Reconciliation of Process Data with Process Simulation

The SACDA group at the University of Western Ontario has developed an equations-oriented modular process simulation program called MASSBAL. A model of a process is constructed by selecting and flowsheeting standard building blocks describing fundamental operations such as the mixing and separating of streams. Building blocks are also provided by which equipment operating or design equations may be incorporated into the model. Reconciliation of the inconsistency and redundancy of process measurements is an optional feature of the program. The measurements are reconciled by minimizing a weighted least-squares criterion while satisfying the model equations and any modeling constraints. The minimum is obtained directly, avoiding the need for laborious searching techniques.

G. R. STEPHENSON and

C. F. SHEWCHUK

SACDA
Engineering Science Building
The University of Western Ontario
London, Ontario, Canada N6A 5B9

SCOPE

Process simulation has become a valuable tool for designing, characterizing, and monitoring the performance of industrial processes. It can be broadly defined as the use of mathematical models to formulate and solve the steady state material and heat balances, equipment operating or design equations, and equations providing information on production, consumption of feed stocks, costs, and similar data for a process.

Most process simulation programs use the sequential modular approach to solving the model equations. It has become apparent, however, that the assumptions of this technique limit its application to design and optimization problems. These limitations can be overcome by an equations-oriented approach. Several equations-oriented programs have been developed or are under development. Some of the more advanced of these are ASCEND (Carnegie Mellon University), FLOWSIM (University of Connecticut), MASSBAL (SACDA), QUASILIN (Cambridge), and SPEEDUP (Imperial College).

For the process simulation model to be used effectively, it must be validated. This validation or reconciliation involves comparing actual instrument readings and analyses with calculated values from the model. Because the measurements are subject to random and systematic error, possibly gross, they are not normally consistent with the model equations nor indeed with the redundancy within themselves. To solve the reconciliation problem a methodology is required which insures that the model equations are satisfied, the difference between the measured and calculated values is minimized, and gross errors are detected. Excellent reviews of the published work on this problem have been presented by Hlavacek (1977) and Mah (1981).

The objectives of this paper are to characterize the modular implementation of the equations-oriented approach to process simulation used in the MASSBAL program, to present the methodology by which the MASSBAL program solves the data reconciliation problem, and to demonstrate the effectiveness of this methodology through practical applications.

CONCLUSIONS AND SIGNIFICANCE

The MASSBAL program employs an equations-oriented approach to process simulation. This technique expresses the complete model of the process as a single large system of nonlinear algebraic equations, termed the model equations. The model equations are solved simultaneously.

The equations-oriented approach is implemented in a modular environment in the MASSBAL program. A model of a process is constructed by selecting and flowsheeting standard building block modules that set up, but do not solve, the equations for such fundamental operations as stream mixing and separating, addition or consumption of heat, and reaction. Building block modules that set up equipment operating or design equations and equations relating production, consumption of feed stocks, cost, etc. to process operation are also provided. The inclusion of such equations is only limited by the requirement that they do not create redundancy or inconsistency in the equation set. This provides a great deal of flexibility. For example, operating costs can be determined for various modes of operation, and production rates can be used to directly determine feed stock requirements.

The model equations are solved by a Newton-Raphson iterative procedure. The algorithm used to solve the linearized equations takes advantage of the sparsity of the Jacobian matrix, the invariance of the partial derivatives of the linear terms of the model equations, and the concept of symbolic and algebraic solutions to minimize computer memory requirements and computation time. This algorithm is used routinely to

Correspondence concerning this paper should be addressed to C. F. Shewchuk.

solve equations sets comprised of 200 to 4,000 equations. Convergence is usually rapid and computation time is relatively short.

Reconciliation of process measurements is an optional feature of the MASSBAL program. Operating data can be input directly into an underconstrained model. An optimization is performed whereby the model equations are satisfied and the deviations of the measured and calculated values are minimized in a least-squares sense. Gross errors are detected by statistical examination of the deviations.

The optimization is solved using the method of Lagrange multipliers. It is shown that the equations-oriented approach is well suited for the optimization. All that is necessary is to augment the solution vector with the Lagrange multipliers, transpose the Jacobian matrix for the model, and add the measurements that link the partitions of the augmented equation set for the optimization. The set of minimum deviations is found directly; searching is not required.

The data reconciliation feature of the MASSBAL program has been used in process troubleshooting, monitoring process operation on an on-going basis, and "back-calculating" equipment parameters for predictive models. The MASSBAL program is mounted on several computer service bureaus that make it commercially available throughout North America and Europe. Users of the program are drawn from the pulp and paper, mineral processing, pharmaceutical, and petrochemical industries.

INTRODUCTION

Process simulation has become an accepted and valuable tool for designing, characterizing, and monitoring the performance of industrial processes. It is also becoming an important part of the curriculum of many engineering schools. A recent review of this subject has been presented by Shacham et al. (1982) and a number of textbooks are also available, notably Westerberg et al. (1979) and Meyers and Seider (1976).

The problems that can be solved using process simulation fall into three broad categories: simulation, design, and optimization. In the simulation problem, the process feeds and the equipment or design variables for the processing units are completely defined. The unknowns are the variables associated with all other process streams and tag-along variables such as operating costs. Determining the effect of changes in feed rate and/or composition and determining the effect of changes in process configuration fall into this category. In the design problem, some of the equipment variables are left unspecified and an equivalent number of stream variables are constrained. The calculated variables can be used to size and/or specify equipment. In the optimization problem, any of the stream or equipment variables may be left unspecified. The unspecified variables are determined so as to minimize an objective function. The data reconciliation problem is included in this classification.

Most process simulation programs use the sequential modular approach. In this technique, the modeling equations for each unit in the flowsheet are formulated so that the outlet stream variables are calculated in terms of the inlet stream and equipment variables, and solved in process sequence. When recycle streams are present, an iterative scheme is required. The technique is based on two assumptions. First, the equipment variables and the process stream variables associated with streams entering the flow sheet are completely defined and are not treated as unknowns. Second, the flow of the information in the mathematical model coincides with the material flow. Although this approach has some advantages for the simulation problem, it is not well suited for the design and optimization problems. In both cases, the above assumptions no longer apply and its use becomes cumbersome. The sequential modular approach also eliminates the use of balance equations for several units together or for the whole plant. This may lead to the total material balance being far off for converged solutions. Shacham et al. (1982) characterize the different techniques for process simulation.

The equations-oriented approach overcomes the limitations of the sequential modular technique. In this approach the complete model is expressed as a single large system of nonlinear algebraic equations that are solved simultaneously. All equipment and stream variables are treated as unknowns. No assumptions are made regarding what variables must be specified or about the flow of information in the model. What is required is that the model equations be independent and consistent.

For a process simulation model to be of practical use as an engineering tool, it must be validated. This validation or reconciliation involves comparing process measurements with calculated values from the model. Differences in these values arise from two main sources. First, the measurements are subject to random and systematic errors, possibly gross, arising from instrument faults, reading error, inaccurate laboratory analyses, and similar problems. Such errors result in data that are not only inconsistent with the simulation model, but are inconsistent within themselves. Second, the model may not adequately represent the process. This is often caused by the basic simplifying assumptions of the model. In some situations, however, the process might in fact be different from that perceived by the modeler. Multiple-effect evaporators are widely used in the pulp and paper industry for concentrating spent cooking liquor and in the food processing industry for concentrating products such as orange juice. An evaporator body for which the instruments indicate a negative boiling point rise is an example of the first source of difference between the measured and calculated values. An evaporator body with a tube leak, the perceived process being a body with no leak, is an example of the second source of difference. Shewchuk et al. (1980) report that data reconciliation can be both time consuming and expensive. Industrial applications are discussed by Ham et al. (1979).

The reconciliation problem has received consideration in the literature for more than twenty years. Kuehn and Davidson (1961) used Lagrange multipliers to solve for optimal adjustments to the measurements for the case when either all or none of the component flow rates are measured. Excellent reviews on this problem have been presented by Hlavacek (1977) and Mah (1981). Recently, Crowe et al. (1983) have proposed an approach based on matrix projection. The treatment is restricted to balances that are linear, although an extension to bilinear balances is presented. It is assumed for the linear case that for any stream in which a concentration or temperature is measured, the total flow is also measured. This permits the calculation of the flow rate of enthalpy or of a component. These values are then used as measurements to be adjusted.

THE PROCESS MODEL

The equations-oriented approach is implemented in a modular environment in the MASSBAL program. Each of the stan-

dard building block modules sets up the equations associated with it. For example, consider a stream splitter having in general K outlet streams and C components per stream. The subset of $K(C+1)+1$ equations in $K(C+2)$ variables that would be set up by invoking the standard building block for a splitter is

Component mass balances:

$$f_{ik}/F_k = f_{io}/F_o \text{ for } i = 1, C \text{ and } k = 1, K \tag{1}$$

Total mass balance:

$$\sum_{k=1}^{K} F_k - F_o = 0 \tag{2}$$

Temperature relationships:

$$T_k - T_o = 0 \text{ for } k = 1,K. \tag{3}$$

This building block has $K-1$ variables for which equations are not formulated. That is, there are $K-1$ degrees of freedom. These are the relative flow splits between the outlet streams. A special building block module is included in the MASSBAL program by which the user provides equations, termed modeling constraints, that satisfy the degrees of freedom associated with the standard building block modules. The modeling constraints generated by this building block module can set variables to fixed values, equate variables, linearly relate two or more variables, relate two variables as a fixed ratio or product, and relate two variables by a table of values. Modeling constraints of arbitrary complexity can be accommodated through user-supplied subroutines. These equations are only restricted by the requirement that they do not create redundancy or inconsistency in the equation set. This provides a great deal of flexibility. For example, production rate can be used directly to determine feed stock requirements.

The relationships that model the operation of a proposed or existing process include mass and energy balances, equipment specific operating equations, modeling constraints and, optionally, equations that provide management information on production, consumption of feed stocks, costs, and related factors. These relationships form a set of N nonlinear simultaneous model equations which can be written as

$$f(x) = 0. \tag{4}$$

The solution vector, which may be expressed as

$$x = (x_1, x_2, \ldots, x_M)^T, \tag{5}$$

is comprised of the process stream, equipment, and other related variables of the model.

The solution of a set of nonlinear simultaneous equations can be accomplished by a number of methods. These are classified as precedence-ordering methods, tearing methods, iterative methods without partial derivatives, and iterative methods with partial derivatives. The Newton-Raphson method, which falls in the last classification, is used in the MASSBAL program. This method approximates the functions f by Taylor series expansions terminated after the first derivatives, thus providing the linearized set of equations

$$J(x)|_{x^*} \cdot \Delta x = -f(x)|_{x^*} \tag{6}$$

where,

$$J_{ij}(x) = \partial f_i(x)/\partial x_j \tag{7}$$

and

$$\Delta x = x - x^*. \tag{8}$$

If the partial derivatives of the terms of a model equation are only slightly affected by one or more of the variables, a quasi-Newton linearization may be used. Equation 6 can be solved for Δx provided that M and N are equal and $J(x)$ is well-conditioned. This solution is used to refine the estimate of the solution vector according to

$$x = x^* + \phi\, \Delta x \tag{9}$$

Equations 6 and 9 are evaluated iteratively until

$$|\Delta x_j / x_j^*| < \epsilon \text{ for } J = 1, N \tag{10}$$

at which point the solution to Eq. 4 is determined. The relaxation factor can be used to assist convergence. A value less than one may be required for the first few iterations when x^* may deviate significantly from the solution. The initial estimate of x can be internally generated, partially user-supplied, or the result from a previous similar simulation. For many MASSBAL models this method obtains convergence for a value of ϵ equal to 0.00001 in approximately 10 iterations.

It is well established that iterative methods that use partial derivatives converge in fewer iterations than iterative methods not using partial derivatives. This is a primary reason for choosing the Newton-Raphson method. However, the decrease in the number of iterations must be weighed against an increase in computation time for evaluating the partial derivatives. This effect can be offset by taking advantage of the concept of symbolic and algebraic solutions and the invariance of the partial derivatives of the linear terms of the model equations.

The distribution of nonzero terms in the Jacobian matrix for an equation set typical of process simulation is illustrated in Figure 1. One of the most striking features of the matrix is its sparsity. The MASSBAL program employs an equation-solving algorithm developed by Bending and Hutchison (1973). It uses a pivot selection strategy which minimizes fill-in — that is, the generation of nonzero elements during decomposition of the Jacobian matrix — and exploits the sparsity to efficiently utilize computer memory, storing only the nonzero elements of the matrix. A flowsheet for a brown stock washer-knotter subsystem of a chemical pulping process is shown in Figure 2. The model generated by the MASSBAL program for this subsystem has 339 equations. The Jacobian matrix has 1,150 nonzero elements, which is only 1.0% of the total. The solution procedure generates a further 700 nonzero elements, which corresponds

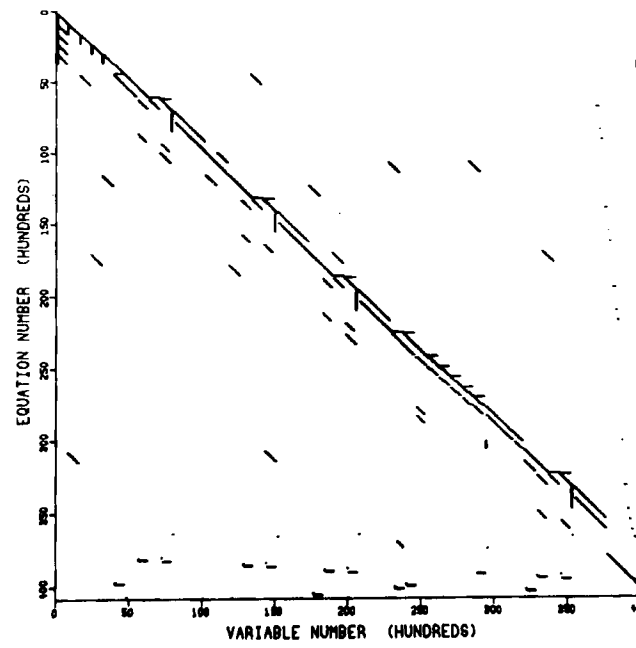

Figure 1. Distribution of nonzero terms in the Jacobian matrix for an equation set typical of process simulation.

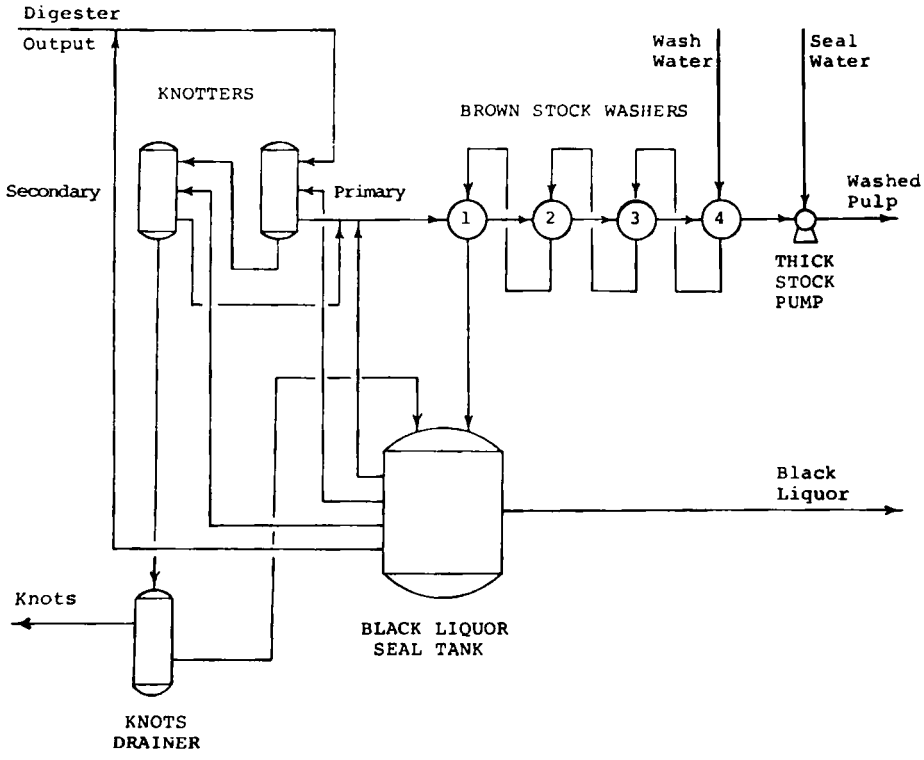

Figure 2. Flowsheet for a brown stock knotter-washer subsystem of a chemical pulping process.

to a fill-in of only 0.6%, or an increase in nonzero elements of 60.9%.

The equation-solving algorithm used by the MASSBAL program also uses the concept of symbolic and algebraic solutions of linear algebraic equations to dramatically reduce computation time. While obtaining the first solution, the elementary row operations, which represent the symbolic decomposition of the matrix, are coded in a list. Because the topology of the Jacobian matrix does not change from one iteration to the next, this list may be used to obtain the solution on subsequent iterations by simply performing the algebra. It has been found that several algebraic iterations can be performed in the computation time required for obtaining a single symbolic solution. For the model of the brown stock knotter-washer subsystem, the symbolic solution requires 1.440 s computation time on a CDC Cyber 835, while the algebraic solution requires 0.158 s. That is, about nine algebraic solutions are performed in the same computation time as one symbolic solution.

The MASSBAL program maintains the Jacobian matrix between iterations and calculates the derivatives of only the nonlinear terms of the model equations for algebraic iterations. The partial derivatives of the linear terms of the model equations are invariant. Since only from 10 to 40% of the terms in many process simulation equation sets are nonlinear, a significant saving in computation time is achieved. For the model of the brown stock knotter-washer subsystem referred to above, about 33% of the terms of the model equations are nonlinear.

THE DATA RECONCILIATION PROBLEM

The MASSBAL program permits the input of redundant and inconsistent measured data directly into an underconstrained model. The only restriction is that a subset of the measured values must be sufficient to satisfy the unconstrained degrees of freedom. The measurements are reconciled by minimizing a weighted sum of the squares of the normalized differences between the measured and calculated values while satisfying the model equations and any modeling constraints.

To express the reconciliation optimization mathematically, the solution vector is first partitioned as

$$x = (u:v)^T. \tag{11}$$

u and v are the subsets of the measured and unmeasured variables, having lengths P and $M-P$ respectively. The problem can then be stated as: minimize

$$g(u) = \sum_{p=1}^{P} \sum_{q=1}^{Q_p} w_{pq}((m_{pq} - u_p)/r_{pq})^2 \tag{12}$$

subject to Eq. 4. The weighting factor is an arbitrary measure of the relative confidence of the measured value. A weight of zero effectively eliminates the measurement from the analysis. The measurement range is used to normalize the deviation between the measured and calculated value. Using normalized deviations accommodates mixing of various types of process variables in the measured subset.

Using Lagrange multipliers, the optimum is found by obtaining a stationary point of the Lagrangian

$$G(x,\lambda) = g(u) + \lambda^T f(x). \tag{13}$$

Setting the derivatives of $G(x,\lambda)$ with respect to the Lagrange multipliers to zero forms the set of N nonlinear equations

$$f(x) = 0, \tag{14}$$

which are identical to Eq. 4 except for the reordering of the terms of f implied by Eq. 11. Setting the derivatives of $G(x,\lambda)$ with respect to the process variables to zero yields

$$\left[\begin{array}{c|c} A & 0 \\ \hline 0 & 0 \end{array}\right]\left[\begin{array}{c} u \\ \hline v \end{array}\right] + J^T(x)\lambda = \left[\begin{array}{c} B \\ \hline 0 \end{array}\right]. \tag{15}$$

The matrix A links Eqs. 14 and 15. It is a $P \times P$ diagonal matrix

for which

$$A_{pp} = \sum_{q=1}^{Q_p} 2w_{pq}/r_{pq}^2 \tag{16}$$

The vector B has length P and is defined by

$$B_p = \sum_{q=1}^{Q_p} 2w_{pq}m_{pq}/r_{pq}^2 \tag{17}$$

Equations 14 and 15 form a set of $N + M$ nonlinear equations in $M + N$ unknowns for which the solution minimizes $g(u)$ and satisfies Eq. 4. The solution of this equation set proceeds as described for the process simulation model. Equation 14 can be linearized as in Eq. 6. For computation it is more expedient, however, to write the linearized equation set in terms of x. Assuming a value of unity for ϕ results in the linearized equation

$$J(x)|_{x^*} \cdot x = -f(x)|_{x^*} + J(x)|_{x^*} \cdot x^* . \tag{18}$$

A quasi-Newton linearization of Eq. 15 which neglects the effects of the second-order partial derivatives with respect to the process variables results in the equation

$$\left[\begin{array}{c|c} A & 0 \\ \hline 0 & 0 \end{array}\right]\left[\begin{array}{c} u \\ \hline v \end{array}\right] + J^T(x)_{x^*} \cdot \lambda = \left[\begin{array}{c} B \\ \hline 0 \end{array}\right]. \tag{19}$$

This linearization provides two important benefits. First the Lagrange multipliers do not appear in any of the coefficients of the linearized equations. Therefore, they do not require an initial guess. Second, time-consuming evaluation of the second derivatives is avoided. In augmented form the linearized equations set appears as

$$\left[\begin{array}{c|c} J(x)|x^* & 0 \\ \hline \begin{array}{c|c} A & 0 \\ \hline 0 & 0 \end{array} & J^T(x)|x^* \end{array}\right]\left[\begin{array}{c} x \\ \hline \lambda \end{array}\right] = \left[\begin{array}{c} -f(x)|_{x^*} + J(x)|_{x^*} \cdot x^* \\ \hline B \\ \hline 0 \end{array}\right] \tag{20}$$

This representation demonstrates that the equations-oriented approach is well suited for the data reconciliation optimization.

Under the assumption that the absolute deviations of the measured and calculated values are normally distributed, the MASSBAL program annotates any measurements that lie outside the 95% confidence limit. Although the assumption of normality has been shown to be violated in practice, it has been found that this examination detects any gross errors. There is no substitute, however, for engineering judgment. The deviations may all be within the expected error tolerance from an engineering point of view, but a measurement may be annotated because it is statistically larger than the others.

The formulation of the data reconciliation problem described herein is computationally highly efficient. The optimum solution is obtained directly; no costly trial and error simulations are required. Typically, a data reconciliation problem requires about the same number of iterations as the corresponding simulation problem and about one-and-a-half times the computation time.

A problem that is encountered with unconstrained optimization problems is that a solution of the equations which also minimizes the objective function may not be realizable in practice. The very fact that the measured values represent, in general, the physical reality helps insure that this will not occur.

APPLICATIONS

The data reconciliation feature of the MASSBAL program is a tool for troubleshooting the operation of a process. A significant deviation between a measured and calculated value may yield an indication of a potential instrument problem. The deviations between the measured and calculated values along with the detailed results of the simulation may pinpoint a unit that is not functioning as expected. The resolution of the discrepancies between the process and the simulation results is in essence the basics of troubleshooting that a process engineer would perform.

A second use of the data reconciliation feature is monitoring the operation of a process on an on-line basis. The simulation

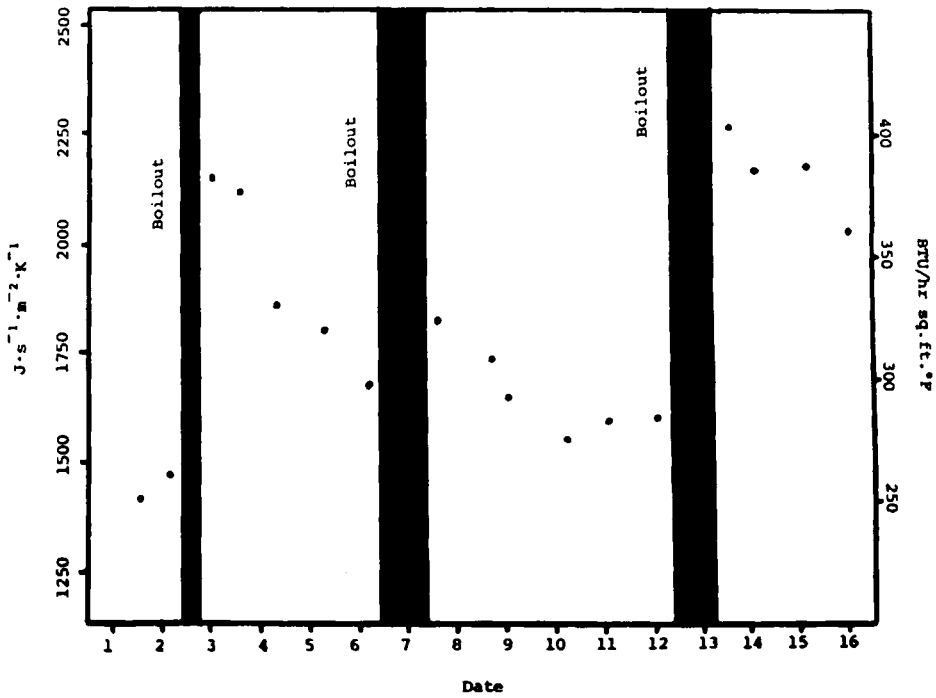

Figure 3. Trend of the overall heat transfer coefficient for an evaporator set.

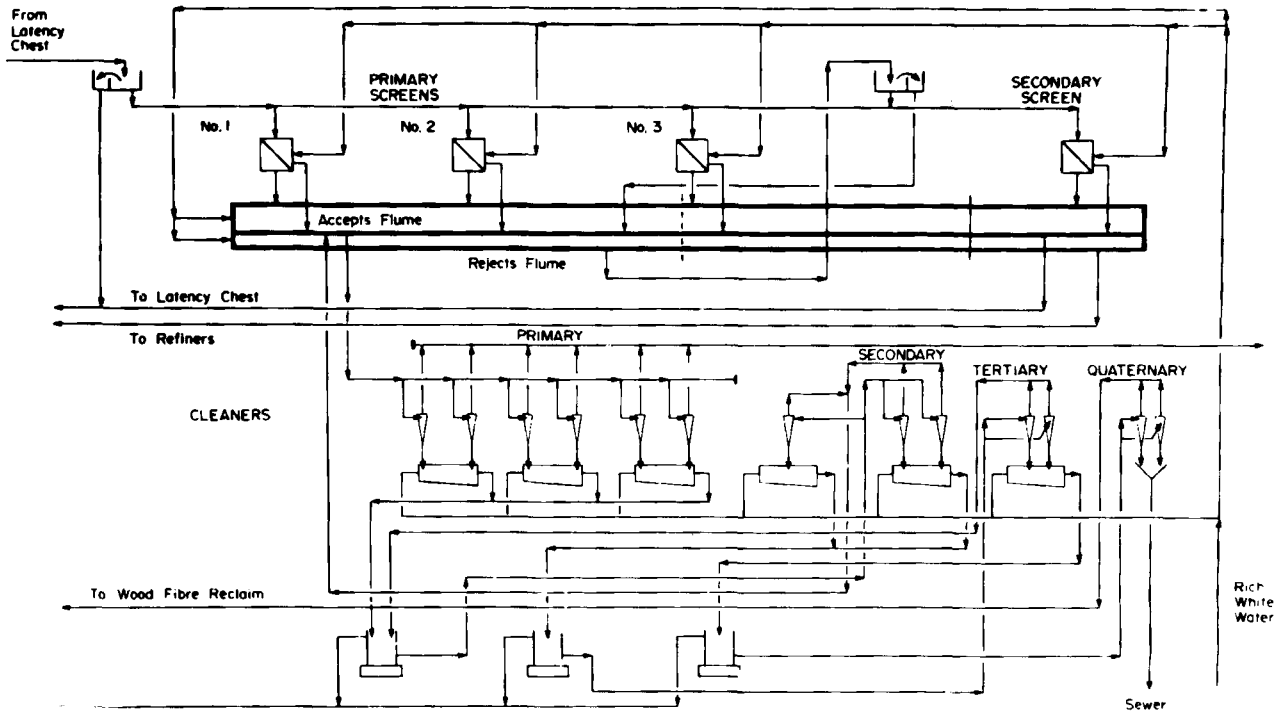

Figure 4. Screening and cleaning system for a CTMP pulp mill.

results may be obtained regularly and automatically if the computer on which the program is mounted can communicate with the process control system. Trends can be generated and used to track the performance of the process. Also, unexpected changes in the operation of the process may be identified. A typical application is the monitoring of the overall heat transfer coefficient of an evaporator set reported by Shewchuk et al. (1980). A plot of the overall heat transfer coefficient based on the daily log sheets for a 16-day period is shown in Figure 3. Fouling of the heat transfer surfaces causes the overall heat transfer coefficient to decrease with time. The trend is used to indicate when cleaning of the surfaces using boilout is required.

The above applications of the data reconciliation feature have a common characteristic. If sufficient redundancy exists, they may be employed using simple heat and material balance models with *no requirement* for detailed mathematical models of process equipment. The generality of the method, however, does not preclude the inclusion of equipment models of arbitrary complexity in the process models. The MASSBAL program leaves this option open to the user.

Some applications of process simulation such as evaluation of alternate operating strategies and sensitivity testing require a predictive model. By including the predictive model in the reconciliation optimization, the parameters of the predictive model that best fit the process operation are determined. Since a variable can have more than one corresponding measurement, sets of process measurements collected over a period of time can be used directly to obtain values of the parameters which more closely represent steady state than is possible by using a single set or an average of a number of sets. This model can then be used in subsequent simulations to represent the process operation at different conditions.

As an illustration of this application consider the screening and cleaning system of a typical CTMP pulp mill shown in Figure 4. The objective of the modeling is to obtain a model that will predict shive removal efficiency under different operating conditions. The shive removal of a screen or cleaner can be described by

$$\epsilon_s = aR_w/[(a-1)R_w + 1]. \tag{21}$$

Figure 5 is a graphical representation of this equation for various values of the shive removal constant. The MASSBAL program has a feature whereby a group or macro, defined in terms of the fundamental building blocks, can be declared. The macro defined for the screens and cleaners would incorporate Eq. 21 with the shive removal constant left unconstrained. This allows the constant to either be fixed externally or be calculated from measured values. This macro is then used with the standard building blocks to construct a block diagram of the process as shown in Figure 6. The measurements summary generated by the MASSBAL program for the reconciliation optimization for this example is shown in Figure 7. Figure 8 is the output for the

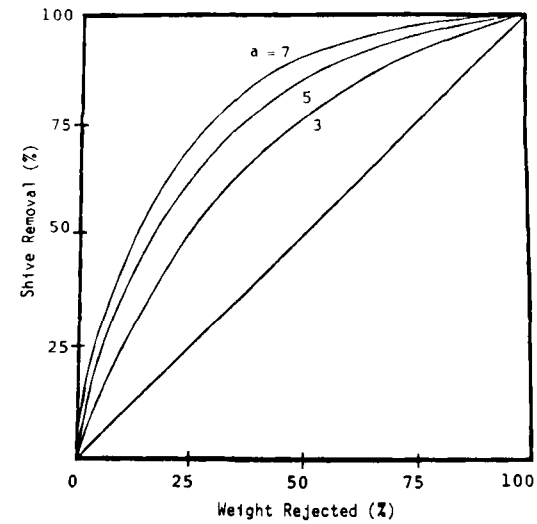

Figure 5. Shive removal model for screens and cleaners.

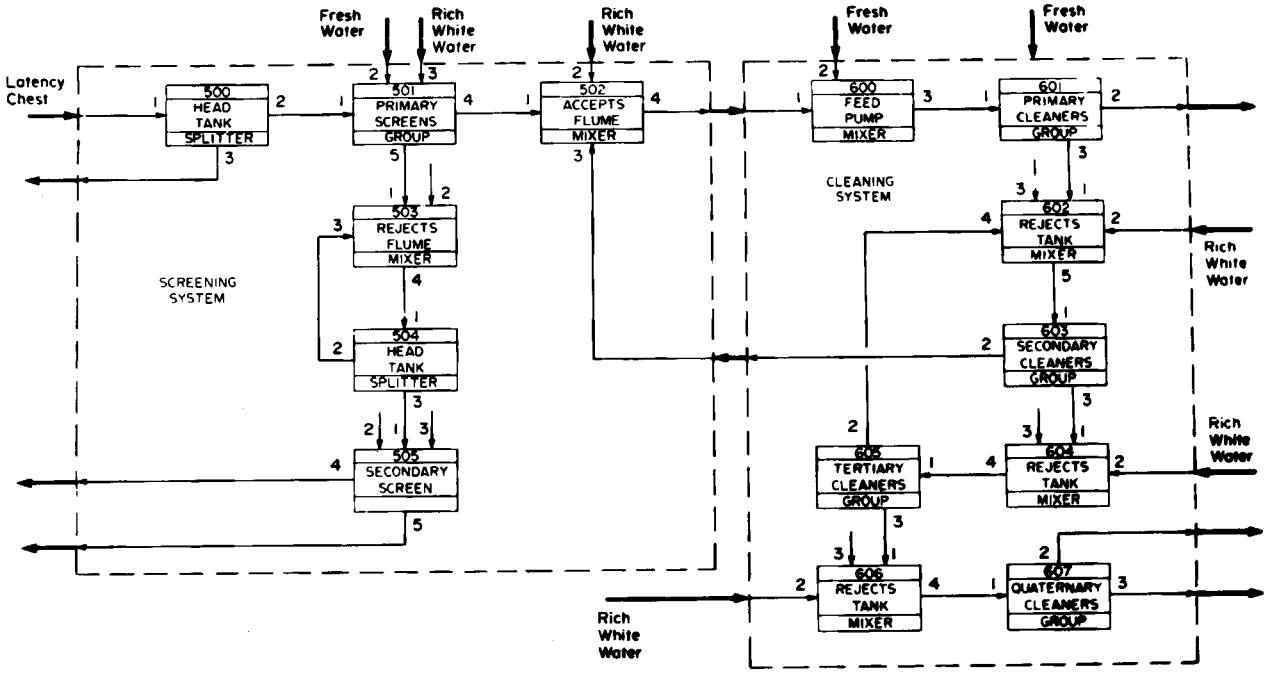

Figure 6. Block diagram for screens and cleaners flowsheet.

macro representing the secondary cleaners. The value of the shive removal constant is that which best fits the process measurements. The results of this analysis can be used to investigate alternative operating conditions or flow sheet arrangements in a predictive mode.

MEASUREMENTS

NAME	UNIT	STREAM	VARIABLE	MEASUREMENT	CALCULATED	
FRESH WATER	1	1	12	85.000	80.000	*
LATENCY CHEST	400	1	12	4000.000	4031.038	
LATENCY CHEST	400	1	11	1.150	1.185	
LATENCY CHEST	400	1	14	.350	.355	
LATENCY CHEST	400	1	13	1500.000	1515.968	
PRIMARY CLEANERS	601	2	12	8800.000	8957.159	
PRIMARY CLEANERS	601	2	13	1900.000	1817.740	
SECONDARY SCREEN	505	4	12	700.000	741.201	*
SECONDARY SCREEN	505	5	12	100.000	99.512	
SECONDARY SCREEN	505	4	13	1800.000	1820.100	
QUATERNARY CLEANER	607	2	12	100.000	90.629	*
QUATERNARY CLEANER	607	3	12	5.000	4.814	
QUATERNARY CLEANER	607	2	13	1800.000	1794.698	
RICH WHITE WATER	700	1	12	6000.000	5862.899	
RICH WHITE WATER	700	1	11	4.000E-02	2.982E-02	*
RICH WHITE WATER	700	1	13	2000.000	2043.657	
PRIMARY SCREENS	501	4	11	.800	.800	
PRIMARY SCREENS	501	5	11	1.900	1.878	
PRIMARY SCREENS	501	4	14	.200	.201	
PRIMARY SCREENS	501	5	14	1.100	1.143	
PRI. SCR. ACC. FLUME	502	4	12	9500.000	9533.606	
PRI. SCR. REJ. FLUME	503	4	12	650.000	616.094	
SECONDARY SCREEN	505	4	11	.750	.772	
SECONDARY SCREEN	505	5	11	2.000	1.978	
SECONDARY SCREEN	505	4	14	.700	.672	
SECONDARY SCREEN	505	5	14	2.500	2.440	
PRIMARY CLEANERS	601	2	11	.500	.443	*
PRIMARY CLEANERS	601	3	11	1.700	1.719	
PRIMARY CLEANERS	601	2	14	.130	.125	
PRIMARY CLEANERS	601	3	14	.450	.465	
PRI. CLNRS REJ. TANK	602	5	12	1650.000	1689.281	
SECONDARY CLEANERS	603	2	11	.600	.589	
SECONDARY CLEANERS	603	3	11	3.200	3.149	
SECONDARY CLEANERS	603	2	14	.200	.186	
SECONDARY CLEANERS	603	3	14	1.000	1.070	*
SEC. CLNRS REJ. TANK	604	4	12	325.000	325.581	
TERTIARY CLEANERS	605	2	11	.750	.809	*
TERTIARY CLEANERS	605	3	11	4.000	3.765	*
TERTIARY CLEANERS	605	2	14	.350	.302	
TERTIARY CLEANERS	605	3	14	2.500	2.599	
TER. CLNRS REJ. TANK	606	4	12	100.000	95.443	
QUARTERNARY CLEANER	607	2	11	.600	.673	*
QUARTERNARY CLEANER	607	3	11	12.000	11.646	
QUARTERNARY CLEANER	607	2	14	.800	.778	
QUARTERNARY CLEANER	607	3	14	5.000	4.504	*
RICH W.W. HEADER	703	2	12	1400.000	1398.033	
RICH W.W. HEADER	703	3	12	200.000	200.858	
RICH W.W. HEADER	703	4	12	225.000	221.940	
RICH W.W. HEADER	703	5	12	3000.000	2994.223	
RICH W.W. HEADER	703	6	12	800.000	787.915	
RICH W.W. HEADER	703	7	12	200.000	205.148	
RICH W.W. HEADER	703	8	12	50.000	54.781	*

Figure 7. Measurements summary.

SUMMARY

The MASSBAL program implements the equations-oriented approach to process simulation in a modular environment. Standard building blocks, which set up equations for such fundamental operations as stream mixing and separation, are used to represent the process. The model equations form a large set of nonlinear algebraic equations which are solved simultaneously using the Newton-Raphson iterative technique.

Reconciliation of process measurements is an optional feature of the MASSBAL program. The associated optimization is solved using Lagrange multipliers. It is shown that for the equations-oriented approach data reconciliation is a straightforward extension of the simulation problem. This feature makes process simulation more directly usable by in-plant engineers for detecting instrument problems, troubleshooting operating problems, and monitoring performance. It also provides a mechanism for specialists in process simulation to more easily generate validated process models.

UNIT 603 - SECONDARY CLEANERS

STREAM TONS PER DAY	1 INLET	2 OUTLET	3 OUTLET
SHIVES	.327	.104	.223
FIBRE	76.457	55.791	20.666
WATER	10049.660	9408.526	641.135
SOLIDS	19.389	18.152	1.237
TOTAL FLOW	10145.833	9482.572	663.261
PULP ODT/DAY	76.784	55.895	20.889
CONSISTENCY	.757	.589	3.149
USGPM	1689.281	1578.848	110.433
PPM SOLIDS	1929.274	1929.274	1929.274
% SHIVES	.426	.186	1.070

CLEANER PARAMETERS -

% TOTAL REJECTS	6.537
% PULP REJECTS	27.029
% SHIVES REMOVED	68.258
CLEANER CONSTANT [A]	5.805
A X R	156.916
[A-1] X R + 1	229.887
ANR/[[A-1]XR+1]	68.258
NO. BANKS OPERATING	3.000

Figure 8. Output for secondary cleaners.

ACKNOWLEDGMENT

This paper is based in part upon the paper "The Reconciliation of Process Simulation and Actual Operation," by C. F. Shewchuk, which is in the Proceedings of the Technical Association of the Pulp and Paper Industry, 1984 Annual Meeting, TAPPI Press, Atlanta.

NOTATION

a = screen/cleaner shive removal constant

$A = P \times P$ diagonal matrix defined by $A_{pp} = \sum_{q=1}^{Q_p} 2w_{pq}/r_{pq}^2$

B = vector of length P defined by $B_p = \sum_{q=1}^{Q_p} 2w_{pq}m_{pq}/r_{pq}^2$

C = number of components in a stream

f = lefthand side vector of model equations

f_{io} = flow of component i in inlet stream

f_{ik} = flow of component i in outlet stream k

F_o = total flow in inlet stream

F_k = total flow in outlet stream k

g = objective function for data reconciliation

G = Lagrangian

i = model equation index

j = solution vector index

J = Jacobian matrix

k = outlet stream index for splitter building block

K = number of outlet streams for splitter building block

m_{pq} = qth measurement for u_p

M = number of variables in solution vector

N = number of model equations

p = measured variables vector index

P = number of measured variables

q = measurements for u_p index

Q_p = number of measurements for u_p

r_{pq} = measurement range for the qth measurement of u_p

R_w = screen/cleaner weight reject ratio

T_o = temperature of inlet stream

T_k = temperature of outlet stream k

u = subset of x for which measurements exist

v = subset of x for which no measurements exist

w_{pq} = arbitrary weight for qth measurement of u_p

x = solution vector for model equations

x° = estimate of x

Δx = vector of corrections to x

ϵ = convergence tolerance

ϵ_s = screen/cleaner shive removal efficiency

λ = vector of Lagrange multipliers

ϕ = relaxation factor

LITERATURE CITED

Bending, M. J. and H. P. Hutchison, "The Calculation of Steady-State Incompressible Flow in Large Networks of Pipes," *Chem. Eng. Sci.*, 28, 1857 (1973).

Crowe, C. M., Y. A. G. Campos, and A. Hrymak, "Reconciliation of Process Flow Rates by Matrix Projection. I: Linear Case," *AIChE J.*, 29(6), 881, (1983).

Ham, P. G., G. W. Cleaves, and J. K. Lawlor, "Operation Data Reconciliation: An Aid to Improved Plant Performance," *Proc. 10th World Petroleum Congr.*, Bucarest, 4, 281 (1979).

Hlavacek, V., "Analysis of a Complex Plant – Steady-State and Transient Behavior," *Compute. Chem. Eng.*, 1(1), 75 (1977).

Kuehn, D. R., and H. Davidson, "Computer Control II Mathematics of Control," *Chem. Eng. Prog.*, 57(6), 44 (1961).

Mah, R. S. H., "Design and Analysis of Process Performance Monitoring Systems," *Proc. Eng. Found. Conf. on Chem. Process Control* 2, Sea Island, GA (1981).

Myers, A. L., and W. D. Seider, *Introduction to Chemical Engineering and Computer Calculations*, Prentice-Hall, Englewood Cliffs, NJ (1976).

Shacham, M., et al., "Equations-Oriented Approach to Process Flowsheeting," *Compute. Chem. Eng.*, 6(2), 79 (1982).

Shewchuk, C. F., S. J. Waite, and R. A. Hinton, "A Practical User-Oriented Program for Evaporator Analysis," *AIChE Symp. Ser.*, 76(200), 143 (1980).

Westerberg, A. W., et al., *Process Flowsheeting*, Cambridge Univ. Press, Cambridge (1979).

Manuscript received Jan. 3, 1984, and revision received Apr. 22, 1985.