Parallel Algorithms for Multicomponent Separation Calculations

Tearing and simultaneous correction techniques coupled with an odd-even cyclic reduction parallel algorithm are used to carry out calculations of multicomponent separation problems. The old-even algorithm implements effectively on most parallel processors. No noticeable differences are found when numerical results are compared with those obtained using serial algorithms. The results for three example problems are presented to illustrate the method. Calculations were carried out using single precision arithmetic.

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Introduction

Naphtali (1965) has shown that for distillation problems involving many stages but relatively few components, the most efficient grouping of the discrepancy functions is according to stage location. Naphtali and Sandholm (1971) implemented the method with the application of the Newton-Raphson technique and since then the method has been used widely. The method is capable of solving almost all types of multicomponent, multistage separation problems. Another method, due to Wang and Henke (1966), is of relative importance in the petroleum industry; it has a different approach to the solution of the resulting nonlinear equations that model the process. Convergence is fast for conventional distillation of fairly narrow boiling, nearly ideal mixtures.

The main features of both methods rest on the kind of algorithm used for resolving the resulting tridiagonal and block tridiagonal matrices. The Wang and Henke method and other related methods use the well-known and efficient Thomas algorithm. The Naphtali-Sandholm and similar methods use an implementation of Gaussian elimination of submatrices (Henley and Seader, 1981). With the advent of parallel computers it is possible to tackle larger and more complex problems in the petrochemical and chemical industry, but all the algorithms above are serial by nature. In this paper, we present parallel implementations of algorithms for resolving multicomponent separation calculations.

The odd-even cyclic reduction is a popular alternative to the standard sequential algorithms. Cyclic reduction was discussed by Hockney (1965) for the block tridiagonal systems arising from the five-point difference approximation for Poisson's equation. Subsequently, several authors, including Hockney (1970) and Ericksen (1972), pointed out that the algorithm could also be adapted to general tridiagonal systems.

Cyclic reduction for block tridiagonal matrices has been studied for parallel computers by Kapur and Browne (1981, 1984), who consider implementation on the TRAC computer. They also consider a variant of cyclic reduction known as odd-even introduced by Heller (1976, 1978). In simple terms, this results in the off-diagonal entries moving away from the diagonal so that after $\log_2 N$ steps a diagonal matrix remains and the solution is obtained immediately without a back substitution process. Gannon et al. (1983) recognized the potential superiority of odd-even elimination in their study of implementing parallel algorithms on the CHiP systems. In a recent paper Johnsson (1984) gives a thorough analysis of the implementation of cyclic reduction on a family of parallel computers. These designs are of multiple-instruction-stream, multiple-data-stream (MIMD) type using simple processors and no global memory.

Solving the MESH and HME equations

As with all models of chemical processes, the analysis of the equilibrium stages starts with the construction of energy, material, and phase equilibrium relationships. Methods of solving the equilibrium stage equations fall into two groups:

1. Tearing methods, where subsets of the complete set of equations are solved in sequence
2. Simultaneous correction (SC) methods, where all the equations are solved simultaneously

Stages are numbered from the top down. A partial reboiler counts as a stage and the condenser is numbered as a stage even if the distillate is liquid.

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The MESH equations are as follows:

$$M_{ij} = L_{j-1}x_{i,j-1} + V_{j+1}y_{i,j+1} + F_j z_{ij} - (L_j + U_j)x_{ij} - (V_j + W_j)y_{ij} = 0 \quad (1)$$

$$E_{ij} = y_{ij} - K_{ij}x_{ij} = 0 \quad (2)$$

where K_{ij} is the phase equilibrium ratio,

$$(S_y)_j = \sum_{i=1}^{C} y_{ij} - 1.0 = 0 \quad (3a)$$

$$(S_x)_j = \sum_{i=1}^{C} x_{ij} - 1.0 = 0 \quad (3b)$$

and

$$H_j = L_{j-1}H^L_{j-1} + V_{j+1}H^V_{j+1} + F_j H^F_j - (L_j + U_j)H^L_j - (V_j + W_j)H^V_j + Q_j = 0 \quad (4)$$

where V denotes internal vapor flow rate, L is the internal liquid flow rate, U and W are the liquid and vapor sidestream flow rates, F is the feed flow rate, x is the liquid mole fraction, and y is the vapor mole fraction. H^V is the vapor -phase enthalpy, H^L is the liquid-phase enthalpy, H^F is the enthalpy of the feed streams, and Q is the rate of heat addition. This model is restricted to two-phase flow and will break down if two or more liquid phases are present. Finally, C is the number of components in the system, N is the number of stages, and i and j denote the component and stage indices, respectively.

The HME equations are:

$$H_j = (1 + S_j)V_j H^V_j - V_{j+1}H^V_{j+1} + (1 + s_j)L_j H^L_j - L_{j-1}H^L_{j-1} - F_j H^F_j - Q_j = 0 \quad (5)$$

$$M_{ij} = (1 + S_j)v_{ij} + (1 + s_j)l_{ij} - v_{i,j+1} - l_{i,j-1} - f_{ij} = 0 \quad (6)$$

$$E_{ij} = K_{ij}l_{ij}\frac{V_j}{L_j} - v_{ij} = 0 \quad (7)$$

where in addition to the previously named variables, s is the ratio of liquid sidestream to liquid interstage flow, S is the ratio of vapor sidestream to vapor interstage flow, v_{ij} is the vapor component flow rate, and l_{ij} is the liquid component flow rate.

In equilibrium stage calculations the above equations are solved subject to the requirement that the vapor and liquid streams leaving stage j are in complete thermal, mechanical, and chemical equilibrium. Consequently the steady-state behavior of the column is modeled by a large and sparse system of nonlinear equations.

Briefly, the method developed in detail by Wang and Henke implies the partition of all equations and solves them sequentially except for the modified M equations, which are solved separately for each component by a tridiagonal matrix technique (the Thomas algorithm). The method developed by Naphtali and Sandholm resolves the collection of discrepancy functions written as $\boldsymbol{F}(\boldsymbol{X}) = 0$ using a Newton-Raphson iterative method in which successive sets of the output variables are produced until the values of the $\boldsymbol{F}(\boldsymbol{X})$ (i.e., HME) functions are reduced to zero. Let

$$\boldsymbol{X} = [\boldsymbol{X}_1, \boldsymbol{X}_2, \ldots, \boldsymbol{X}_j, \ldots, \boldsymbol{X}_N]^T$$

and

$$\boldsymbol{F} = [\boldsymbol{F}_1, \boldsymbol{F}_2, \ldots, \boldsymbol{F}_j, \ldots, \boldsymbol{F}_N]^T$$

where $\boldsymbol{X}_j$ is the vector of output variables for stage j arranged in the order $\boldsymbol{X}_j = (v_{ij}, T, l_{ij})$, and $\boldsymbol{F}_j$ is the vector of $2C + 1$ functions for stage j arranged in the order $\boldsymbol{F}_j = (H_j, M_{ij}, E_{ij})$.

The Newton-Raphson iteration is performed by solving for the corrections $\Delta\boldsymbol{X}$ to the output variable, which in matrix form becomes

$$\Delta\boldsymbol{X}^{(k)} = -\left[\left(\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{X}}\right)^{-1}\right]^{(k)} \boldsymbol{F}^{(k)}$$

These corrections are used to compute the next approximation to the set of output variables from

$$\boldsymbol{X}^{(k+1)} = \boldsymbol{X}^{(k)} + \theta\Delta\boldsymbol{X}^{(k)}$$

where θ is a nonnegative scalar step factor; its use is explained by Henley and Seader (1981).

The Jacobian matrix $\boldsymbol{J} = (\partial \boldsymbol{F}/\partial \boldsymbol{X})$ is here very large, but its evaluation is greatly facilitated by the fact that the conditions on stage j are only influenced directly by the conditions on stages $j + 1$ and $j - 1$; as a result, the Jacobian becomes block-tridiagonal in structure. This permits rapid solution by the odd-even cyclic reduction algorithm. For details of the Jacobian elements refer to Naphtali and Sandholm (1971).

Odd-Even Cyclic Reduction Method

The Jacobian $(\partial \boldsymbol{F}/\partial \boldsymbol{X})$ is a block-tridiagonal $N \times N$ matrix of partial derivatives of all functions with respect to all the output variables. Figure 1 shows the block-tridiagonal structure of the Jacobian. The submatrices $\boldsymbol{A}_j$, $\boldsymbol{B}_j$, and $\boldsymbol{C}_j$ are extremely sparse; $\boldsymbol{A}_j$ and $\boldsymbol{C}_j$ are almost empty. Each of the above blocks represents a $(2C + 1) \times (2C + 1)$ submatrix of partial derivatives. For example, for a 16-stage column separating a mixture of five components the equilibrium stage model comprises 176 equations.

The main ideas of the odd-even algorithm are given by Hockney (1965) for the solution of tridiagonal matrices and by Meis and Marcowitz (1978) for the solutions of block-tridiagonal matrices. What is new, however, is the identification of a class of calculations in chemical process design where the odd-even cyclic reduction method is potentially profitable.

Hockney (1965) describes an algorithm that successively decouples the tridiagonal system into a sequence of smaller systems. The number of steps required to complete the decoupling is $O(\log_2 N)$, where N is the dimension of the matrix. The basic ideas of the reduction method are presented by Heller (1976) and it can be understood by writing down three successive equations in the tridiagonal set,

$$a_{j-1}x_{j-2} + b_{j-1}x_{j-1} + c_{j-1}x_j = d_{j-1} \quad (8a)$$

$$a_j x_{j-1} + b_j x_j + c_j x_{j+1} = d_j \quad (8b)$$

$$a_{j+1}x_j + b_{j+1}x_{j+1} + c_{j+1}x_{j+2} = d_{j+1} \quad (8c)$$

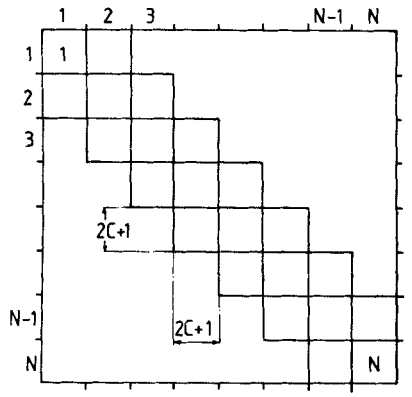

Figure 1. Jacobian matrix for complex column.
All elements outside of the square areas are zero
Each square contains one or more nonzero elements

or

$$A = (a, b, c)$$

and

$$Ax = d$$

We can eliminate x_{j-1} and x_{j+1} from the second equation to yield an equation for x_{j-2}, x_j, and x_{j+2} that can be written as

$$a_j^{(1)}x_{j-2} + b_j^{(1)}x_j + c_j^{(1)}x_{j+2} = d_j^{(1)} \tag{9}$$

where

$$a_j^{(1)} = \alpha_j a_{j-1} \tag{10a}$$

$$b_j^{(1)} = b_j + \alpha_j c_{j-1} + \gamma_j a_{j+1} \tag{10b}$$

$$c_j^{(1)} = \gamma_j c_{j+1} \tag{10c}$$

$$d_j^{(1)} = d_j + \alpha_j d_{j-1} + \gamma_j d_{j+1} \tag{10d}$$

and

$$\alpha_j = -a_j/b_{j-1} \tag{10e}$$

$$\gamma_j = -c_j/b_{j+1} \tag{10f}$$

Therefore, we have a system of equations $A^{(1)}x = d^{(1)}$, where the structure of $A^{(1)}$ is shown in Figure 2b. Doing this for all even and again for all odd j yields two sets of equations, each of size $N/2$, for the even and for the odd unknowns, each of which involves only three unknowns. Renumbering them, we have two sets of tridiagonal equations, and clearly we can repeat the process $\log_2 N$ times. The method can be repeated recursively to give $A^{(2)}x = d^{(2)}$ as shown in Figure 2c, and so on. In general if A is strictly diagonal dominant, as is frequently the case when solving distillation, absorption, and stripping column calculations, the off-diagonal terms decrease at a quadratic rate, i.e., $a_j^{(q+1)} \simeq [a_j^{(q)}]^2 < 1$. Therefore, if $n = \log_2 N$, it is possible to terminate the process in fewer than n steps when the off-diagonal terms are sufficiently small.

Meis and Marcowitz (1978) describe the Buneman method for resolving a set of block-tridiagonal matrices. Following the previous reasoning we write down three successives blocks in the block-tridiagonal set as,

$$A_{j-1}\Delta_{j-2} + B_{j-1}\Delta_{j-1} + C_{j-1}\Delta_j = F_{j-1} \tag{11a}$$

$$A_j\Delta_{j-1} + B_j\Delta_j + C_j\Delta_{j+1} = F_j \tag{11b}$$

$$A_{j+1}\Delta_j + B_{j+1}\Delta_{j+1} + C_{j+1}\Delta_{j+2} = F_{j+1} \tag{11c}$$

where A_j, B_j, and C_j are matrices, and Δ_j and F_j are vectors. Similarly, we can eliminate Δ_j and Δ_{j+2} to yield an equation for Δ_{j-2}, Δ_j and Δ_{j+2}. The resulting equation may be written as

$$A_j^{(1)}\Delta_{j-2} + B_j^{(1)}\Delta_j + C_j^{(1)}\Delta_{j+2} = F_j^{(1)} \tag{12}$$

where

$$\tilde{A}_j = B_j^{-1}A_j \tag{13a}$$

$$\tilde{C}_j = B_j^{-1}C_j \tag{13b}$$

$$\tilde{F}_j = B_j^{-1}F_j \tag{13c}$$

and

$$B_j^{(1)} = I - \tilde{A}_j\tilde{C}_{j-1} - \tilde{C}_j\tilde{A}_{j+1} \tag{13d}$$

$$F_j^{(1)} = F_j - \tilde{A}_j\tilde{F}_{j-1} - \tilde{C}_j\tilde{F}_{j+1} \tag{13e}$$

$$A_j^{(1)} = -\tilde{A}_j\tilde{A}_{j-1} \tag{13f}$$

$$C_j^{(1)} = -\tilde{C}_j\tilde{C}_{j+1} \tag{13g}$$

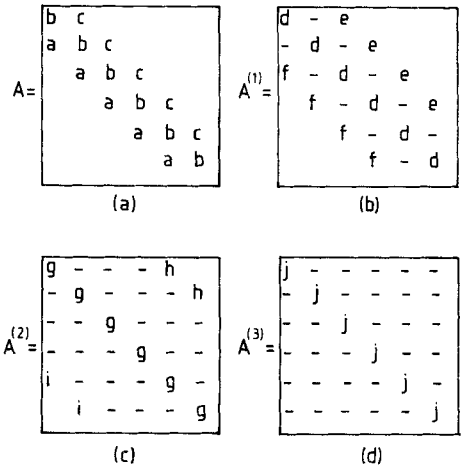

Figure 2. Routing of tridiagonal matrix elements.

where I is the identity matrix. The method can be repeated recursively as for the simple tridiagonal solver. Finally, we solve the diagonal block equation of the form

$$B_j^{(n)}\Delta_j = F_j^{(n)} \tag{14}$$

to obtain the unknown vector Δ_j. Details of the odd-even cyclic reduction algorithm used can be found in the supplementary material.

Numerical Results and Discussions

The reason for considering alternative forms of solution for the block-tridiagonal systems was to construct a method that was appropriate for implementation on the present generation of multiprocessor computers. For multicomponent separation analysis the optimum configuration is a processor interconnection network in the form of a two-dimensional lattice in which processors are connected to their nearest (i.e., north, south, east, west) neighbors. There are a number of machines (such as the AMT DAP 500 series) that are hardwired as a two-dimensional lattice. Other machines based on a hypercube topology are more general interconnections that include two-dimensional lattices as subnetworks. In addition, the Inmos transputer microprocessor is designed with four links and so can be naturally formed into a rectangular lattice processor array.

With nearest-neighbor connectivity between the processors it is possible to associate each stage of the separation process with a row of the processor array and each component with a column. This assumes an array of at least $N(2C + 1)$ processors, which is not a significant restriction on a DAP with (at present) a 32×32 array or on a transputer network that can be constructed of any size. In a tearing method the cyclic reduction algorithm is then implemented separately on each column of processors with each processing element in the array associated with a row of the tridiagonal matrix. In a simultaneous correction (SC) method each row of blocks is associated with a column of processing elements and the block cyclic reduction is implemented across the rows. The Gauss-Jordan algorithm to solve systems within the block structure (i.e., invert the diagonal blocks) is implemented on a column of processors and in general is more efficient than Gauss elimination when implemented on a linear processor array.

In both the cyclic reduction and Gauss-Jordan algorithms all the (active) processing elements are performing the same sequence of computation and it is possible to implement the method on a SIMD (single-instruction-stream, multiple-data-stream) type of machine. In view of the automatic synchronization of operating in this mode the scheme provides an efficient algorithm for MIMD (multiple-instruction-stream, multiple-data-stream) machines. The relatively small amount of data communication involved makes this computation ideally suited to message-passing architecture with no global memory.

For the numerical experiment the method was coded for the DAP (in DAP-Ada) and the results quoted below were obtained via a DAP simulator on a microVAX. The algorithm has been tested in the design of a distillation column using data for three systems. System I is formed by ethane, propane, *n*-butane, *n*-pentane, and *n*-hexane. This system has been studied by Johansen and Seader (1972) and the final results are in agreement with those published. Table 1 shows the final results using the tearing method and Table 2 displays results when an SC method is used. Convergence is reached with only three iterations, in comparison with 19 iterations using the tearing method.

Table 1. Results for Five-Component System Using the Tearing Method

Stage	Phase	Temp. K	Flow Rate gmol/s	Component* Mol Frac. (1)	(2)	(3)	(4)	(5)
1	VAP	322.24	2.52	0.1487	0.8252	0.0261	0.0000	0.0000
3	LIQ	336.21	0.38	0.0122	0.7560	0.2282	0.0013	0.0000
13	VAP	402.19	4.66	0.0001	0.0341	0.7115	0.2413	0.0131
16	LIQ	426.58	5.04	0.0000	0.0008	0.2362	0.6515	0.1129

Condenser duty = −2.53455E+05 J/s
Reboiler duty = 4.72663E+05 J/s

*Ethane (1), propane (2), *n*-butane (3), *n*-pentane (4), *n* = hexane (5)

A second example involving the separation of acetone with water from a quaternary feed mixture of methanol, ethanol, acetone, and water by extractive distillation is given in the supplementary material. This system has been studied by Gallun and Holland (1976). A third example, also in the supplementary material, involves the separation of ethyl-acetate from a feed mixture of ethanol, ethyl-acetate, and water by azeotropic distillation. Pure-component molecular parameters, pure-component fugacity, vapor heat capacity, and UNIQUAC parameters for these systems were obtained from Prausnitz et al. (1980). Complete specification of the packages used to illustrate the odd-even algorithm can be found in the supplementary material.

The quantities with complex derivatives for the construction of the Jacobian were approximated with finite difference. Originally we sought to approximate the Jacobian by adapting a quasi-Newton method described by Lucia and Macchieto (1983) based on the sparse update method of Schubert for block-tridiagonal matrices. However we have found the same dissatisfaction as pointed out by Westman et al. (1984).

In summary, we have presented a number of promising preliminary results which support the suitability of the odd-even cyclic reduction method for replacing serial algorithms in the design of vapor-liquid separators. First and foremost, we have presented a way of resolving tridiagonal and block-tridiagonal matrices that appear from the analysis of chemical processes.

Notation

a_j, b_j, c_j = coefficients tridiagonal matrix
A_j, B_j, C_j = coefficients block-tridiagonal matrix

Table 2. Results for Five-Component System Using the SC Technique

Stage	Phase	Temp. K	Flow Rate gmol/s	Component* Mol Frac. (1)	(2)	(3)	(4)	(5)
1	VAP	322.45	2.52	0.1481	0.8243	0.0276	0.0000	0.0000
3	LIQ	336.62	0.38	0.0121	0.7495	0.2372	0.0013	0.0000
13	VAP	402.27	4.66	0.0001	0.0333	0.7116	0.2419	0.0131
16	LIQ	426.63	5.04	0.0000	0.0008	0.2352	0.6511	0.1128

Condenser duty = −2.53455E+05 J/s
Reboiler duty = 4.72663E+05 J/s

*Ethane (1), propane (2), *n*-butane (3), *n*-pentane (4), *n* = hexane (5)

C = number of components
E = equilibrium discrepancy function
H_j = energy discrepancy function on stage j, J/s
F = total feed rate, gmol/s
f = component feed rate, gmol/s
$\boldsymbol{F}$ = discrepancy function vector
H = enthalpy, J/gmol
$\boldsymbol{I}$ = identity matrix
$\boldsymbol{J}$ = Jacobian matrix of partial derivatives
K = phase equilibrium ratio
l = component liquid flow, gmol/s
L = total liquid flow, gmol/s
M = mass discrepancy function, gmol/s
N = number of stages
O = heat added
s = ratio of liquid sidestream to liquid interstage flow
S = ratio of vapor sidestream to vapor interstage flow
T = temperature, K
v = component vapor flow, gmol/s
V = total vapor flow, gmol/s
x = liquid-phase compositions
$\boldsymbol{X}$ = vector of variables
y = vapor-phase compositions

Greek letters

Δ_j = vector of output variables v, T, l
α_j, γ_j = defined by Eqs. 10e, 10f

Subscripts

i = component number
j = stage number
q = odd-even number

Superscripts

k = simultaneous correction iteration number
L = liquid phase
V = vapor phase

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