problems, and obtain solutions quickly. Also, with GINO it is possible to assign to the students a larger number of numerical problems during a course and for which they can examine different cases and sensitivities of solutions.

A limitation of GINO is that the solution time can be rather significant for the larger problems (e.g. 30×50). This is mainly due to the fact that the program evaluates the gradients numerically. However, we have not found this to be a serious limitation for teaching since many assignment problems do not involve more than 10 variables.

An extensive comparison of GINO with other similar programs can be found in the paper "Nonlinear Programming on a Microcomputer" by B.L. Golden and E.A. Wasil, Computers and Operations Research, 13(2), pp. 149-166 (1986).

Although GINO has on-line documentation, it is useful for the instructor to have a copy of the book "Modeling and Optimization with GINO" by J. Liebman, L. Lasdon, L. Schrage and A. Waren, The Scientific Press, Palo Alto, CA (1986). This book has many good examples of optimization problems, and it provides useful guidelines for using GINO more effectively.

Information on GINO can be obtained from Professor Leon Lasdon, Department of General Business CBA 5.202, University of Texas, Austin, TX 78712-1175. Tel: (512) 471-3322. The program is also distributed by LINDO Systems, Inc., P.O. Box 148231, Chicago, IL 60614. Tel: (312)871-2524.

MICROCOMPUTER/PERSONAL COMPUTER NOTES

Peter Rony
Virginia Polytechnic Institute and State University

In the spirit of David Himmelblau's Computing in Chemical Engineering Award Address last November 1986, the March 1986 issue of **Computer** presents "St. Patrick's Almanack" in The Open Channel feature of the magazine. The theme of The Open Channel is a quote attributed to Charles McCabe in the San Francisco Chronicle: "Any clod can have the facts, but having opinions is an art." Some quotes, along with their authors, from the Almanack include: "One picture is worth a thousand reels of tape" (B.N. Fraizer); "The trapdoors to failure outnumber the shortcuts to success" (L.B. Johnson); "I've finally learned what 'upward compatible' means. It means we get to keep all our old mistakes." (Dennie van Tassel); "The VAX-11/785 is bug-for-bug compatible with the 780."(Anonymous); "Remember, the best ideas originate in the U.S.; other people have to think and talk in a foreign language. This gives you a tremendous technical edge." (B.S. Benson); "Time sharing is the junk mail part of the computer business." (H.R.J. Grosch); "Maybe Computer Science should be in the College of Theology." (R.S. Barton); "The good Christian should beware of mathematicians and all those who make empty prophecies. The danger already exists that mathematicians have made a covenant with the devil to darken the spirit and confine man in the bonds of Hell." (St. Augustine); and finally, "Hell must be isothermal; for otherwise the resident engineers and physical chemists (of which there must be some) could set up a heat engine to run a refrigerator to cool off a portion of their surroundings to any desired temperature." (Henry Albert Bent). Additional quotes will be published in this column is six months.

Readers interested in learning about programs and divisions of the National Science Foundation (whose support contributes significantly to advanced scientific computing) should see a

three-issue series, "Advanced Scientific Computing I, II, and III," published in Vol. 16 (Nos. 3 and 4) and Vol. 17 (No. 1) of **Mosaic** during 1985 and 1986. Single copies can be obtained at a cost of $2.75 each. Mail your order form to: Superintendent of Documents, Government Printing Office, Washington, D.C. 20402. Topics covered in the three issues include: "A Third Kind of Science," "The Pursuit of Parallelism (Architectures, Topologies, Pipelining)," "New Languages for Old (Algorithms)," "Access to Supercomputers," "Biology's Computation Future," "Computers to Go with the Flow (Engineering with multiphase flow, A turbulent superfuture)," "Expert Chemical Systems," "Mathematicians at the Receiving End," "Physicists: More Problems than Approaches," "Many-body Problems," "Taunting the Computer (Computer Vision, A Marr Sampler)," "A Picture is Worth ...(Architecture and Algorithms)," and "The Problem of Macrovariables."

The English microcomputer journal, **Microcomputers and Microsystems**, has always been a source of practical articles. The following from Vol. 10, Nos. 1 through 10, may be of interest: "Design and evaluation of a dual-microcomputer shared memory system with a shared I/O bus" (pp. 3-10); "Microprocessor-based delay generators" (pp. 25-27); "32008-based single-board microcomputer" (pp. 28-32); all of the articles in Vol. 10, No. 2 (March 1986), a special issue on backplane bus standards; "The physics of driving backplane buses" (March 1986, pp. 61-64), which explains and applies transmission line theory; "Exception Handling in the 68000, Part 1 and 2" (pp. 202-210 and 258-267); "Flexible interface based on the peripheral interface structure" (pp. 222-225); "Microprocessor processing of 10 MHz acoustic signals" (pp. 273-277); "Data acquisition and control system for laboratory experiments" (pp. 325-331); "Assembler-monitor package to teach assembly language" (pp. 336-339); "Simulation experiences in the development of software for digital signal processors" (pp. 419-426); "Cross-assembler for the TMS32010 digital signal processor" (pp. 434-441); "Software controller for an arithmetic processor [that is interfaced to a 6802]" (pp. 442-449); and "Microprocessor-based digital controller for DC motor speed (pp. 543-552).

Dr. Dobb's Journal of Software Tools has always been one of your editor's favorite computer magazines. It is oriented towards software tools in a variety of languages--Pascal, C, Forth, assembly, Modula-2, etc. Occasionally, a superbly written and illustrated hardware article, e.g., "Bringing Up the 68000--A First Step" (Jan 1986) appears. For the period of January 1986 through February 1987, readers may be interested in: "COM: An 8080 Simulator for the MC68000" (Jan, Mar 1986); "A Simple Multitasking Operating System for Real-Time Applications" (Jan 1986); "Fast Integer Powers for Pascal" (Feb 1986); "The Problems of Parallelism" (Mar 1986); "Speeding MS DOS Execution" (Mar 1986); "Automatic Porting Between Pascal Dialects" (Mar 1986); Annual Artificial Intelligence Issue (Apr 1986); "A Modula-2 68000 Cross Assembler" (Apr, May, Jun 1986); "BRIE--The Boca Raton Inference Engine" (Apr 1986); "The Cryptographer's Toolbox" (Apr 1986); "Direct Access to the IBM Video Display" (Apr 1986); Special FORTH issue (Jul 1986); "Benchmarking C Compilers" (Aug 1986); "Algorithms: Curve Fitting with Cubic Splines" (Sep 1986); "Turbo Prolog: The Language" (Sep 1986); "High-Speed Thrills" (turbo-boards for the IBM PC) (Sep 1986); "Programming on the 80386" (Oct 1986); "Modula-2 Compilers for the IBM PC" (Oct 1986); special issue on PC graphics (Nov 1986); "New Issues in PC Graphics" (Nov 1986); "A Mandelbrot Program for the Macintosh" (Nov 1986); "A Digital Dissolve for Bit-Mapped Graphics Screens" (Nov 1986); "A Multitasking Kernel" (for the 8086 and 8088) (Dec 1986); annual 68K issue (Jan 1987); "Macintosh Buttons and Amiga Gadgets" (Jan 1987); "Text Editors: In Matters of Taste ..." (the baby duck syndrome) (Feb 1987); "Artificial Intelligence" (Feb 1987); "Hashing for High Performance Searching" (Feb 1987).

Colleagues who are tempted to program in the C language would appreciate the extensive article, "Benchmarking C Compilers," by Relph, Hahn, and Viles in the August 1986 issue of Dr. Dobb's Journal. Seventeen C compilers were tested, and tables of benchmarks were provided of regular EXE time, floating-point EXE time, and memory-model EXE time. The Dr. Dobb's article states the following about Microsoft C: "Microsoft doesn't take many steps, but the ones it takes are big ones. Last year, just before we started working on our review, it discontinued marketing a repackaged Lattice compiler and released its own product. In one step it went from als-ran status to supplying the most professional package with perhaps the best C compiler available ... Now, just barely in time for this year's review, comes a beta copy of the upcoming Microsoft C, Version 4.0, and it is another bit step."

Computer magazine, the flagship publication of the IEEE Computer Society, generally requires a higher degree of literacy in computer science and engineering than many other computer magazines. The best way to treat the year of magazines at hand is to list issue themes that may be of interest: "An Introduction to GaAs Microprocessor Architecture for VLSI" (Mar 1986); Design Automation (integrated circuits, languages, analog circuits) (Apr 1986); Computer Science Education in the U.S. (Jun 1986); Expert Systems in Engineering (Jul 1986); Domesticating Parallelism (parallel processors) Aug 1986; "Peak vs. Sustained Performance in Highly Concurrent Vector Machines" (Sep 1986); GaAs Microprocessor Technology (Oct 1986); New Computers for Artificial Intelligence Processing" (Jan 1987).

An article by Ware Myers, an experienced contributing editor to **Computer**, "Getting the Cycles out of a Supercomputer," is concerned with writing software that maximizes productivity, the central problem of supercomputer use. See pages 89-93, 100 in the March 1986 issue. Tables 1 and 2 illustrate how the "minisupers" stack up.

Extra tracks, extra sectors, fake sectors, spiral tracking, supersectors (write-splicing), sector alignment, wide tracks, and weak bits. For those of you who are interested in how manufacturers copy protect disks, these are the techniques discussed in "How disks are 'padlocked'" on pages 32-40 in the June 1986 issue of **IEEE Spectrum**. An interesting and superbly illustrated article.

The **IEEE Spectrum** special January 1987 issue on "Technology '87" contains articles on: minis and mainframes, personal computers, software, design automation, communications, solid state, instrumentation, industrial electronics, power and energy, consumer electronics, transportation, aerospace and military, medical electronics, and the specialities. An excellent issue that provides perspective on a wide range of topics.

The **IEEE Spectrum** special May 1986 issue on "Personal Computers: Lessons Learned" is also worth reading. Six feature articles are dedicated to this topic.

IEEE Spectrum, which is sent to the more than 200,000 members of the IEEE, is one of the finest technical magazines published. Articles of potential interest include: "The compact disk ROM: how it works" (Apr 1986); "The compact disk ROM: applications software" (Apr 1986); "MAP protocols for communicating in the factory" (Apr 1986); "Optical dectors: three contenders" (May 1986); "Communicating from the edge of the solar system" (Jun 1986); special issue on "Peacekeeping by technical means" (Jul 1986); special issue on "Optical computing: a field in flux" (Aug 1986); "Burning coal more cleanly and efficiently" (Aug 1986); "Amorphous silicon: from promise to practice" (Sep 1986); "Transducers: Optical-fiber sensors challenge the competition" (Sep 1986); "The lure of molecular computing" (Oct 1986); "Expert systems: Software 'doctor' prescribes remedies" (Oct 1986); "A framework for computer design," which makes the point that instead of starting off with a microprocessor, equipment designers must now choose a bus standard before hardware and software (Oct 1986); "Making your PC behave like another" (Oct 1986); "Discrete-event simulation" (Dec 1986); "Helping engineers help themselves" (Dec 1986); "Coherent optical detection: a thousand calls on one circuit (Feb 1987); and "Designing micro-based systems for failsafe travel" (Feb 1987).

"With this issue (July 10, 1986), **Electronics** returns to a biweekly publishing schedule." So ends an ill-fated transition to a weekly, with reduced technical detail in articles, that represented a classic editorial misjudgement by McGraw-Hill. **Electronics** is back, almost, as one of the finest magazines in its field. The publisher continues: "For example, you proved that we are right when we boast of having the most loyal readers in the business." In a telephone survey of several thousand readers (from among 300,000 subscribers), editors learned the following: 92% read each issue from cover to cover, 81% placed technology news at the top of the list, 79% voted for in-depth technology developments and analysis, 43% voted for business and industry news, and 22% voted for company and marketing strategy. Perhaps there are lessons to be learned from this reader survey that can be applied to chemical engineering magazines.

Electronics' annual Technology Outlook is in the October 16, 1986 issue of **Electronics**. Topics covered include computers, microsystems, software, semiconductors, chip processing, telecommunications, data communications, CAD and CAE, test and measurement, packaging, manufacturing, and consumer products.

For the hardware oriented among you, here is a list of articles of potential interest from **Electronics**. "How the PC is changing testing" (Mar 24, 1986); "At last: Parallel-engine benchmarks" (Apr 7); "VLSI gives bipolar a second wind" (Apr 7); "Motorola tailors a DSP for filtering" (Apr 21); "Speech processing: hearing better, talking more" (Apr 21); "Ultradense chips: the drive quickens" (Apr 28); "Is RISC a good idea or just hype?" (May 5); "How IBM designed its RISC-technology PC" (May 5); "A 3-way tug of war hits 32-bit micro business" (May 5); "NASA hangs in with space-factory program" (May 5); "Apple finally gives up: it's adding MS-DOS to the Mac" (May 12); "Intel graphics IC targets CAD and business use" (May 19); "Solid-State sensors tap IC technology to add functions," an interesting article (Jun 2); "This could be the year that clones outsell IBM" (Jun 9); "Turning a PC into a silicon compiler" (Jun 16); "Long live the minicomputer!" (Jun 16); 65,000 processors tackle biggest data jobs," an article on the Connection Machine from Thinking Machines Corp. (Jun 23); "Multibus II heads for the fast track" (Jul 10); "A new class of DSP chip--vector signal processors" (Jul 24); "At last, it's easy to design RS-232C modems" (Jul 24); "The boom starts in smart power products" (Jul 24); a nifty new electronic device, the Motorola SENSEFET, is advertised on page 23 (Aug 7); "What's holding back expert systems?" (Aug 7); "A new way to speed up circuit simulation," an algorithm called Cinnamon that outruns the Spice2 circuit simulator by 100 to 1 (Aug 7); "The exploding role of nonvolatile memory" (Aug 21); "DSP boards tackle a tough class of Artificial Intelligence tasks" (Aug 21); "Software is the challenge in better graphics" (Sep 4); "GaAs LSI goes commercial" (Sep 18); "What makes Compaq's new PC so important?" (Sep 18); "First look at Motorola's latest 32-bit processor, the 68030" (Sep 18); "Texas Instrument's blazing-fast CMOS logic takes on Schottky bipolar" (Sep 18); "This smart power chip breaks the 100-V barrier" (Oct 2); "The Apple II: Teaching an old dog new tricks" (Oct 2); "A new easy way to design ASICs" (Oct 16); "How Weitek's chips run Fortran and C at 25 megaflops" (Oct 30); "How to boost floppy-disk capacity to 11 megabytes" with standard 5¼-inch floppies (Nov 13); "This CPU does floating point faster than any 2-chip set," a story on the T800 single-chip transputer, which has a speed of 4 million single-precision Whetstone instructions per second (Nov 27); "Will smart cards create a billion dollar IC business?" (Dec 18, 1986); "How designers are building denser linear ICs" (Dec 18); "Everyman's LAN: fast, easy to install, affordable," about the 1 megabyte/sec TOKENSTAR network that uses phone lines and costs $130 per connection (Jan 8, 1987); "How to boost an IBM PC to 4 MIPs" (there is a catch: it has to be programmed in Forth) (Jan 8); "A modem chip that needs only one 5-V power supply" (Jan 8); "Intel's $35 chip set has Hayes modem commands in firmware" (Jan 22); "What's new in laboratory instruments: Traditional products get squeezed by newer gear" (Feb 5).

Have you kept up with amazing developments in superconductors in recent months? A brief summary of superconductor research and development is reported in the Feb 19, 1987 issue of **Electronics**, pp. 54-56. New ceramics that contain compounds of lanthanum, barium or strontium, copper, and oxygen are producing critical temperatures above 30 and 40 degrees Kelvin. A superconductor that operates above the boiling point of liquid nitrogen would likely lead to revolutionary developments in electronics and computer hardware. Its discovery was announced on CBS News on February 19, 1987. Look for a discussion of this exciting work in **Science**.

The smart memory is a new breed of logic-memory chip that is beginning to take over special-purpose tasks from the high-volume, 'jelly-bean' chips such as DRAMs. What are these strange new electronic beasties? Examples are the VT16AM8 dual-port SRAM, with one port being 8 bits wide and the second being 16 bits wide; multiport video dynamic RAMs; multiport static RAMs; semaphore RAMs; SRAM-based first-in, first-out (FIFO) buffers; content-addressable memories (CAMs); cache-tag RAMs; and cache-data RAMs. Read all about them in **Electronics**, Feb 5, 1987, pp. 65-69.

The contents of **Byte** magazine can be summarized in terms of the theme of each issue: "Number Crunching" (micro-based supercomputer, computer approximations, inversion of large

matrices, Runge-Kutta methods, and the ATOMCC Toolbox) in April 1986; "Optical and Other Types of Mass Storage" (evolution of mass storage, CD-ROM software development, application interface of optical drives, optical disk error correction, roundup of optical disk drives, tape backup systems, and laser libraries) in May 1986; "Computers and Music" (music software, digital music synthesis, digital sampling on the Macintosh, musical fractals, MIDI project) in June 1986; the "Engineer's Toolbox" (computer circuit simulation, analog circuit analysis, structural analysis, stress analysis, material selection, small-scale engineering applications) in July 1986; "Object-Oriented Languages" (object-oriented programming, Smalltalk, objects, icons, software ICs, object-oriented languages for the Macintosh, programming experiences, object-oriented FORTH) in August 1986; "68000 Machines" (UNIX and the MC68000, trips and traps, comparison of MC68000 family processors, Atari ST software development, Amiga animation, Amiga vs Macintosh) in September 1986; "Public Domain Powerhouses" (PD PROLOG, an icon tutorial, enhanced console driver, Abundance--a FORTH-based database language that can run backward in time, Z80MU, CP/M hall of fame) in October 1986; "Representing Knowledge" (finding rules in data, bit-mapped classifier, handling conflicts in data, art of deduction, rule-based programming, machine learning) in November 1986; "Graphics Algorithms" (Henon mapping with Pascal, abstract mathematical art, TMS34010 graphics system processor, plotting the Mandelbrot set, graphic quadric surfaces, free-form curves on your micro) in December 1986; "Programmable Hardware" (overview, introduction to programmable array logic, getting started with PALs, microcoded vs. hard-wired control; PALs simplify complex circuits; a PAL programmer) in January 1987; and "Educational Computing" (using computers for instruction, the difference in higher education, the quiet revolution, educational software, potential for interactive technology) in February 1987.

Notable quote: "The flood of word processors for MS-DOS machines continues." See August 1986 **Byte**, p. 319.

Other useful articles in issues of **Byte** include: "Software review: PCTEX and MicroTEX," two typesetting packages (Apr 1986, pp. 267-272); "68000 Wars: Rounds 2 and 3" (May and Nov 1986); "Decoding MacPaint on the IBM PC" (Jun 1986); "Five Laboratory Interfacing Packages: SALT, LABPAC, PCLAB, Labtech Notebook, ASYST, and ILS" (Jul 1986, pp. 303-312); "The Definicon 68020 Coprocessor, Parts 1 and 2," which provides 32-bit computing power as a plug-in board to an IBM PC (Jul and Aug 1986); "Mathematics of Programming," the text of a speech given by C.A.R. Hoare at the Boston Computer Museum on Byte's 10th anniversary celebration (Aug 1986); two reviews of Turbo Prolog (Sep 1986); "Real Time under Real Pascal" (Sep 1986, pp. 145-154); "Product Review: The COMPAQ Deskpro 386" (Nov 1986); "Product Preview: Lotus Manuscript" (Nov 1986); "Memory Management Units for 68000 Architectures" (Nov 1986); "A Program for Approximating Integrals" (Dec 1986); "Using DOS Functions from Turbo Pascal" (Dec 1986); "An Introduction to Relaxation Methods" (Jan 1987); "Look it Up Faster with Hashing" (Jan 1987); "High-Performance Software Analysis on the IBM PC" (Jan 1987); "Speed and Compatibility Tests on 12 IBM PC AT Compatibles" (Jan 1987); and "Another Approach to Data Compression (Nyquist Sampling Theorem)" (Feb 1987).

Chemical NAND gates and memories? A news item in Microbytes (**Byte**, Aug 1986, p. 9) reports on Carnegie-Mellon University chemistry research. The NAND gate is based on two cyanine/quinone complexes joined to a porphyrin molecule. If both cyanine groups are excited by two lasers, the porphyrin molecule becomes excited. The excited porphyrin can in turn excite a chromaphore molecule that can be read by a third laser or serve as an input for another NAND gate. The memory is based upon a three-molecule cluster of the biological molecule, bacteriorhodopsin, that can hold a single bit of data. The triad exists in two states, each of which absorbs light at a different frequency. The state of each molecule can be read and flipped with a laser tuned to one of these frequencies.

How about lab simulators? Vose and Williams report on "LabVIEW, a laboratory virtual instrument engineering workbench" that exploits Macintosh graphics in **Byte**, Sep 1986, pp. 84-92. LabVIEW today, no lab instructors tomorrow.

An interesting software product that is described in **Byte**, Sep 1986, pp. 299-300 is Software Carousel, a virtual memory manager that allows you to shift between programs instantly. Costs $49.95, and is available from SoftLogic Solutions, Inc., 530 Chestnut St., Manchester, NH 03101, (603) 627-9900. A hard disk is recommended but not required.

Are you curious about "The State of Soviet Microelectronics"? If so, read an article with this title in the Nov 1986 issue of **Byte**, pp. 137-143. Undergraduate engineering students at my university probably have more IBM PCs and clones than can be found in all of Moscow.

SUPERCRITICAL FLUID EXTRACTION LESSON

The supercritical fluid extraction lesson is an educational computer program developed for an IBM PC. The program introduces design concepts to undergraduate chemical engineering students while at the same time teaching them about supercritical fluid extraction, a relatively new separation process. The lesson is divided into three parts. The first two sections introduce the student to the theory of supercritical extraction and explain how to design the process. Part III of the lesson consists of a menu driven program that allows the student to design a simplified supercritical extraction process. With the easy to use menus and on-screen instructions, students may easily vary any of the design parameters such as flowrates, compositions, pressure, temperature, and solvent to feed ratio.

For more information contact:

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220 S. 33rd St.
Philadelphia, PA 19104-6393

CALL FOR PROPOSALS FOR THE PREPARATION OF A CACHE PROCESS DESIGN CASE STUDY

Over the course of the last two years the CACHE Process Design Case Study Task Force has published the following three case studies:

1. Separation System for Recovery of Ethylene and Light Products from a Naphtha Pyrolysis Stream.
2. Design of an Ammonia Synthesis Plant.
3. Design of an Ethanol Dehydrogenation Plant.

These case studies which were developed entirely by members of the task force have been well received. As a result CACHE is seeking to expand the project to include high quality contributions from our faculty colleagues at large.

Therefore we are seeking proposals for the development of a CACHE Process Design Case Study and are willing to provide funds up to a maximum of $5,000. This money can be used, for example, to pay the stipend of an undergraduate/graduate student, to contribute to the summer salary of the supervisor or to cover other office expenses.

Proposals involving nontraditional chemical engineering tasks, e.g., semi-conductor processing, bio-processing and materials will be given preference. Projects with industrial participation are viewed favorably. Proposals should be directed to Professor Manfred Morari, Chemical Engineering 206-41, Caltech, Pasadena, CA 91125 and Professor Ignacio E. Grossmann, Dept. of Chemical Engineering, Carnegie-Mellon University, Pittsburgh, PA 15213.

As a reminder, the goal of the Design Case Study Task Force is the development of case studies to aid process design education. Though no two design problems are alike, there is a general logical sequence of basic steps which lead to a good design. It is the chief objective of the CACHE Case Studies to demonstrate and elucidate this thought and decision process. The CACHE Case Studies should be different from final student or industrial project reports in that they do not only present one final solution, but show the whole solution procedure leading from the problem statement to the final solution(s) in an organized manner. Within that philosophy, neither the scope is fixed nor is the methodology limited. Eventually, a library of case studies is sought ranging from small ones to large ones and covering a variety of design aspects.

For more details, please contact Manfred Morari or Ignacio Grossmann.

ANNOUNCEMENT

Two enhancements to DSS/2 were recently completed that might be of interest:

(1) A set of subroutines and associated test problems for computing second derivatives directly, rather than by stagewise differentiation, in the solution of second-order partial differential equations (PDEs). Initial experience has indicated that the new subroutines produce solutions to PDE problems when stagewise differentiation either fails or gives solutions with spurious effects.

(2) A set of subroutines and associated test problems for orthogonal collocation on finite element solutions to PDE problems, on one and two-dimensional spatial domains. Orthogonal collocation is a well established numerical method in engineering research for the solution of PDE problems, but has the reputation of being complicated and difficult to apply to each new problem. The new subroutines essentially automate orthogonal collocation and therefore make it straightforward to use.

Each set of software is thoroughly documented internally with comments, and includes a set of test problems to demonstrate the use of the software, and verify that it is working correctly on the user's local computer(s). The software is written as single and double precision Fortran 77 source code, and can be provided on nine-track tape or 360 kb diskettes. The price is $125.00 for each set.

Please direct any questions you may have about the software to the following:

Professor W.E. Schiesser
Lehigh University
Whitaker Laboratory 5
Bethlehem, PA 18015
(215) 758-4264

COMPARISON OF OPERATING SYSTEM COMMANDS FOR SEVERAL DIFFERENT COMMONLY USED COMPUTERS

J.D. Seader
University of Utah

On March 28, 1985, CACHE issued a position paper entitled, "Expectations of the Competence of Chemical Engineering Graduates in the Use of Computing Technology." This paper has attracted much attention among educators, ABET, and AIChE. Among the expectations listed and discussed in the paper, one is, "...the chemical engineering graduate must be familiar with at least one operating system for personal and mainframe computers." A significant aspect of this expectation is that, like programming languages, different operating systems have many types of commands in common. Thus, once one learns what can be done with one operating system, one can quite readily learn the commands of another operating system. This is particularly true with respect to the following types of operating system commands:

1. Logging on and off
2. File specifications
3. Use of wildcard characters
4. Managing directories and files
5. Creating and editing files
6. Running program, command, and executable files

The accompanying table (on page 25) compares these types of commands for five commonly used operating systems: DEC VMS, UNIX, Univac EXEC, IBM VM/CMS, and IBM PC-DOS (and MS-DOS). It may prove useful as a reference for those who must use two or more different operating systems.

Comparison of Operating System Commands for Different Campus Computers

Command	ChE MicroVAX	GOULD 9080	UNIVAC 1100/72	IBM 4381	IBM PC
LOGGING IN	Username: Password:	login: password:	Enter Userid/Password;	Type L userid ENTER PASSWORD	No account or password needed
OPERATING SYS.	VMS	UNIX 4.2	EXEC 8	VM/CMS	PC-DOS or MS-DOS
OPER. SYS. PROMPT	$	n vlsi>	>	====>	A>, B>, C>etc.
LOGGING OFF	LOGOUT	logout	@FIN	LOG	No loggoff needed
OBTAIN ON-LINE HELP	HELP	man command	@HELP	HELP HELP	No help facility
FILE SPECIFICATION	node-name :: storage device: [dir-name] file-name. file-type; version	/dir-name /subdir-name /sub-subdir-name /file-name	qualifier* file dir-name file-name	filename filetype filemode	drive: filename. extension
WILDCARD CHARACTERS	*%	*?	$	*	*?
SHOW CURRENT DIRECTORY	SHOW DEF	pwd	@DIR, N	Always stay	CD
CREATE A DIRECTORY	CREATE/DIR [dir-name]	mkdir dir-name	@CAT,P dir-name	in current	MD dir-name
MOVE TO A DIRECTORY	set def [dir-name]	cd dir-name	@CONNECT dir-name	directory	CD\dir-name
LIST A FILE	TYPE file	cat file	@PRINT file	x file	TYPE file
PRINT A FILE	PRINT file	lpr file	@PRINT,C file	PR file	PRINT file
CREATE AND EDIT A FILE	EDIT file	jove file	@EDIT file	XEDIT file	EDLIN file
EDITOR PROMPT	*	No prompt	n*	No prompt	*
EXIT THE EDITOR	<ctrl/z> EXIT	<ctrl/x> <ctrl/z>	E	FILE	<ctrl/z> E
APPEND ONE FILE TO ANOTHER	APPEND file1 file2	cat file1 >> file2	Must be done in the editor	file1 file2 (AP	COPY file1 + file2
COPY A FILE	COPY file1 file2	cp file1 file2	@EDIT file1, file2 E	COPY file1	COPY file 1 file 2
RENAME A FILE	REN file1 file2	mv file1 file2	@CHG,S file1, file2	RENAME file1 file2	REN file1 file2
DELETE A FILE	DEL file	rm file	@SCRATCH file	ERASE file	DEL file
LIST FILES IN CURRENT DIRECTORY	DIR	ls -a	@DIR, L	FILEL	DIR
FORTRAN COMMANDS:					
COMPILE	FORTRAN file	f77 file.f -o fileout	@COMPILE, file	RUNFORT	PROFORT file
LINK	LINK file1, file2		@LINK file		LINK file1, file2
RUN	RUN file		@XQT file		file
RUN A COMMAND FILE	@file	source file	@ADD file	file	file
RUN AN EXECUTABLE FILE	file	source file	@XQT file	file	file

FLOWTRAN OPTIMIZATION PROJECT

L.T. Biegler
Carnegie-Mellon University
Large-Scale Systems Task Force

At the last two CACHE receptions a FLOWTRAN optimization option was described as part of the poster presentation. The Large-Scale Systems Task Force is pleased to announce that work on the FLOWTRAN option has been completed. FORTRAN source code for this package will be available at nominal cost and will probably be distributed via BITNET. Final decisions regarding availability and distribution of this software, however, will be made at the CACHE trustees' meeting this summer. Moreover, documentation on the optimization option will be included in the next edition of the FLOWTRAN manual, which is currently in the last stages of production and should be available by this summer.

The FLOWTRAN optimization option was developed at Carnegie-Mellon University and is based on state-of-the-art SQP (Successive Quadratic Programming) algorithms. It allows for a great deal of flexibility in posing the optimization problem and in choosing the appropriate strategy for solving the problem efficiently. Since its development the code has been tested on a number of computers at various locations, including:

Carnegie-Mellon University, VAX 11/780, VAX 8650, MicroVax II
Monsanto Corporation, IBM 30XX
Purdue University, IBM 43XX
University of Pennsylvania, VAX 11/750
University of Utah, UNIVAC 1100/71

A battery of seven optimization problems has been solved successfully at all testing sites.

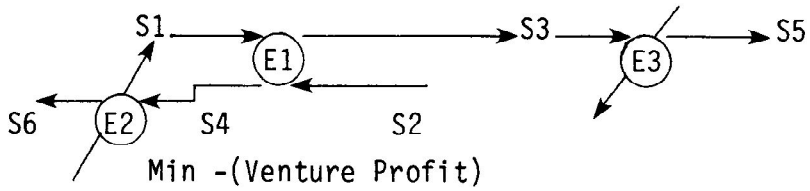
At this stage, potential users will probably be interested in the answers to the following questions:

- How easy will it be install the optimization option on my current version of FLOWTRAN?

- How easy will it be for me (and my students) to set up and solve flowsheet optimization problems with this option?

The answer to the first question depends to some extent on the particular FLOWTRAN implementation you have, but it is conceptually no different than adding a user-written FLOWTRAN block. Most users will find it convenient to keep the optimization block in compiled (relocatable or object) form and link it to FLOWTRAN at run time. This can be done simply by modifying the LINK (or equivalent) statement in the FLOWTRAN command file. This was very easy to do on the implementations tested above. You may want to consult your systems programmer or user consultant if you foresee any problems in your particular implementation.

The second question is perhaps best answered by considering a very simple optimization problem. Posed by Prof. Seader and presented in the figure below, this one variable optimization maximizes the venture profit for three heat exchangers by adjusting the approach temperature of E1.



Min -(Venture Profit)

s.t. temp in S4 ≤ 300 °F
temp in S3 ≤ 100 °F

For FLOWTRAN input the optimization block is treated as any other NEW BLOCK and is either added at the end of the calculation sequence (as in this example) or is substituted for the stream convergence block when tear streams are present. Without the optimization block, the example can be simulated on FLOWTRAN using the following input data.

```
TITLE HEAT EXCHANGER SIMULATION
PROPS 2 1 2 1 1
PRINT TABLES INPUT
RETR TOL STYR

BLOCK E1 EXCH3 S1 S2 S3 S4
BLOCK CE1 CEXC3 E1
BLOCK E2 HEATR S4 S6
BLOCK CE2 CHETR E2
BLOCK E3 HEATR S3 S5
BLOCK CE3 CHETR E3

PARAM E1 1 25 5 5 50 1 1 0
PARAM CE1 1 -2 1 1 1 335
PARAM E2 1 350 5 0 0 1
PARAM CE2 1 -2 1 1 1 335 1000 75 366
PARAM E3 1 100 5 0 0 1
PARAM CE3 1 -2 1 1 1 335 200 75 80 20

POUNDS S1 2 25000
POUNDS S2 1 25000
TEMP S1 300
TEMP S2 100
PRESS S1 50
PRESS S2 90

END CASE
END JOB
```

Note that here no recycle streams are present and the calculation sequence is fairly straightforward. To solve the optimization problem posed in the figure, the FLOWTRAN input file is expanded to include the optimization block SCOPT, additional PUT statements as well in-line FORTRAN statements need to be added. This is described in detail in the next edition of the FLOWTRAN manual. The resulting input file (with appropriate comments) then becomes:

```
TITLE HEAT EXCHANGER OPTIMIZATION
PROPS 2 1 2 1 1
PRINT TABLES INPUT
RETR TOL STYR
```

```
C
C **** INCLUDE NEW STATEMENTS FOR NEW OPTIMIZATION BLOCK
C
NEW BLOCK SCOPT 160 1 3 3 2
DIM   COMMON/OPTVAR/ID(40), SV(10), C(50), FX
DIM   COMMON/OPTCNT/IPASS, INF, DELTA, ST(10),V(40),ORD(40)
DIM   INTEGER V,ORD
DIM   COMMON/CONTRL/N, KOUT, KSKIP, KONV

C
C **** IDENTIFY DECISION VARIABLE
C
F 600 ID(1) = IDTA

BLOCK E1 EXCH3 S1 S2 S3 S4
BLOCK CE1 CEXC3 E1
BLOCK E2 HEATR S4 S6
BLOCK CE2 CHETR E2
BLOCK E3 HEATR S3 S5
BLOCK CE3 CHETR E3
C
C **** SET UP OPTIMIZATION PROBLEM USING IN-LINE FORTRAN
C **** USE VENTURE PROFIT AS OBJECTIVE FUNCTION
C
F     CAPC = RRRRR(CCE3) + RRRRR(CCE2) +RRRRR(CCE1)
F     UTILC = (RRRRR(CUE3)+RRRRR(CUE2) + RRRRR(CUE1)) * 8000.
F     FX = 0.5*CAPC +UTILC
C
C **** INCLUDE TWO INEQUALITY CONSTRAINTS FROM PROBLEM
C
F     C(1) = S4(4) - 300.
F     C(2) = S3(4) - 200.

C
C **** ADD SCOPT BLOCK
C
BLOCK OPTIT SCOPT 3*0 E1 3*0 600
C
C **** ADD PUT STATEMENTS TO IDENTIFY DECISION
C **** AND RETENTION VARIABLES
C
PUT PDEX E1 1 IDTA
PUT RDEX CE1 1 CCE1
PUT RDEX CE2 1 CCE2
PUT RDEX CE3 1 CCE3
PUT RDEX CE1 2 CUE1
PUT RDEX CE2 2 CUE2
PUT RDEX CE3 2 CUE3

PARAM CE1 1 -2 1 1 1 335
PARAM E2 1 350 5 0 0 1
PARAM CE2 1 -2 1 1 1 335 1000 75 366
PARAM E3 1 100 5 0 0 1
PARAM CE3 1 -2 1 1 1 335 200 75 80 20
```

```
C
C **** SPECIFY PARAMETERS FOR SCOPT BLOCK
C
PARAM OPTIT 1 0 1 0 2
PARAM OPTIT 10 0.0005
PARAM OPTIT 16 1
PARAM OPTIT 56 1
PARAM OPTIT 106 50

POUNDS S1 2 25000
POUNDS S2 1 25000
TEMP S1 300
TEMP S2 100
PRESS S1 50
PRESS S2 90
END CASE
END JOB
```

Although quite a few statements have been added to the input file, these are as easy to specify as any other FLOWTRAN simulation task. This file now produces the following output.

```
UNIT TABLE
    UNIT NAME   UNIT TYPE
      E1          EXCH3
      CE1         CEXC3
      E2          HEATR
      CE2         CHETR
      E3          HEATR
      CE3         CHETR
      OPTIT       SCOPT

FLOW TABLE
  STREAM NAME  FROM
       S1                E1
       S2                E1
       S3       E1       E3
       S4       E1       E2
       S5       E3
       S6       E2

INPUT STREAMS
       S1
       S2
OUTPUT STREAMS
       S5
       S6
                                                          8-FEB-87

HEAT EXCHANGER OPTIMIZATION
PHYSICAL PROPERTY OPTION
   ANTOINE VAPOR PRESSUR
   REDLICH-KWONG VAPOR FUGACIT
   UNCORRECTED LIQUID FUGACIT
   IDEAL SOLUTION ACTIVITY
```

```
    OPTIMAL SOLUTION FOUND AFTER     8 ITERATIONS
    KUHN-TUCKER ERROR IS           0.372649E+02
    AT FINAL ITERATION,  OBJECTIVE FUNCTION IS  0.943332E+05

    DECISION VARIABLES
 0.119451E+02

    INEQUALITY CONSTRAINTS
-0.119451E+02 -0.842856E+02

    FINAL PROCESS REPORT OF OPTIMAL POINT FOLLOWS...

                                                                  8-FEB-87

HEAT EXCHANGER OPTIMIZATION


E1     - EXCH3 - HEAT EXCHANGED =  0.2142E+07 BTU/HR
    CORRECTED  LMTD (DEG F) =    13.74 , OVERALL U =  50.0
    CALCULATED AREA (SQ FT) =  3116.36
    INLETS =   S1          S2        OUTLETS =    S3          S4
    DEG F     300.00      100.00                 115.71      288.05
CE1   (EXCHC)  COST FOR EXCHANGER UNIT E1
    TYPE OF EXCHANGER    -2.00     MAT OF CONST FACTOR       1.00
    PRESSURE FACTOR       1.00     TUBE LENGTH FACTOR        1.00
    COST INDEX           335.0     UTILITIES COST FACTOR    0.000
    EXCHANGER AREA FT2  3116.36     EXCHANGER DUTY BTU/HR  2141515.
    EXCHANGER COST,    $ =     41980.00
    UTILITIES COST, $/HR =         0.00
E2     - HEATR - INLET = S4    , OUTLET = S6
    OUTLET TEMP =  350.00 DEG F , PRESSURE DROP =    5.00 PSI
    DUTY =  0.8118E+06 BTU/HR
CE2   (EXCHC)  COST FOR EXCHANGER UNIT E2
    TYPE OF EXCHANGER    -2.00     MAT OF CONST FACTOR       1.00
    PRESSURE FACTOR       1.00     TUBE LENGTH FACTOR        1.00
    COST INDEX           335.0     UTILITIES COST FACTOR  *******
    EXCHANGER AREA FT2   276.66     EXCHANGER DUTY BTU/HR   811750.
    EXCHANGER COST,    $ =      7410.00
    UTILITIES COST, $/HR =         8.12
E3     - HEATR - INLET = S3    , OUTLET = S5
    OUTLET TEMP =  100.00 DEG F , PRESSURE DROP =    5.00 PSI
    DUTY = -0.1639E+06 BTU/HR
CE3   (EXCHC)  COST FOR EXCHANGER UNIT E3
    TYPE OF EXCHANGER    -2.00     MAT OF CONST FACTOR       1.00
    PRESSURE FACTOR       1.00     TUBE LENGTH FACTOR        1.00
    COST INDEX           335.0     UTILITIES COST FACTOR  200.000
    EXCHANGER AREA FT2   123.01     EXCHANGER DUTY BTU/HR   163948.
    EXCHANGER COST,    $ =      4150.00
    UTILITIES COST, $/HR =         0.33
```

8-FEB-87

HEAT EXCHANGER OPTIMIZATION

STREAM NAME:	S1	S2	S3	S4	S5
	LBMOL/HR	LBMOL/HR	LBMOL/HR	LBMOL/HR	LBMOL/HR
1 TOLUENE	0.0	271.344	0.0	271.344	0.0
2 STYRENE	240.052	0.0	240.052	0.0	240.052
TOTAL LBMOL/HR	240.052	271.344	240.052	271.344	240.052
TOTAL LB/HR	25000.0	25000.0	25000.0	25000.0	25000.0
1000 BTU/HR	-1453.20	-3711.78	-3594.72	-1570.27	-3758.67
DEGREES F	300.00	100.00	115.71	288.05	100.00
PSIA	50.000	90.000	45.000	85.000	40.000
DENSITY, LB/FT3	48.7021	53.1678	54.9814	46.5569	55.5012
MOLE FRAC VAPOR	0.0000	0.0000	0.0000	0.0000	0.0000

STREAM NAME:	S6
	LBMOL/HR
1 TOLUENE	271.344
TOTAL LBMOL/HR	271.344
TOTAL LB/HR	25000.0
1000 BTU/HR	-758.52
DEGREES F	350.00
PSIA	80.000
DENSITY, LB/FT3	44.0463
MOLE FRAC VAPOR	0.0000

As can be seen, the output gives a clear description of the process at its optimum point. Further information about the optimization for diagnostic purposes can be found in the HISTORY file which has not been included here. The program was run using most of the default specifications for SCOPT. Advanced users will also be able to take advantage of a number of options that enhance FLOWTRAN's simulation and optimization capabilities. These include:

- simultaneous convergence of control loops and tear streams by either Broyden or Newton methods.

- full flowsheet optimization using the infeasible path approach.

- variants of the infeasible path approach include the complete feasible variant (CFV) and embedded Broyden optimization (EBOPT).

As mentioned above, the program, with all necessary documentation, will be available before the fall semester. More complete information regarding costs and distribution will be available in the next newsletter. We also look forward to the application of this optimization program in undergraduate and graduate curricula and invite comments, questions and experience on test problems from interested chemical engineering faculty.

STATUS OF FLOWTRAN LOAD MODULES FOR UNIVERSITY COMPUTERS

J.D. Seader

As part of a continuing program of support to education, Monsanto Company announced on August 19, 1982, that load modules for the FLOWTRAN simulation program would be made available on magnetic tape to departments of chemical engineering to install on their own in-house computers. Thus, departments would be able to run FLOWTRAN on their own computers at no charge other than that of their own computer center. CACHE is continuing the supervision of the preparation of FLOWTRAN load modules for a wide variety of main-frame, supermini, and supermicro-type digital computers and the distribution of the modules on magnetic tape to those departments that order them. Instructional books on FLOWTRAN are already available through CACHE by using the order form at the end of this newsletter.

FLOWTRAN tapes are now available for the following computers:

1. **DEC VAX** computers running with the VMS operating system.
2. **DEC 20XX** mainframe computer running with the FORTRAN-20, Version 7 compiler (9-track, 1600 BPI tape).
3. **UNIVAC 1100** series computers running under the EXEC 1100 (38R2/08) operating system with the FORTRAN 77-SID (1OR/A) compiler (9-track, 1600 BPI tape).
4. **Amdahl** computers running under the MTS (Michigan Terminal System) operating system with a FORTRAN Level G or H compiler (9-track, 6250 BPI tape).
5. **IBM** and IBM-Plug-Compatible mainframe computers such as the 370, 30XX, and 43XX with the following operating system and FORTRAN compiler combinations:

Version	Operating System	FORTRAN Compiler
a	VM/CMS	VS
b	OS1/MVS	IV-H ext
c	OS/VS2 MVS	VS
d	CMS	IV-G1

6. **IBM PC-XT-370** personal computer operating in conjunction with an IBM mainframe.
7. **CDC Cyber** mainframe computers with the NOS operating system and a FORTRAN V compiler.
8. **Apollo Domain** with stations running with AEGIS operating system (program on floppy disks).
9. **Data General MV** superminicomputer running with AOS/VS operating system.
10. **DEC MicroVAX II** with the VMS operating system.
11. **Honeywell** computers with CP6 operating system.

Conversions are also underway for the Sun workstation, DEC 10, Sperry 90/80, DEC VAX under UNIX, and Prime machines. Each FLOWTRAN tape contains either load and/or relocatable code, test problems and solutions, and installation instructions. The FLOWTRAN program may be used for educational purposes, but not for consulting. A total of 147 FLOWTRAN tapes have already been distributed. The following universities have received FLOWTRAN during the current academic year:

University	Computer	Operating System
Univ of Dayton	DEC MicroVAX II	VMS
Univ of Louisville	IBM 3081D	VM/CMS
Tulsa Univ	Honeywell T6600	CP6
Youngstown State	Amdahl 5868	VM/CMS
Univ do Porto	CYBER 170-720	NOS 2.0
Indian Inst Tech Kharagpur	Apollo Domain	AEGIS
Northeastern Univ	Sun-3/160C-P2	UNIX V2.0
Carnegie-Mellon	DEC MicroVAX II	VMS

If you would like to obtain a FLOWTRAN tape for your computer and have not already expressed that desire to CACHE, complete and submit the form, FLOWTRAN TAPE, at the end of this newsletter. You will be required to sign a User's Agreement that must be approved by Monsanto. The cost of the tape, payable to CACHE, is $250. However, the charge to CACHE-supporting departments listed near the end of this newsletter is only $175.

MICROCACHE SOFTWARE-MODULE MATBAL

Brice Carnahan
The University of Michigan

We have now distributed the basic MicroCACHE software and an assortment of modules produced at The University of Michigan to nearly thirty schools in the U.S., Canada, and Europe. Sales continue at a modest but encouraging rate (see ORDER FORM at the end of the News).

Recently, we received the first non-Michigan module named MATBAL, authored by PROF. DENIZ KARMAN of the Chemical Engineering Department at the University of New Brunswick in Fredericton, NB. This is a very attractive module for introducing students in the first chemical engineering course to open and closed systems, identification of the SYSTEM for analysis, selection of UNITS and a BASIS, MASS and MOLE FRACTIONS, and the writing of MATERIAL BALANCES (for open steady-state processes with reaction).

A chlor-alkali plant consisting of three principal subsystems:

A) brine saturation and purification,
B) electrolysis, and
C) amalgam-decomposition,

is used as the teaching vehicle. Any of seven subsystems (A, B, C, A+B, A+C, B+C, and A+B+C) can be chosen for analysis.

The calculation basis can be selected from several species quantities (e.g., salt charged, caustic or chlorine produced) or time period (hour or day). Mass units can be any of the following: gm, kgm, lb, metric ton, g mol, kgm mol, lb mol, metric ton mol.

Once a system and basis have been chosen, the stream quantities for the chlor-alkali plant are computed and displayed in tabular form along with the appropriate flowsheet.

A powerful feature of the module is the presentation of the appropriate material balance in SYMBOLIC form for any selected system for any desired element or compound (Cl, H, Hg, Na, O, Cl2, H2, H20, NaCl, and NaOH) or the total mass present in the process, i.e., the student can choose the specie and immediately see the appropriate material balance written in equation form.

Programs in the module are written in BASICA and require that the BASICA interpreter be available (comes with virtually any IBM/PC) in addition to the MicroCACHE system software. The module can be run on the PC, XT, AT, or IBM/PC compatible. Student-machine interaction is essentially instantaneous. If you teach the first chemical engineering course, I think you will like Prof. Karman's module.

I would like to encourage any faculty with modules they have written and thoroughly tested (preferably with students) to send me a copy for review and possible distribution via the current CACHE channels. We will pay a small royalty fee of $20 directly to the module author for each copy of a module that is sold.

In a related matter, there will be a workshop on MicroCACHE at the ASEE Chemical Engineering Professors school in August. We hope to have several PCs on site so that those in attendance can run some of the modules and try out the module preparation software.

LIST OF CHEMICAL ENGINEERING DEPARTMENTS SUPPORTING CACHE

Last fall, CACHE solicited universities for funds to carry out on-going CACHE activities and to provide seed money for new projects. Departments providing support for the 1986-88 period, as well as for the 1985-87 period, are as follows:

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University of Delaware
ETH, Switzerland
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University of Illinois, Chicago
Kansas State University
Katholieke University Leuven, Belgium
King Abdulaziz University, Saudi Arabia
Lamar University
Lehigh University

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Wayne State University
University of Western Ontario
West Virginia University
University of Wisconsin-Madison
Worcester Poly. Institute
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LIST OF INDUSTRIAL CONTRIBUTORS TO CACHE

The following companies have contributed financial support to specific CACHE activities during 1986-1987:

Chevron Research Corporation
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Exxon Education Foundation
Shell Companies Foundation
Xerox Foundation

FLOWTRAN BOOKS

TO: ULRICH'S BOOKSTORE
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549 East University Avenue
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FLOWTRAN SIMULATION-AN INTRODUCTION,
2nd Edition, by J.D. Seader, W.D. Seider, and A.C. Pauls
No. of copies _____ @ $13.95/each

EXERCISES IN PROCESS SIMULATION USING FLOWTRAN,
2nd Edition, Edited by J.P. Clark, T.P. Koehler, and J.T. Sommerfeld
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CACHE USE OF FLOWTRAN ON UCS,
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☐ I am interested in **obtaining** a FLOWTRAN tape.

If you have checked either of the above squares, please complete the following information. If you have two computers you want to consider, duplicate this form, submit both completed forms and your preference.

1. Computer make and complete model number
   _____
2. Operating system version _____
3. FORTRAN compiler version _____
4. Magnetic tape facility:
   No. of tracks _____
   Drive speed in bits/inch _____

Name: _____

Address: _____

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Send the form to:

Professor J.D. Seader
CACHE
3062 MEB
University of Utah
Salt Lake City, UT 84112

Send this form only if you have not previously contacted Professor Seader.

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CACHE PROCESS DESIGN CASE STUDY VOLUME 1

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CACHE Process Design Case Study Vol. 2
DESIGN OF AN AMMONIA SYNTHESIS PLANT

Preliminary Design and Economic Analysis

Summary: The objective of the case study is the design of an ammonia synthesis plant that is to be built in 1990, and that uses hydrogen and nitrogen feedstocks from a coal gasification plant. All stages of the design procedure starting from preliminary calculations down to the detailed flowsheet calculations are described. Emphasis is placed on the following steps: screening of key flowsheet decisions (pressure of synthesis loop, ammonia recovery, synthesis of gas recycle, hydrogen recovery from purge stream), selection of reactor configuration, cost minimization, and synthesis of heat exchanger network.

The proposed design incorporates a medium-pressure synthesis loop with water absorption/distillation for ammonia recovery, and with membrane separation for hydrogen recovery. The process was designed with the simulator PROCESS from Simulation Sciences, and the ammonia reactor was designed with the special purpose package QBED. A listing of this program is included in the case study. Depending on the required detail and the availability of process simulation software, the case study is suitable as a one-term assignment for a single student or a group of students. The preliminary calculations of the case study were performed by a group of three students, while the final design report is based on the work of a group of five students.

The problem statement was supplied by Philip A. Ruziska from Exxon Chemicals, and the case study was prepared under the supervision of Ignacio E. Grossmann from Carnegie-Mellon University.

CACHE Process Design Case Study Vol. 3
DESIGN OF AN ETHANOL DEHYDROGENATION PLANT

Preliminary Design and Economic Analysis

Summary: The objective of this case study is the preliminary design of an acetaldehyde synthesis process by ethanol dehydrogenation. The project covered all stages of the design procedure starting from consideration of qualitative aspects of the flowsheet and preliminary calculations to detailed process simulations and final economic evaluations. In this study emphasis is placed on synthesizing a workable flowsheet and justifying its configuration, simulating and evaluating the design using a commercial process simulator, and deriving a heat recovery network for the final process.

The main reaction in this process is the endothermic dehydrogenation of ethanol to acetaldehyde. However, under the specified reactor conditions, a number of byproducts are produced and their presence determines a number of interesting alternatives for separation. Once these alternatives have been screened and a workable flowsheet has been synthesized, the study centers on the simulation of this flowsheet using PROCESS from Simsci, Inc. Here, some of the features, advantages and limitations of this simulator are presented. Finally, the study concludes with a complementary presentation of this process simulated with the CACHE version of FLOWTRAN. While the aim of this study is not to provide a detailed comparison between PROCESS and FLOWTRAN, a useful description of the relative merits of both simulators can be readily observed.

This project is suitable for a one-term project by a five or six person team of senior design students. The results of two such teams are given in this study.

This problem was posed by the Union Carbide Corporation and the case study was prepared under the supervision of L.T. Biegler of Carnegie-Mellon University and R.R. Hughes of the University of Wisconsin.

CACHE PROCESS DESIGN CASE STUDY VOLUME 3

"Design of an Ethanol Dehydrogenation Plant"

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3. MicroCACHE McCabe-Thiele **MOD**ule (MCCABE) Diskette
4. MicroCACHE McCabe-Thiele Module **Source** File Diskette

Documentation:

1. *Overview*
2. *User's Manual*
3. *Instructor's Manual*
4. *Module Writer's Manual*
5. *Graphics Packages Manual*

Videotapes (VHS Format):

1. *The MicroCACHE CAI System*
2. *Module Preparation I*
3. *Module Preparation II*

Modules

1.	a) Interactive Graphical Flowsheet Preparation b) Steady-State Process Simulator (Mat. Bal. Only) (CLASS)	$ 150.	_____
2.	Material Balance Exercises (MATBAL)	$ 90.	_____
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10.	Linear Programming (LINPRO)	$ 90.	_____
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12.	Gas Reservoir Simulation (GASSIM)	$ 90.	_____

TOTAL _____

*Module requires that a copy of the MicroSoft FORTRAN-77 compiler be available. These modules should be used only on PCs with hard disks (e.g., XT,AT).

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Foundations of Computer-Aided Process Design

Contents