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An Introduction to the CONCEPT
Program for Controller-Run
Solvent Extraction
Process Testing

A. D. Mitchell

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AN INTRODUCTION TO THE CONCEPT PROGRAM FOR CONTROLLER-RUN
SOLVENT EXTRACTION PROCESS TESTING

A. D. Mitchell⁷⁷
Chemical Technology Division

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AN INTRODUCTION TO THE CONCEPT PROGRAM FOR CONTROLLER-RUN
SOLVENT EXTRACTION PROCESS TESTING

A. D. Mitchell

ABSTRACT

The CONCEPT program is a new computer model for controller-run solvent extraction process testing. The program can currently be used for the Purex and Thorex processes. Although CONCEPT was tailored to model centrifugal contactors, other types of contactors can also be simulated. The major features of this program include its provisions for variable flow rates and volumes and its implementation of automatic process controllers. A listing of the program and instructions for its use are presented.

1. INTRODUCTION

The CONCEPT program is a new computer model for controller-run solvent extraction process testing. The program was developed as a tool for testing ideas in the reprocessing of nuclear fuel. The basic concepts and methods used in the CONCEPT program are similar to those in the SEPHIS programs.¹⁻³ The new abilities of this program make it especially useful in certain modeling applications; but due to some very specific limitations, the CONCEPT program should not be viewed as a replacement for the SEPHIS-MOD4 program.

The CONCEPT program is built on a stage model similar to that of the SEPHIS-MOD4 program. The differences arise in the specific assumptions used to limit the stage model. The SEPHIS programs assumed that both the flow rates and the volumes were constants set by the user. The CONCEPT program calculates the stream flow rates and stage volumes using equations that describe their interrelationship.

The concentrations in the CONCEPT program are calculated in a manner similar to that of the SEPHIS-MOD4 program. In SEPHIS-MOD4 the stages are

tailored to resemble mixer-settler stages with explicitly defined mixers and settlers. However, the CONCEPT program uses stages that are tailored to act like centrifugal contactors with instantaneous mixing and phase separation.

One of the major features of the CONCEPT program is its use of process controllers. In SEPHIS-MOD4 the feed stream variables are treated as constants, but in the CONCEPT program, each of the feed stream variables (i.e., flow rates, concentrations, and temperatures) can be automatically and independently controlled based on some other variable in the system. These controllers can be employed in optimization, flowsheet development, plant monitoring, and safeguards testing.

In adapting the ideas of the SEPHIS-MOD4 program to the stage model in the CONCEPT program, certain procedures had to be revised or removed. This prevents the use of the CONCEPT program as a replacement to the SEPHIS-MOD4 program for the Purex process. In the SEPHIS-MOD4 program for the Purex process, the conversion of units from a molar to a molal basis was done to bypass the effects of changes in volume due to changes in concentration. This conversion does not seem to be feasible in the CONCEPT program. The assumption of where and when chemical equilibrium occurs is very similar for the two programs, but the printed results for the SEPHIS program are equilibrium results, whereas those of the CONCEPT program are not necessarily equilibrium results. In addition, the assumptions made in adapting plutonium reduction reactions in the CONCEPT program are different from those made in the SEPHIS-MOD4 program, and consequently the results differ. For these reasons the CONCEPT program is not a replacement for the SEPHIS-MOD4 program and should be used primarily when its extra abilities are required.

The program has been converted to use SI-metric units. The only significant change involved changing the time basis from minutes to seconds. For those comfortable with the SEPHIS-MOD4 program, this will entail a change in the ratio of flow rate to volume and in the corresponding time increment.

The CONCEPT program was originally designed to test solvent extraction flowsheets proposed for centrifugal contactors with process controllers. However, implementation of the stage model in the program now allows the user to test many ideas in addition to those originally intended. In conjunction with experimental testing, the program should become a useful aid in developing flowsheets for nuclear fuel reprocessing.

2. STAGewise IDEAS AND MATHEMATICS IN THE CONCEPT PROGRAM

The ideas and mathematics in the CONCEPT program make it distinct from other solvent extraction modeling programs. Although the general description of the stages with their associated feed streams is similar to that of other models, the use of equations to calculate changes in flow rates and volumes, and the particular method of calculating concentrations distinguish this program from its predecessors. The CONCEPT program also employs automatic process controllers on the feed-stream variables if specified by the user. The correlation for calculating distribution coefficients and the mechanics of plutonium reduction reactions are adapted from the SEPHIS-MOD4 program. The variables used in the equations are defined in Appendix A.

2.1 General Model of a Stage

The model of a stage in the CONCEPT program is subdivided into the description of fluid flows through the stage and the description of solute flows through the stage. The description of fluid flows is primarily a volume balance problem where the changes in stage volumes are regulated by the flow rates in the stage. The description of solute flows is in the application of unsteady-state mass balances in the stage. Once one stage has been described, it is easy to group many such stages to describe any desired solvent extraction system.

The volumes and flow rates of the two phases comprise the fluid-flow problem to be described. Figure 1 shows the idealized stage (j) used in the description. Four streams may enter each stage: the aqueous stream from the preceding stage (A_{j-1}), the organic stream from the succeeding stage (O_{j+1}), the aqueous feed stream (A_{fj}), and the organic feed stream (O_{fj}). The aqueous and organic streams which leave the stage (A_j , O_j) either flow to the next stage or leave the system as product streams. Under normal conditions, the position of the phase interface will vary between the aqueous volume set point (V_S) and the total stage volume (V_T). The aqueous volume set point is the maximum aqueous volume that could be found in the stage without having an aqueous stream flowing out of the stage. The aqueous volume set point can be zero if the stage

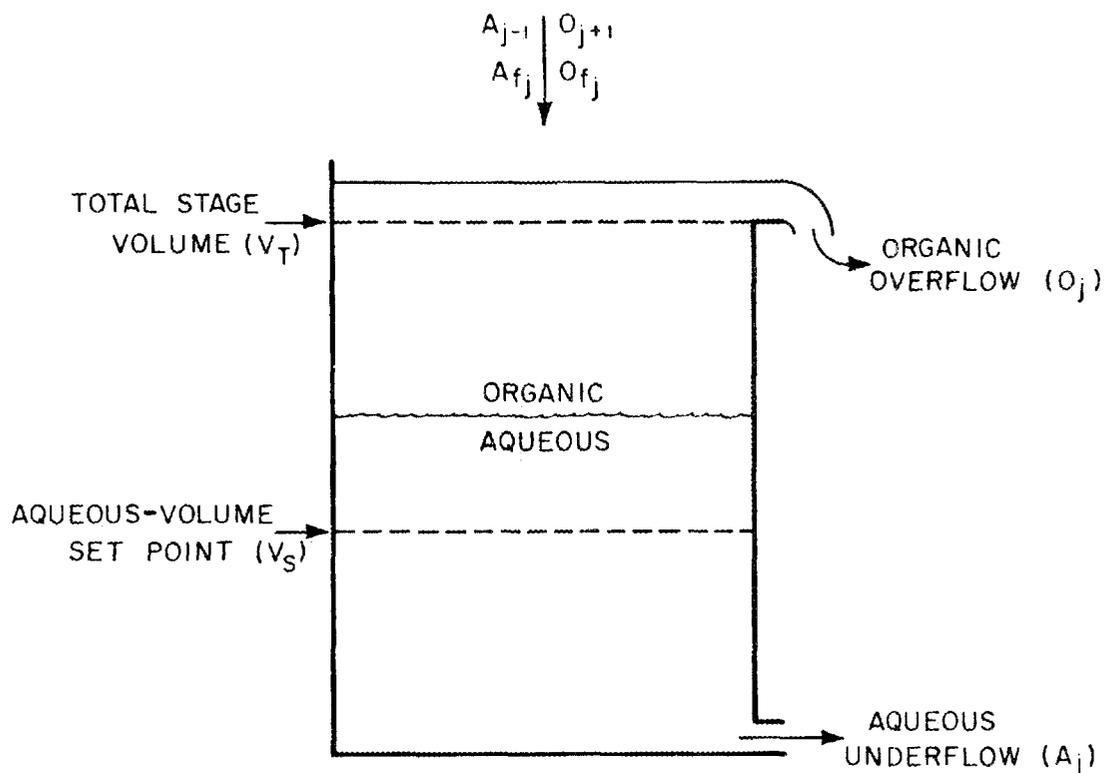


Fig. 1. General model of volumes and flow rates in a stage.

drains completely; values greater than zero indicate that there would be a residual volume due to back-pressure or a trap or jackleg on the aqueous underflow. The total stage volume is the volume up to the organic overflow weir.

The solute-flow problem can be visualized more easily with a group of stages as shown in Fig. 2. The stages in the CONCEPT program are arranged so that the aqueous phase flows toward higher numbered stages while the organic phase flows toward lower numbered stages. The solutes enter the system in the feed streams (identified by the subscript f). The feed streams are combined with streams from neighboring stages in what can be called a mixer. Because the CONCEPT program tries to mimic centrifugal contactors where the mixing time is essentially zero, the mixer in the CONCEPT program has no volume and no residence time. It is used only to equilibrate the streams entering the stage. The products of the mixer are combined with the stage contents in what can be thought

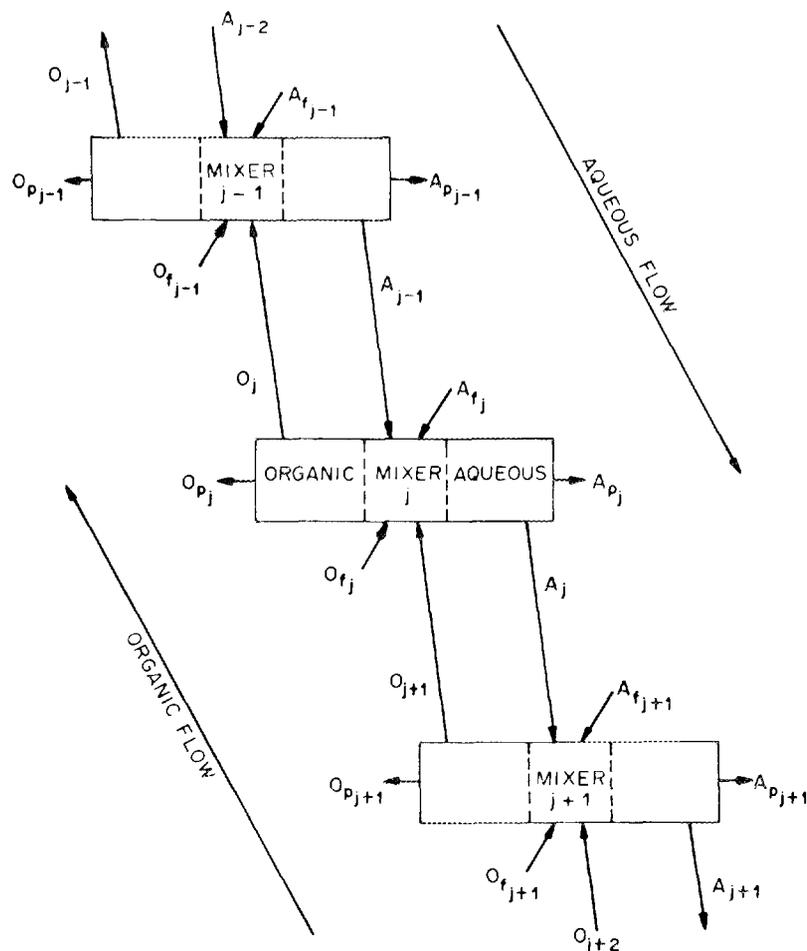


Fig. 2. A group of stages showing interconnecting streams.

of as settlers. Except for considering reactions, the aqueous and organic phases in the settler are kept separate and the solutes are not allowed to change phase. In the case of plutonium reduction reactions, the organic-phase plutonium(IV) is allowed to cross from the organic to the aqueous portion of the settler. The products of the settler leave the stage and proceed to the next mixer, or leave the system as a product stream (identified by the subscript p). It should be noted that the interstage flow rate (i.e., A_j in Fig. 2) is actually $A_j - A_{p,j}$, and A_j is the total phase flow rate out of the stage. (Figure 2 was simplified for clarity.)

The feed-stream variables in the CONCEPT program can be varied automatically by use of process controllers. The controllers can vary the solute concentrations, temperatures, and flow rates of the feed streams. The variable monitored by the controller can be any concentration, temperature, flow rate, volume, or density in the system. The controller can use either three-mode or on/off controlling schemes. Feed-stream variables can also be constants (noncontrolled).

2.2 Mathematical Model of Mass Balances in a Stage

The general description of a stage indicates how the separate components fit into the overall scheme. However, the computer must be given equations with which to work. In this case, volume and mass balances must be written for the fluid-flow and solute-flow problems. It should be noted that the following mass balances neglect the product streams. The product streams constitute a constant term subtracted from the flow rate arriving from the preceding or succeeding stages (A_{j-1} or O_{j+1}), and they are treated as such by the program.

The differential volume balances for each phase describe how the volumes depend on the flows. For the aqueous phase

$$\frac{dV_{aj}}{dt} = A_{j-1} + A_{fj} - A_j, \quad (1)$$

or the rate of change of the volume is equal to the difference between the flow rates of the streams entering the stage and the flow rate of the stream leaving the stage. Similarly for the organic phase,

$$\frac{dV_{oj}}{dt} = O_{j+1} + O_{fj} - O_j. \quad (2)$$

Assuming that the flow rates into the stage are given, the only variables remaining are A_j and O_j . These are described by

$$A_j = k_{aj}(V_{aj} - V_{Sj}), \quad (3)$$

and

$$O_j = k_{oj}(V_{oj} + V_{aj} - V_{Tj}). \quad (4)$$

These equations assume that the aqueous flow rate out of the stage is proportional to the aqueous volume in excess of the set-point volume, and the organic flow rate out of the stage is proportional to the organic volume over the overflow weir. The program imposes other restrictions, namely:

$$V_{aj} \leq 0.95 V_{Tj} ; \quad (5)$$

$$k_{aj} > 0 ; \quad (6)$$

$$k_{oj} > 0 ; \quad (7)$$

$$A_j \geq 0 ; \quad (8)$$

and

$$O_j \geq 0 . \quad (9)$$

These restrictions derive from the mathematical requirements of the program and from practical limitations on the system. The restriction in Eq. (5) keeps the aqueous level from going above the overflow weir. Although the program would not allow an aqueous stream to flow over the weir, the large aqueous volume would produce problems in Eq. (4). If the restriction in Eq. (5) were removed, there could conceivably be a calculated organic flow out of a stage [from Eq. (4)] without any organic being present in the stage. The factor of 0.95 was chosen arbitrarily. Equations (6) and (7) are used to prevent division by zero and negative flow rates. Equations (8) and (9) restrict the flow rate to non-negative values. A negative flow rate would mean that a stream was flowing in the wrong direction, and the mass balances in the program are not designed to handle such a stream.

Considering the aqueous phase, Eq. (3) is substituted into Eq. (1) giving

$$\frac{dV_{aj}}{dt} + k_{aj} V_{aj} = A_{j-1} + A_{fj} + k_{aj} V_{Sj} . \quad (10)$$

This is a first-order linear differential equation, and the solution to the general case is of the form

$$V_{aj} = \exp(-fk dt) [C + \int \exp(fk dt) (A_{j-1} + A_{fj} + k_{aj} V_{Sj}) dt] . \quad (11)$$

The program uses an integrated form of Eq. (11), which explicitly defines the new aqueous volume in terms of the previous volume and the parameters in Eq. (11). The integration of Eq. (11) is over one time interval, Δt ; V_{Sj} and k_{aj} are treated as constants, but A_{j-1} and A_{fj} are assumed to vary linearly over the time increment Δt . The integration is performed for the general case of Eq. (11), for the special case $V_{aj} \leq V_{Sj}$, and for the transition case. The equations for the organic phase are treated similarly. The accuracy of these methods is discussed in Sect. 4.

The calculation of flow rates and volumes is followed by the calculation of concentrations, which is accomplished in two steps. The streams entering the stage are equilibrated in the mixing zone of the contactor. After being equilibrated, the entering streams are combined with the contents of the aqueous and organic settlers. These settlers are treated as well-stirred tanks with the volumes defined above.

Equilibration of streams entering the stage is performed by applying a steady-state mass balance. This mass balance dictates that the amount of solute leaving the mixer is equivalent to the amount entering the mixer, or

$$A_{mj}x_{mj} + O_{mj}y_{mj} = A_{j-1}x_{j-1} + A_{fj}x_{fj} + O_{j+1}y_{j+1} + O_{fj}y_{fj} . \quad (12)$$

Further requirements are imposed that

$$A_{mj} = A_{j-1} + A_{fj} , \quad (13)$$

and

$$O_{mj} = O_{j+1} + O_{fj} . \quad (14)$$

To equilibrate the streams, the aqueous and organic concentrations are related by a distribution coefficient

$$y_{mj} = D x_{mj} . \quad (15)$$

The distribution coefficient is calculated as a function of the aqueous concentrations, the tributyl phosphate (TBP) content of the organic phase, and the temperature. The temperature in this case is calculated by a simple heat balance

$$T_{mj}(A_{mj} + O_{mj}) = A_{j-1}T_{j-1} + A_{fj}T_{fj} + O_{j+1}T_{j+1} + O_{fj}T_{fj}, \quad (16)$$

with consideration given to the different specific heat of the organic phase. In Eqs. (12) through (16) the temperatures, concentrations, and flow rates of the streams entering stage j are taken to be the average of the values at the start and at the end of the time increment. The concentrations subscripted by m are taken to be constant over the time increment. It should be noted that Eqs. (12) and (15) are not used for extreme flow ratios

$$A_{mj} \geq 25 O_{mj} \quad (17)$$

nor

$$O_{mj} \geq 25 A_{mj}. \quad (18)$$

In these cases the mass balance is simply

$$A_{mj}x_{mj} = A_{j-1}x_{j-1} + A_{fj}x_{fj}, \quad (19)$$

with a similar equation for the organic phase. With extreme flow ratios, unrealistic solute concentrations are calculated during the start-up of a process. This is generally not a problem after each stage has an adequate flow of each phase, but the restrictions in Eqs. (17) and (18) were added as a housekeeping measure during start-up. This completes the equilibration of streams entering the stage, so these streams now flow to the settlers.

The equilibrated streams are combined with the contents of the settlers according to a mass balance for a well-stirred tank. For the aqueous phase,

$$\frac{d(V_{aj}x_j)}{dt} = (A_{j-1} + A_{fj})x_{mj} - A_jx_j + G, \quad (20)$$

or the change in the amount of a solute in the stage is equal to the difference between the amount flowing in and the amount flowing out of the stage, with consideration given for any amount generated by reactions in the stage. To simplify this equation, the differential is expanded according to

$$\frac{d(V_{aj}x_j)}{dt} = V_{aj} \frac{dx_j}{dt} + x_j \frac{dV_{aj}}{dt}, \quad (21)$$

or by substituting from Eq. (1)

$$\frac{d(V_{aj}x_j)}{dt} = V_{aj} \frac{dx_j}{dt} + x_j (A_{j-1} + A_{fj} - A_j). \quad (22)$$

Using algebraic relationships on Eqs. (20) and (22)

$$V_{aj} \frac{dx_j}{dt} - (A_{j-1} + A_{fj})(x_{mj} - x_j) = G. \quad (23)$$

In this equation, x_{mj} and G are considered to be constants for a time increment; V_{aj} , A_{j-1} , and A_{fj} are considered to vary linearly from the start of the time increment to the end of it. The solution to Eq. (23) for the general case is

$$z = \exp[-\int P(t) dt] \{C + \int Q(t) \exp[\int P(t) dt] dt\}, \quad (24)$$

where

$$z = x_{mj} - x_j, \quad (25)$$

$$P(t) = \frac{A_{j-1} + A_{fj}}{V_{aj}}, \quad (26)$$

and

$$Q(t) = -G/V_{aj}. \quad (27)$$

The CONCEPT program uses an integrated form of Eq. (24). The integration of Eq. (24) is over one time interval, Δt . Because of the complexity of the integration, certain liberties were taken to simplify the expressions where necessary. The integration was performed for the general case and for a number of important special cases. Similar equations are used for the organic phase. The accuracy of these methods is discussed in Sect. 4.

2.3 Process Controller Operation

Implementation of process controllers is a major feature of the CONCEPT program. Properly employed, the process controllers in the pro-

gram can automatically determine flowsheet conditions; simulate unit operations; transfer streams from one place to another; add, subtract, multiply, divide; act as timers or alarms; or simply simulate process controllers. Their proper specification requires thoughtful consideration on the part of the user, but their potential usefulness should warrant this degree of consideration.

The CONCEPT program uses three-mode (PID) and on/off-type controllers. In both cases the goal is to control some particular feed-stream variable based on a controlling scheme and the value for a system variable being monitored. In the input to the program, the user must specify which variable is being controlled, which variable is being monitored, and the controlling scheme to be used. Any number or combination of these process controllers can be used, and any variable in the system can be monitored.

2.3.1 Three-mode controllers

The controlling scheme for three-mode controllers is shown in Fig. 3. When the computer evaluates a process controller, it first finds the value

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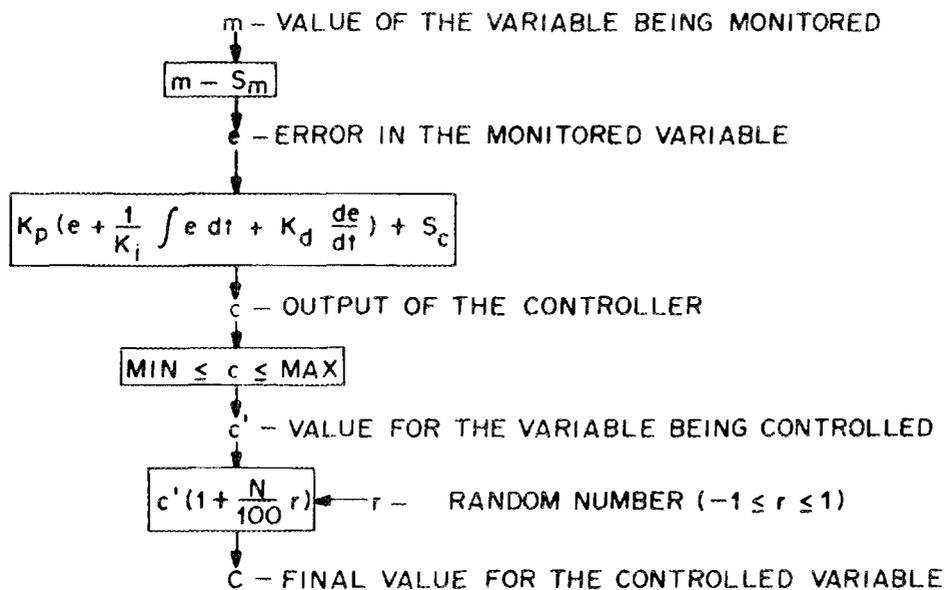


Fig. 3 Controlling scheme for a three-mode controller.

of the variable being monitored. This value is compared with the set point for the monitored variable. For regular controller operation, the set point is the target value for the controller. However, for many controller uses, the set point is just a number to subtract from the value of the monitored variable. Subtracting the set point from the value of the monitored variable results in an error in the monitored variable. This error is used in a standard three-mode controller equation

$$c - S_c = K_p [e + (1/K_i) \int e dt + K_d (de/dt)] , \quad (28)$$

where c is the output of the controller. The initial value for the integral term in Eq. (28) is set to zero when the feed streams are reinitialized. The value for the integral is approximated as a summation

$$\int_0^t e dt = \sum_{t=0}^t \frac{e_{t+\Delta t} + e_t}{2} \Delta t . \quad (29)$$

The derivative term is approximated as

$$\frac{de}{dt} = \frac{e_{t+\Delta t} - e_t}{\Delta t} . \quad (30)$$

The four constants in Eq. (28) are determined by the user. Controllers generally have limitations on their operation (a valve may be opened no further than all the way, nor closed further than off). Thus the value of c is constrained by a minimum and a maximum value which must be specified by the user. After the limits have been imposed, some amount of noise or an error band may be applied to the value of the variable being controlled. The size of the error band, N , is determined by the user. This noise can be viewed either as a degree of measurement uncertainty or as an error in valve placement. The position within the error band is determined by a random number. The noise is applied according to

$$C = c' [1 + r(N/100)] , \quad (31)$$

so the error band is some fraction of c' rather than an absolute amount. The final value for the controlled variable, C , is also constrained to be greater than zero (except in the case of temperature).

2.3.2 On/off controllers

The controlling scheme for on/off controllers is shown in Fig. 4. As for three-mode controllers, the computer starts by finding the value of the variable being monitored. This value is compared with two set points (referred to as upper and lower set points). If the monitored value is higher than the upper set point, the controller turns the controlled variable to the "on" value. If the monitored value is below

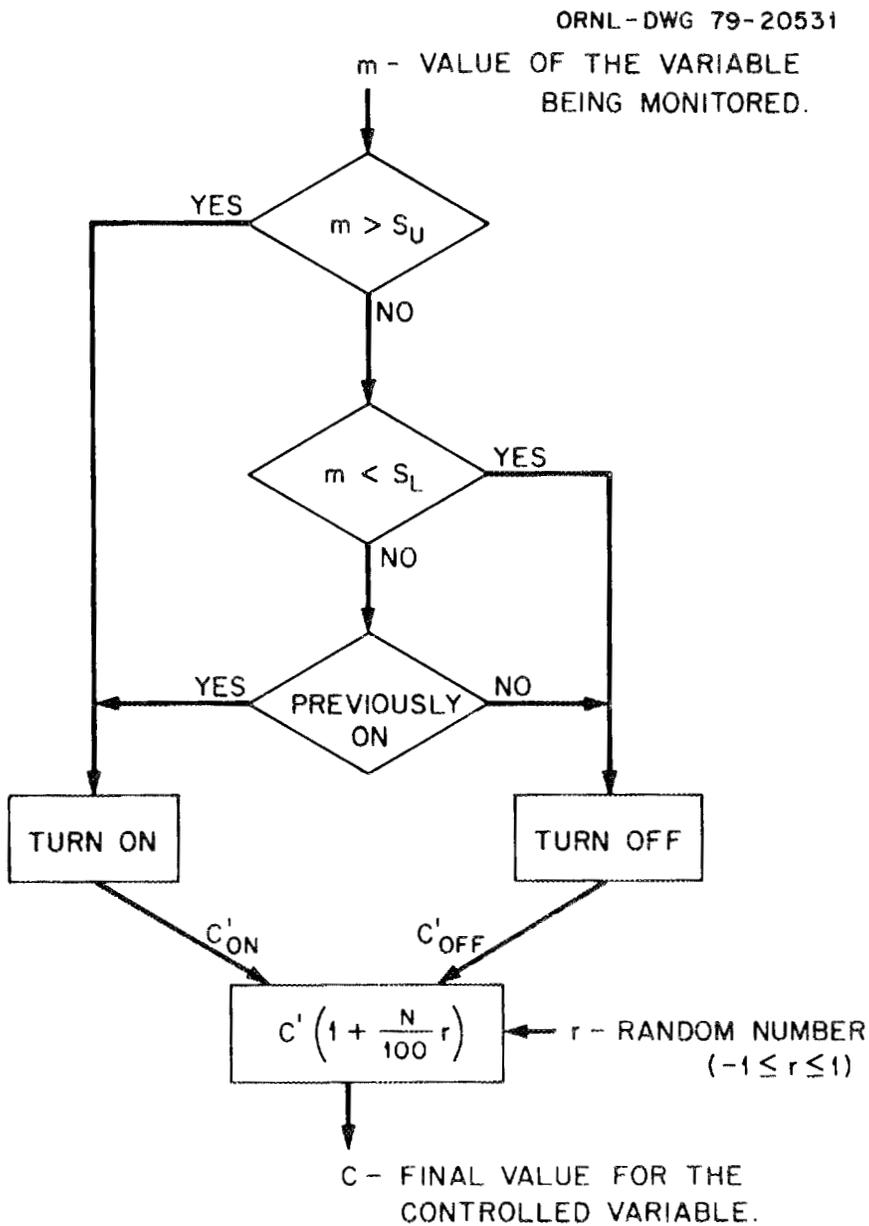


Fig. 4. Controlling scheme for an on/off controller.

the lower set point, the controlled variable is turned to the "off" value. If the monitored value is between the upper and lower set points, the controlled variable is turned to whichever state it was already in. After determining whether the controlled variable is "on" or "off," the controller imposes the noise or error band in the same way as with the three-mode controller.

It should be noted that when the monitored value is between the upper and lower set points, the computer determines whether the controlled variable was "on" or "off" by determining whether the previous value for C is closer to c'_{on} or c'_{off} . This has consequences only when the noise or error bands for c'_{on} and c'_{off} overlap. In such a case, the controlled variable may switch between "on" and "off" when the random number causes C to be in the overlapping region. This switching is generally an unimportant consequence, and may be a useful property.

2.3.3 Variables that can be controlled or monitored

To give the user a large amount of flexibility in devising his system, every feed-stream variable kept by the program may be controlled independently and simultaneously. The feed-stream variables kept by the program are concentrations, temperature, and flow rate.

An even more extensive variety of variables can be monitored. A controller can monitor variables directly or indirectly. The directly monitored variables include the concentrations, temperature, or flow rate of any feed stream, and the concentrations, temperature, flow rate, density, or volume of either phase in any stage in the contactor bank. The flow rate of a stage in this case is the flow rate out of the stage (such as A_j) rather than the flow rate to the next stage ($A_j - A_{pj}$).

Certain variables (such as elapsed time or feed-stream density) can only be monitored indirectly by using careful thought and subterfuge. For example, monitoring elapsed time is useful in setting timers for events such as a stream turnoff, or for setting alarms for events such as unacceptable product concentrations. What is needed is a variable that can be simply related to time. An obvious choice is volume. If a

feed stream with a small flow rate is directed into a large, empty tank (a stage used exclusively for this purpose), the accumulated volume in the tank will be a direct measure of elapsed time. The feed stream and tank combination are easily specified by proper use of the stage volume parameters.

Monitoring the density of a feed stream is even easier. A feed stream (identical to the desired stream) can be run through a stage used exclusively for this purpose, and the density of the solution in the stage can be monitored. This will introduce a small time delay in the measurement, but that is generally unimportant. Ratios of plutonium to heavy metal, sums of component concentrations, or stage inventories can be monitored through use of similar, but more complicated, tricks.

These indirect measurements, when so specified, could have been accommodated by simple changes in the program. However, it is very difficult to know what variables would be most desired by the general user. It is even more difficult to devise a general scheme to specify, for example, that the required variable is the ratio of plutonium leaving in the product to the plutonium leaving in the waste. The user has the options of modifying the program to his special needs, or contriving to get the same information by indirect methods or clever tricks. Several tricks with controllers are described more fully in Sect. 7.

2.4 Distribution Coefficients

The CONCEPT program can currently work with the Purex process or the Thorex process. For the most part, the correlations used to calculate distribution coefficients are the same as those used in the SEPHIS-MOD4 program.

For the Thorex process the program calculates distribution coefficients for uranium, thorium, and nitric acid. The distribution coefficient for inextractable nitrates is assumed to be zero. The correlations used are identical to those in the SEPHIS-MOD4 program, and the steady-state results should also be identical.

For the Purex process the program calculates distribution coefficients for uranium, plutonium, and nitric acid. The coefficients for

reduced plutonium, plutonium reductant, and inextractable nitrates are assumed to be zero. A correction for the plutonium distribution coefficient as described by Jubin⁴ has been added. Because the correlations in the SEPHIS-MOD4 program are in terms of molal units whereas those in the CONSEPT program are in molar units, the molar concentrations are converted before using the correlations, and the resulting distribution coefficients are converted back to molar units before they are used. This method of conversion produces small discrepancies between the results of the CONSEPT program and the SEPHIS-MOD4 program.

2.5 Plutonium Reduction Reactions

The mechanics of plutonium reduction are adapted largely from the SEPHIS-MOD4 program. The CONSEPT program allows instantaneous reduction, reduction by uranium(IV), and reduction by hydroxylamine. The results of the two programs differ moderately, and this difference is thought to be due to two differences in the program. First, in the SEPHIS-MOD4 program the reaction rate is determined by molal concentrations, whereas in the CONSEPT program the rate is determined by molar concentrations. This should result in small, but noticeable, discrepancies.

The second difference is in the method of factoring the extent of reaction into the amount of solute initially present. In the SEPHIS-MOD4 program the extent of reaction is defined in terms of some amount of solute reacted. This amount is then added (or subtracted) to the amount of that solute in the stage. In the CONSEPT program the extent of reaction is converted to a rate or generation term in Eq. (24). This rate, multiplied by a weighting factor determined by the mass balance in Eq. (24), is added (or subtracted) to the concentration in the stage. Ideally, these two methods should produce the same results, but the different assumptions and approximations produce discrepancies.

The differences between the two programs should not be overstated. They are generally small; and, as often happens in cases like this, it is difficult to determine which method is truly more correct.

3. OVERVIEW OF THE CALCULATIONAL ROUTINES

The equations for the mass balances are only the first hurdle toward completing a model of solvent extraction. These equations must then be fit into a coherent calculational routine so that every argument in a particular equation has a previously computed value when that equation is applied. The calculational routine in the CONCEPT program is primarily in the STAGES subroutine. The subroutines for input and output are important to the program, but they are not complex enough to warrant discussion.

The STAGES subroutine first calculates the aqueous volumes and flow rates by applying the integrated form of Eq. (11) to calculate the volume and Eq. (3) to calculate the flow rate. Equation (11) indicates that the only information required to compute the volume is the volume parameters k_{aj} and V_{Sj} (constants read from the input cards), the feed-stream flow rate, and the flow rate from the preceding stage. The feed-stream flow rate can be either a constant read from input cards or a controlled variable. In the case of a controlled variable, the program uses the value from the input card as an initial value for the first time increment. For all subsequent increments, the program uses the previously calculated value from the controller. The flow rate from the preceding stage was calculated immediately before this stage was considered. The CONCEPT program calculates for only one stage at a time, so when the aqueous volumes are being computed, the program starts with stage one, which has no preceding stage. After stage one has been evaluated, the program moves to stage two, whose preceding stage now has a calculated value for the flow rate.

After all of the aqueous volumes and flow rates have been computed, the organic volumes and flow rates can be evaluated. The organic values must be computed after the aqueous values because of the linkage in Eq. (4). The calculation proceeds in the same manner as for the aqueous phase except that the routine starts with the last stage and moves toward the first stage.

This completes the fluid-flow problem. The flow rates and volumes are evaluated first because they do not depend directly on any other variables in the system as defined in Eqs. (1) through (4). There may be an indirect dependence when a feed-stream flow rate is being controlled. This indirect dependence is taken into account, but the effect of the controllers has an implicit and generally insignificant time delay.

The calculation of concentrations and temperatures requires more work from the computer. From Eq. (12) the concentration in a stage can depend on the concentrations in both the preceding and succeeding stages. Consequently, a direct, accurate calculation, as was used with the volumes, is precluded. One of the variables will always be slightly in error unless a very complex matrix inversion is used. In preference to this method, the CONCEPT program uses a short predictor-corrector type approach.

The program maintains values for variables for two points in time, t and $t + \Delta t$. When the concentrations are being evaluated, the program lacks a value for the succeeding stage for time $t + \Delta t$. To bypass this deficiency, the program makes a rough initial calculation by assuming that the values it lacks for time $t + \Delta t$ have not changed significantly from the values at time t . After the rough calculation has been completed for all the stages, the procedure is repeated. However, for the second calculation, the program now has a much better approximation for the values it lacked in the first calculation. Thus the program first predicts values it lacks, then it corrects its predictions for the final calculation.

Within this predictor-corrector loop is the actual concentration calculation. The calculation is done in three distinct steps. The first step is an iteration between Eqs. (12) and (15). The iteration is to find a consistent set of distribution coefficients and aqueous concentrations. The second step is the partial application of Eq. (24). This initial calculation assumes that the generation term is zero. The result is the concentrations which would be found if there were no reactions. These concentrations are used to determine the extent of

reaction in the third step. The extent of reaction gives the final term in Eq. (24) and the final calculated concentrations.

After the concentrations have been calculated, the program evaluates the feed-stream controllers. The program scans through all of the feed-stream variables to find which ones have process controllers. Upon finding one, the program determines the new value for the controlled variable depending on the controller scheme used and on the value of the monitored variable.

At this point the program has values for every variable at times t and $t + \Delta t$. All of these values are used to check the convergence to steady state. The rate of change for every variable is checked against a tolerance. The maximum change for each phase is printed by stage with the concentration profile, which gives the user an indication of the magnitude and location of the changes in the system.

This completes the calculation for the new point in time, so time is incremented and the calculation is repeated.

4. ACCURACY OF THE MATHEMATICS

Several approximations were made in deriving the mass balance equations. To check the accuracy of the resulting equations and to show the influence of the time increment, several trial calculations were performed. The behavior of the program was compared with ideal behavior for volume balances, solute balances, and controller behavior.

The examples in this section should give the user an indication of the mathematical errors to be expected. These examples are comparisons with mathematical ideality, and should not be misinterpreted as comparisons with actual solvent extraction system behavior.

4.1 Accuracy of Volume Balances

The accuracy of the volume balances was tested by comparing the program results with the analytical solutions. In this way, the influence of the approximations could be ascertained. These comparisons were made for a few values of $\Delta t k$ to show the influence of the time increment on the calculation.

The comparisons were done on a system of three consecutive tanks (Fig. 5). To simplify the problem, the volume proportionality constants were all equal, and the set-point volume was zero. The analytical solution for this problem was obtained by directly integrating Eq. (1) for each stage with the initial conditions that the system is empty and has a constant feed rate. The analytical solutions are:

$$V_1 = \frac{A_{f1}}{k} [1 - \exp(-kt)] , \quad (32)$$

$$V_2 = \frac{A_{f1}}{k} [1 - (1 + kt)\exp(-kt)] , \quad (33)$$

$$V_3 = \frac{A_{f1}}{k} \left[1 - \left(1 + kt + \frac{k^2 t^2}{2} \right) \exp(-kt) \right] . \quad (34)$$

The ideal situation is compared with the program results in Table 1. The results of the program are given for three time increment values for each of the three stages. In the first stage the calculated volumes are

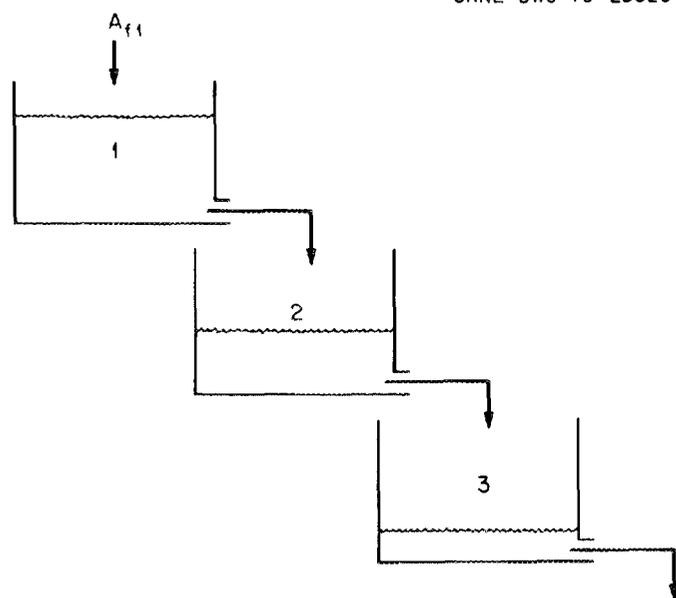


Fig. 5. Three consecutive tanks for testing the mathematical accuracy of the program.

Table 1. Volume balance errors for $k = 1.0$

Elapsed time	Ideal	$\Delta t = 0.25$	$\Delta t = 0.5$	$\Delta t = 1.0$
<u>Stage 1 volume</u>				
1	0.6321	0.6321	0.6321	0.6321
2	0.8647	0.8647	0.8647	0.8647
3	0.9502	0.9502	0.9502	0.9502
4	0.9817	0.9817	0.9817	0.9817
5	0.9933	0.9933	0.9933	0.9933
<u>Stage 2 volume</u>				
1	0.2642	0.2623	0.2565	0.2325
2	0.5940	0.5926	0.5883	0.5707
3	0.8008	0.8001	0.7977	0.7880
4	0.9084	0.9080	0.9069	0.9021
5	0.9596	0.9594	0.9589	0.9567
<u>Stage 3 volume</u>				
1	0.0803	0.0803	0.0806	0.0856
2	0.3233	0.3219	0.3178	0.3029
3	0.5768	0.5753	0.5706	0.5521
4	0.7619	0.7607	0.7573	0.7432
5	0.8753	0.8746	0.8725	0.8637

identical to those from Eq. (32). The size of the time increment seems to have no influence. However, the influence of the time increment is obvious in the results for the second stage. An error is introduced in the second stage because the program assumes that the flow rate out of the first stage varies linearly over a time increment. This approximation becomes more exact as the time increment gets shorter and as the flow rate from the previous stage changes more slowly. Thus the error is initially large but decreases with time. The same is true for the third stage.

Table 2 gives the same results for a larger value of the proportionality constant. The larger value makes the volumes reach their steady-state value much more quickly. In terms of the exponential approach to steady state, the values at $t = 1$ in Table 2 are comparable to those at $t = 4$ in Table 1.

Table 2. Volume balance errors for $k = 4.0$

Elapsed time	Ideal	$\Delta t = 0.25$	$\Delta t = 0.5$	$\Delta t = 1.0$
<u>Stage 1 volume</u>				
1	0.2454	0.2454	0.2454	0.2454
2	0.2499	0.2499	0.2499	0.2499
3	0.2500	0.2500	0.2500	0.2500
4	0.2500	0.2500	0.2500	0.2500
5	0.2500	0.2500	0.2500	0.2500
<u>Stage 2 volume</u>				
1	0.2271	0.2255	0.2201	0.1852
2	0.2492	0.2492	0.2490	0.2477
3	0.2500	0.2500	0.2500	0.2499
4	0.2500	0.2500	0.2500	0.2500
5	0.2500	0.2500	0.2500	0.2500
<u>Stage 3 volume</u>				
1	0.1905	0.1858	0.1708	0.1397
2	0.2466	0.2466	0.2446	0.2315
3	0.2499	0.2499	0.2498	0.2491
4	0.2500	0.2500	0.2500	0.2500
5	0.2500	0.2500	0.2500	0.2500

Again, the values in the first stage are identical to the ideal case regardless of the time increment size. Although the second stage shows errors similar to those in Table 1, the errors are initially more severe than those found in Table 1 but decrease more rapidly. The results from the third stage show the same behavior except that the initial errors are even more severe.

Thus, smaller time increment values result in smaller errors. Larger values for the proportionality constant result in larger errors which diminish more quickly.

4.2 Accuracy of Solute Balances

Testing the solute balances is more difficult because the concentrations depend on both the incoming solute and the volume changes. The concentrations incur errors from the assumptions made in their own equations and from the errors in the volume balance equations. Tests for these errors were performed for both constant volume and variable volume systems. The influence of the size of the time increment was investigated.

The constant volume system is similar to that in Fig. 5 except that the flow rates and volumes have come to steady state. To simplify the system, unit volumes and flow rates were used. The system initially contains only water, and the feed stream is of unit concentration. The resulting concentration in the three stages was followed over time. An analytical solution to the problem indicates that the concentrations should ideally be described by

$$x_1 = x_f \left[1 - \exp\left(\frac{-A_f t}{V}\right) \right], \quad (35)$$

$$x_2 = x_f \left[1 - \left(1 + \frac{A_f t}{V} \right) \exp\left(\frac{-A_f t}{V}\right) \right], \quad (36)$$

and

$$x_3 = x_f \left[1 - \left(1 + \frac{A_f t}{V} + \frac{A_f^2 t^2}{2V^2} \right) \exp\left(\frac{-A_f t}{V}\right) \right]. \quad (37)$$

These equations are very similar to those for the volumes [Eqs. (32)-(34)] except that the proportionality constant k has been replaced by A_f/V . Thus the effect of decreasing the residence time, V/A_f , should be comparable to increasing the proportionality constant.

The results of this test are given in Table 3. As with the volumes, the concentrations in the first stage follow the ideal solution exactly. Concentration errors in the second and third stages show the same dependence as those for the volumes although the concentration errors are larger than the volume errors. The cause of the difference is the assumption that x_{mj} in Eq. (12) is constant over the time increment.

How changing volumes influence errors was tested in a one-stage system. The feed stream had unit concentration and flow rate. Initially,

Table 3. Solute balance errors for a constant volume system

Elapsed time	Ideal	$\Delta t = 0.25$	$\Delta t = 0.5$	$\Delta t = 1.0$
<u>Stage 1 concentration</u>				
1	0.6321	0.6321	0.6321	0.6321
2	0.8647	0.8647	0.8647	0.8647
3	0.9502	0.9502	0.9502	0.9502
4	0.9817	0.9817	0.9817	0.9817
5	0.9933	0.9933	0.9933	0.9933
<u>Stage 2 concentration</u>				
1	0.2642	0.2604	0.2487	0.1998
2	0.5940	0.5912	0.5826	0.5466
3	0.8008	0.7993	0.7946	0.7747
4	0.9084	0.9077	0.9053	0.8956
5	0.9596	0.9592	0.9582	0.9537
<u>Stage 3 concentration</u>				
1	0.0803	0.0784	0.0734	0.0632
2	0.3233	0.3191	0.3066	0.2591
3	0.5768	0.5729	0.5611	0.5129
4	0.7619	0.7592	0.7511	0.7166
5	0.8753	0.8738	0.8689	0.8481

the stage contained a unit volume with zero concentration. The stage volume varied according to

$$V = V_S + \frac{A_f}{k} [1 - \exp(-kt)] , \quad (38)$$

where $V_S = k = 1.0$. The analytical solution for the concentration is

$$x = x_f \left[1 - \exp\left(\frac{-A_f kt}{kV_S + A_f}\right) \left\{ 1 + \frac{A_f}{kV_S} [1 - \exp(-kt)] \right\}^{**} \left(\frac{-A_f}{kV_S + A_f}\right) \right] . \quad (39)$$

More stages would have been tested, but the analytical solution to the mass balance became too complex.

The results of this test are given in Table 4. The stage volume followed Eq. (38) exactly regardless of the size of the time increment. The stage concentration shows reasonably small errors due to the assumption that the stage volume varies linearly over a time increment. [The assumption was made during the evaluation of Eq. (24).] The approximation becomes more exact as smaller time increments are used.

Table 4. Solute balance errors for a variable volume system

Elapsed time	Ideal	$\Delta t = 0.25$	$\Delta t = 0.5$	$\Delta t = 1.0$
1	0.5252	0.5260	0.5279	0.5352
2	0.7306	0.7311	0.7323	0.7358
3	0.8402	0.8405	0.8413	0.8433
4	0.9039	0.9041	0.9045	0.9057
5	0.9419	0.9420	0.9422	0.9430

4.3 Accuracy of Three-Mode Controller

The equations defining the operation of a controller are much simpler than the volume and solute balances. This simple form limits the number of approximations that must be made. To test controller accuracy, simple, well-defined functions were used as the input to the controller, and the controller output was compared with the analytical solution of the controller equation.

When the input to a controller is a constant value, the controller equation [Eq. (28)] simplifies greatly. The analytical form for the output of the controller is

$$c = S_c + K_p e \left(1 + \frac{t}{K_i} \right). \quad (40)$$

This is a linear ramp in time. The calculation used zero values for the set points, and unity for the controller constants. The results are shown in Table 5. As expected, the results match the analytical form exactly, regardless of the time increment.

Table 5. Controller errors for a constant input

Elapsed time	Ideal	$\Delta t = 0.25$	$\Delta t = 0.5$	$\Delta t = 1.0$
1	2.0	2.0	2.0	2.0
2	3.0	3.0	3.0	3.0
3	4.0	4.0	4.0	4.0
4	5.0	5.0	5.0	5.0
5	6.0	6.0	6.0	6.0

When the input to the controller is a ramp, the output on the controller is a quadratic equation. Substituting the ramp

$$e = t \quad (41)$$

into Eq. (28) produces

$$c = S_c + K_p \left(t + \frac{t^2}{2K_i} + K_d \right). \quad (42)$$

The calculation used zero values for the set point, and unity for the controller constants. The results are shown in Table 6. Again, the results match the ideal form exactly for any time increment size.

Using a quadratic equation as the input to the controller should produce a cubic equation as the output. In this case the input function

Table 6. Controller errors for a ramp input

Elapsed time	Ideal	$\Delta t = 0.25$	$\Delta t = 0.5$	$\Delta t = 1.0$
1	2.5	2.5	2.5	2.5
2	5.0	5.0	5.0	5.0
3	8.5	8.5	8.5	8.5
4	13.0	13.0	13.0	13.0
5	18.5	18.5	18.5	18.5

was

$$e = 1 + t + (t^2/2) , \quad (43)$$

and the resulting ideal equation is

$$c = S_c + K_p \left[1 + K_d + t \left(1 + \frac{1}{K_i} + K_d \right) + \frac{t^2}{2} \left(1 + \frac{1}{K_i} \right) + \frac{t^3}{6K_i} \right] . \quad (44)$$

The calculation used zero values for the set points, and unity for the controller constants. The discrepancies between the ideal values and those calculated by the CONCEPT program (Table 7) are due to the approximations made in evaluating the integral and derivative terms in Eq. (28). The errors diminish as the time increment is shortened and the approximations become more exact.

Table 7. Controller errors for a quadratic input

Elapsed time	Ideal	$\Delta t = 0.25$	$\Delta t = 0.5$	$\Delta t = 1.0$
1	6.167	5.922	5.688	6.250
2	13.33	13.09	12.88	12.50
3	24.50	24.27	24.06	23.75
4	40.67	40.44	40.25	40.00
5	62.83	62.61	62.44	62.25

Accuracy of controller operation is related to the functionality of the input error, the size of the time increment, and the controller constants. For simple input errors where the second derivative is always

zero, the controller follows the analytical solution to Eq. (28) exactly regardless of the time increment and the controller constants. When the error has a non-zero second derivative, the controller follows the analytical solution, but not exactly. The difference between the analytical solution and the calculated result is related to the time increment size.

5. INPUT CARDS FOR THE CONCEPT PROGRAM

The formats of the input cards, given in Table 8, are generally comparable to those used for the SEPHIS-MOD4 program. Although the cards are generally self-explanatory, the user is strongly urged to refer to the following sections on using the program. Advice on choosing values for the variables and some examples are given to clarify these cards.

Table 8. Input card formats for the CONCEPT program

Card	Card columns	Variable description
1		FORMAT (I2, I4, 2F8.0, 2I2) start of the next case
	1-2	NTTL = number of title cards (up to 10).
	3-6	NTOST = number of stages (up to 100).
	7-14	CTBP = volume fraction of TBP in the organic phase.
	15-22	TEMPI = initial and default temperature (°C).
	24	IRXN = switch for the plutonium reduction reaction, = 0 for no reduction, = 1 for instantaneous reduction, = 2 for reduction by U(IV), = 3 for reduction by hydroxylamine.
	26	IPROCE = switch for the process being used, = 0 for Purex, = 1 for Thorex.
2		FORMAT (10A8) title cards
	1-80	TITLE = up to 10 cards of text describing the calculation being performed.
3		FORMAT (4F8.0, 5I2) start of the next time period
	1-8	DTHETA = time increment (s).
	9-16	DPRINT = time between successive profile printings (s).
	17-24	TSTOP = time when the calculations will stop if the tolerance is not met (s).
	25-32	TOL = tolerance on the rate of change to determine when a steady state has been achieved (%/s).

Table 8 (continued)

Card	Card columns	Variable description
34	NEWIN	= switch for reading new feed stream cards, = 0 if no feed stream cards are to be read, = 1 if all new feed stream cards are to be read, = 2 if only revisions to the existing feed streams are to be read.
36	NEWOUT	= switch for reading new product stream cards, = 0 if no product stream cards are to be read, = 1 if all new product stream cards are to be read, = 2 if only revisions to the existing product streams are to be read.
38	IVOL	= switch for reading new volume constants, = 0 if no volume constant cards are to be read, = 1 if all new volume constant cards are to be read, = 2 if only revisions to the existing volume constants are to be read.
40	IPRO	= switch for reading an initial profile, = 0 if no profile is to be read, = 1 if an initial profile is to be read.
42	IPNCH	= switch for punching a final profile on cards, = 0 if the final profile is not to be punched, = 1 if the final profile cards are to be punched.
4	FORMAT	(I4, I2, 8F8.0, 2I2) feed stream cards
	1-4	J = stage number where this feed stream enters.
	6	K = phase, = 1 for aqueous, = 2 for organic.
	7-14	CON(1) = nitric acid concentration (mol/L).
	15-22	CON(2) = uranium concentration (g/L).
	23-30	CON(3) = plutonium(IV) concentration (g/L).
	31-38	CON(4) = plutonium(III) concentration (g/L).
	39-46	CON(5) = reductant concentration (mol/L).
	47-54	CON(6) = inextractable nitrate concentration (mol/L).
	55-62	CON(7) = temperature (°C).
	63-70	CON(8) = flow rate (L/s).

Table 8 (continued)

Card	Card columns	Variable description
	72	INDEX = switch for more feed stream cards, = 0 if no cards remain, = 1 if more feed stream cards follow.
	74	ICONTR = switch for controller cards for this feed stream, = 0 if no controller cards follow, = 1 if controller cards follow.
		For the Thorex process CON(3) - CON(5) change
	23-30	CON(3) = thorium concentration (g/L).
	31-38	CON(4) = not defined.
	39-46	CON(5) = not defined.
5		FORMAT (I2, I4, 2I2, 8F8.0, I2) controller cards
	2	L = number of the feed stream variable being controlled; CON(L) on the preceding feed stream card will be controlled as specified by this card.
	3-6	JM = number of the stage being monitored by this controller, > 0 for three-mode control, < 0 for on/off control.
	8	KM = switch for phase being monitored, = 1 for an aqueous bank variable, = 2 for an organic bank variable, = 3 for an aqueous feed stream variable, = 4 for an organic feed stream variable.
	9-10	LM = number of the variable being monitored, = 1-8 same as CON(1) - CON(8) on the feed stream card, = 9 volume (L) only for bank variables, = 10 density (kg/L) only for bank variables.
		For three-mode controlling
	11-18	CON(1) = set point for the monitored variable.
	19-26	CON(2) = proportional gain.
	27-34	CON(3) = integral time (s).
	35-42	CON(4) = derivative time (s).
	43-50	CON(5) = set point for the controlled variable.

Table 8 (continued)

Card	Card columns	Variable description
	51-58	CON(6) = error band on the outgoing value (%).
	59-66	CON(7) = maximum value allowed for the controlled variable (applied before the error band).
	67-74	CON(8) = minimum value allowed for the controlled variable (applied before the error band).
		For on/off controlling
	11-18	CON(1) = upper set point for monitored variable.
	19-26	CON(2) = lower set point for monitored variable.
	27-34	CON(3) = not defined.
	35-42	CON(4) = not defined.
	43-50	CON(5) = not defined.
	51-58	CON(6) = error band applied to the outgoing value (%).
	59-66	CON(7) = outgoing value after the monitored variable is greater than CON(1).
	67-74	CON(8) = outgoing value after the monitored variable is less than CON(2).
	76	ICONTR = switch for controller cards for this feed stream, = 0 if no more controller cards follow, = 1 if other controller cards follow.
6		FORMAT (I4, I2, F8.0, I2) product stream cards
	1-4	J = stage number from which the product stream is removed.
	6	K = phase, = 1 for aqueous, = 2 for organic.
	7-14	PFLO = maximum flow rate for the product stream (L/s).
	16	INDEX = switch for product stream cards, = 0 if no product stream cards follow, = 1 if more product stream cards follow.
7		FORMAT (I4, 4F8.0, I2) volume constant cards
	1-4	J = stage number.
	5-12	VT = total stage volume (L).

Table 8 (continued)

Card	Card columns	Variable description
	13-20	VS = aqueous set point volume (L).
	21-28	CA = aqueous proportionality constant (s^{-1}).
	29-36	CO = organic proportionality constant (s^{-1}).
	38	INDEX = switch for volume constant cards, = 0 if no volume constant cards follow, = 1 if more volume constant cards follow.
8		FORMAT (9F8.0) initial profile cards
		An aqueous card followed by an organic card is required for each stage.
	1-8	CON(1) = nitric acid concentration (mol/L).
	9-16	CON(2) = uranium concentration (g/L).
	17-24	CON(3) = plutonium(IV) concentration (g/L).
	25-32	CON(4) = plutonium(III) concentration (g/L).
	33-40	CON(5) = reductant concentration (mol/L).
	41-48	CON(6) = inextractable nitrate concentration (mol/L).
	49-56	CON(7) = temperature.
	57-64	CON(8) = flow rate out of the stage (L/s).
	65-72	CON(9) = volume (L).
		For the Thorex process CON(3) - CON(5) change
	17-24	CON(3) = thorium concentration (g/L).
	25-32	CON(4) = not defined.
	33-40	CON(5) = not defined.

6. GENERAL USE OF THE CONCEPT PROGRAM

A mere listing of the input card formats cannot indicate the considerations and contingencies that went into the CONCEPT program. Implementation of the ideas in the program led to many potentially useful consequences which are not immediately apparent. Many abilities of the program will not be utilized until the user considers carefully what he would like the program to do. The examples in Sect. 8 should help to broaden the user's understanding of the program's potential.

Before specific examples are given, some advice on choosing values for the variables will probably be useful. The choices for some of the variables are linked through their functionality in the integrated mass balances. Some of the variables need a simple explanation to clarify the impact of a particular choice, or to show the flexibility built into the program.

6.1 Choosing a Value for DTHETA

DTHETA is the time increment used for the calculations. In general, the integration becomes more accurate when smaller values of DTHETA are used. This is a consequence of an implicit approximation that the system is changing fairly slowly from one point in time to the next. As DTHETA is decreased, the magnitude of the changes during one time interval is decreased, making the approximation more exact.

This vague explanation of the effect of DTHETA does little to help in choosing a value. However, the specific equations involving DTHETA show its use in the program and its dependence on other variables. In calculating aqueous volumes and flow rates, the terms used in the equations are $\Delta t k_a$ and $\exp(-\Delta t k_a)$. In these equations a better integration is achieved if the product $\Delta t k_a$ is small ($\ll 0.5$) for each stage. Similarly for the organic phase, it is desirable to keep the product $\Delta t k_o$ small. This means that as larger values for the proportionality constants k_a and k_o are used, smaller values for DTHETA are desirable. A more explicit characterization of the accuracy is given in Sect. 4.

In calculating concentrations the most common form for DTHETA is as a ratio to the residence time. When there is flow into the stage, the terms are $\exp[\pm\Delta t(A_{fj} + A_{j-1})/V_a]$ and $\exp[\pm\Delta t\Delta(A_{fj} + A_{j-1})/\Delta V_a]$. In these cases, the integration becomes more exact as the exponentials approach 1.0. Again, smaller values for DTHETA are desirable. A more explicit example of the effect of DTHETA on accuracy is given in Sect. 4.

DTHETA pervades almost every aspect of the program. As should be expected, a smaller value for DTHETA helps the program more accurately follow the changes taking place in the system. An important conflicting consideration is that as DTHETA is decreased, the computing time is increased. The user must balance these conflicting priorities according to his requirements.

6.2 Other Variables on Card 3

Although DTHETA is probably the most important variable on card 3, the other variables control the input/output functions of the program and require an explanation. DPRINT is the elapsed time between profile printings and as such regulates the amount of printed output. When DPRINT is set equal to DTHETA, every calculated profile is printed. Setting DPRINT to larger multiples of DTHETA results in less printed output when the detail of every calculated profile is not necessary. TOL regulates when the calculations will stop since a steady state has been achieved. A value of 0.0001 is usually sufficient. A negative value for TOL, such as -1.0, requires the program to calculate until TSTOP is reached, regardless of steady state.

The switches on card 3 are generally simple to understand. However, the difference between revisions and all new values needs an explanation. When all new values are to be read in, the program reinitializes all the pertinent variables in preparation for the incoming information. However, when revisions are made, no reinitialization is done so that all the old information is still present and will be used unless the values are overwritten. This can be useful in continued calculations where only one feed stream needs to be changed. Initial profiles cannot be revised;

they can only be replaced. It should also be noted that the entire system is reinitialized after card 1 is read.

6.3 Controller Cards

To specify a controller, the computer must first, and most obviously, be told what is being controlled. Each controller card is associated with the preceding feed-stream card, so the first variable on the controller card indicates to which of the eight feed-stream variables this controller pertains.

As important as which variable is being controlled is which variable is being monitored by this controller. The system used by the program to locate the variable being monitored requires (1) the stage number, (2) whether the variable is in a feed stream or in the contactor bank, (3) the phase, and (4) the variable. By checking whether the stage number is positive or negative, the program determines whether the controller is a three-mode or an on/off controller.

The remaining information on the controller card is the constants defined in Figs. 3 and 4. The constants are generally straightforward in their meaning with one notable exception. The integral time for the three-mode controller [K_i in Eq. (28)] cannot be zero since division by zero is undefined. However, a zero value for the integral time on the input card will be changed to 1.0E+40, effectively removing any integral control.

The mere use of controllers does not imply that the system will be in control. The controller constants can be set as desired, but poorly chosen values can produce an unstable response. Like their real counterparts, when the controllers in the CONCEPT program are not properly tuned, their response will show oscillations that increase in size or simply "peg" at the maximum or minimum value.

6.4 Product-Stream Cards

The product-stream cards describe where streams are removed from the system and the maximum flow rates for those streams. If only a sample product is to be removed, the sample amount should be used for the flow rate. If the entire stream is to be removed, the stream flow rate or, preferably, some larger amount should be used for the flow rate. It is important to understand that although a certain flow rate may be entering a stage or section of equipment, that does not mean that the exiting or product-stream flow rate is limited by that amount. In very many cases, exiting flow rates during transient periods will exceed the flow rate of the entering stream. This is especially true of the organic phase. At the other extreme, if nothing is flowing out of a stage where a product stream has been specified, no product stream will be removed. In this case the maximum flow rate specified on the product-stream card will still be retained for the eventuality that at some time a stream will flow out of that stage.

6.5 Volume Constant Cards

The variables that determine the relationship between flow rates and volumes in a stage are defined in Eqs. (1) through (9). The CONCEPT program does not require that both (or either) phase(s) be found in a stage. One or both phases may be missing; one or both phases may not flow into the stage; and one or both phases may not flow out of the stage. However, the volume parameters are still required for each stage. The total or aqueous set-point volumes may be zero, but the proportionality constants must be greater than zero.

An aqueous stream will not flow out of the stage until the aqueous volume exceeds the aqueous set-point volume. Likewise, an organic stream will not flow out of the stage until the sum of the aqueous and organic volumes exceeds the total volume. These properties can be used to specify in-line tanks in the system. For an aqueous tank, both the total volume and the set-point volume are set to high values. For an organic tank, only the total volume need be set to a high value. Thus, when a phase flows into the tank, it will take a very long time before any flows out.

After all the volume constant cards have been read, the program checks to be sure that every stage has the required values. If a stage lacks a value, the value from the previous stage is used.

6.6 Initial Profile Cards

The initial profile cards are used to specify the initial state of the system. Each stage requires an aqueous card followed by an organic card. If an initial profile is not specified, the previous profile will be used. On the first calculation, the previous profile is a totally empty system.

6.7 Ending Calculations

After the last input card for a time period has been read, the program starts calculating and printing as specified. When the convergence tolerance has been met, or when the elapsed time has reached TSTOP, the calculations stop and another card 3 is read. Here, three choices are possible. If the card is simply giving new values for the various variables, the program will continue working as before. If $D\theta = 0.0$ and $DPRINT = 1.0$, the program starts over again by reading a card 1 and reinitializing the system. If $D\theta = 0.0$ and $DPRINT = 0.0$, the program stops.

7. CREATIVE USE OF THE CONTROLLERS

The variables on the controller cards are defined in Sect. 2.3. Their use as ordinary three-mode or on/off controllers is self-evident and will not be discussed in this section. There are many alternative uses for the controllers which generally disregard the purpose of "controllers" and merely use the controlling schemes as a convenient means to achieve the desired end.

7.1 Routing Streams Within a System

With the SEPHIS-MOD4 program, special variables were used to move an organic stream from one place in the system to another. These variables are not required by the CONCEPT program because the same function can be accomplished with the controllers. It is important to keep in mind that the program does not realize that it is routing a stream within the system. The program just responds to a particular feed stream controlled in a particular way.

For an example, the organic stream leaving stage 5 is to be routed to stage 2. We can consider this as an organic feed stream to stage 2 while the stream leaving stage 5 is a product stream. We would like every aspect of the feed stream to be identical to that of the product stream. In describing the feed stream to stage 2, the values on the feed-stream card are only initial values and can be set as desired. In the subsequent controller cards, the controller for each variable is set to monitor the corresponding variable in stage 5; that is, the controller for the acidity of the organic feed stream to stage 2 is set to monitor the acidity of the organic phase in stage 5 (and hence, the acidity of the product stream leaving stage 5). Recalling the entire action of a three-mode controller, the output of the controller is given by

$$C = \left\{ S_c + K_p \left[(m - S_m) + \frac{1}{K_i} \int (m - S_m) dt + K_d \frac{dm}{dt} \right] \right\} \left(1 + \frac{N}{100} r \right). \quad (45)$$

The overall intent of this particular controller is to require that the acidity of the organic feed to stage 2 be equal to the acidity of the

organic phase in stage 5, or $C = m$ at all times. The only place where m appears alone is in the proportional term, so the integral and derivative control should be removed by setting $K_i = K_d = 0.0$ on the input card. Ignoring the error band ($N = 0.0$) leaves

$$C = S_c + K_p(m - S_m) \quad (46)$$

The obvious solution to the problem is then achieved if $S_c = S_m = 0.0$ and $K_p = 1.0$. The maximum and minimum values must be set to accommodate the expected range. This completes the description of the controller for acidity. The same idea is used for the controllers for each of the other feed-stream components. The following cards are the solution to this example and will have the effect of using any organic solution flowing out of stage 5 as the feed to stage 2.

	2	2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	40.0	0.0	1	1	FEED STREAM CARD
1	5	2	1	0.0	1.0	0.0	0.0	0.0	0.0	0.0	10.0	0.0	1	1	CONTROLLER CARDS
2	5	2	2	0.0	1.0	0.0	0.0	0.0	0.0	0.0	300.0	0.0	1	1	
3	5	2	3	0.0	1.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	1	1	
4	5	2	4	0.0	1.0	0.0	0.0	0.0	0.0	0.0	50.0	0.0	1	1	
5	5	2	5	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1	1	
6	5	2	6	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	1	1	
7	5	2	7	0.0	1.0	0.0	0.0	0.0	0.0	0.0	70.0	20.0	1	1	
8	5	2	8	0.0	1.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0	0	

Minor variations on this idea are numerous. Heaters or coolers on the stream are specified by adjusting the temperature controller. Eliminating the temperature controller will keep the feed-stream temperature constant at its initial value (40°C in this case). Evaporators merely require different values for the proportional gain in Eq. (46). For example, 2.0 for concentrations and 0.5 for the flow rate will double the concentrations as if half of the solution had been boiled away.

7.2 Inserting Errors in "Uncontrolled" Feed Streams

It is sometimes instructive to know how a particular system will react when the feed streams are not accurately known. This can be tested with the use of controllers because many types of errors can be produced by them. Strictly random errors are generated by using the noise on the controller. Systematic errors (square waves or sine waves) can be produced by properly manipulating the on/off and three-mode controlling

schemes. A random walk error results from manipulating the three-mode controlling scheme in yet another manner. Ingenuity will undoubtedly lead to other error forms.

7.2.1 Random errors

Suppose we want to impose a random error on the feed-stream flow rate (2.5 L/s \pm 5%) while leaving the concentrations constant. Using the three-mode operation from Eq. (45), it is immediately apparent that only a small part of the operation is necessary to achieve the simple error. Setting the proportional gain (K_p) to zero leaves only

$$C = S_c \left(1 + \frac{N}{100} r \right). \quad (47)$$

Thus the set point for the controlled variable is equal to the nominal flow rate ($S_c = 2.5$), and the noise is set to the proper level ($N = 5.0$). The other variables on the controller card do not affect the result, but they should still be set to reasonable values. In this case the controller is set to monitor itself, and the other constants are set to zero. The maximum and minimum are set appropriately. The cards to do this are reproduced here.

```

7 1 3.0 300.0 3.0 0.0 0.0 0.0 60.0 2.5 1 1 FEED STREAM CARD
R 7 3 R 0.0 0.0 0.0 0.0 2.5 5.0 2.63 2.37 0 CONTROLLER CARD

```

On/off controllers can be used in a similar manner to give random variations about c'_{on} and c'_{off} .

7.2.2 Systematic errors

When random errors are used as in Sect. 7.2.1, the error changes each time increment so that within a few stages, the impact of the error will be severely moderated. A systematic error or an error that varies in a more predictable manner will affect the system in a different way. Systematic errors can be produced with many different methods. The two examples described here are only illustrations of the more general techniques.

The first method will produce a square wave using an on/off controller; the second method will produce a sine wave using a three-mode controller.

A square wave is a simple consequence of an on/off controller. Recalling the general scheme from Fig. 4, the values for c'_{on} and c'_{off} can be used as high and low conditions for the square wave. The only question remaining is how to switch between the "on" and "off" conditions or how to set S_U and S_L . In the case of the stage 7 feed-stream flow rate ($2.5 \text{ L/s} \pm 5\%$), the switching mechanism can be set by realizing that when the feed rate changes from $2.5 + 5\%$ to $2.5 - 5\%$, the flow rate leaving that stage will also begin to change. Thus if the feed flow rate controller is set to monitor the flow rate leaving stage 7, S_U and S_L can be set near to the expected maximum and minimum flow rates. The cards for this case are shown here.

```

7 1 3.0   300.0  3.0   0.0   0.0   0.0   60.0   2.5   1 1  FEED STREAM CARD
9 -7 1 8 3.60  3.40  0.0   0.0   0.0   0.0   2.375  2.625  0  CONTROLLER CARD

```

When the flow rate leaving stage 7 exceeds 3.60 L/s, the feed-stream flow rate to stage 7 is changed from 2.625 to 2.375 L/s. Decreasing the feed flow rate will eventually decrease the flow rate leaving the stage. The time required for the flow rate to diminish depends on the volume proportionality constants. When the flow rate leaving stage 7 falls below 3.40 L/s, the feed-stream flow rate is changed back to 2.625 L/s, thus completing the cycle that forms the wave.

In this case the square wave is very regular and symmetric, spending as much time "on" as "off." More irregular waves can be formed by adjusting the values for S_U and S_L closer to or further from the absolute extreme flow rates expected for stage 7 (in this case 3.625 and 3.375 L/s since there is a 1.0-L/s stream coming from the previous stage). The controller can be made to change at random intervals by monitoring another feed stream which has a noise band and setting S_U and S_L in relation to that noise band.

Sinusoidal errors or errors with other shapes can be achieved in a more indirect manner. In this method a variable elsewhere in the system

which is changing in some desired fashion is adjusted and added to the nominal value of the feed-stream flow rate. Again in this case the aqueous feed flow rate to stage 7 is to be 2.5 L/s \pm 5%. In this calculation, the temperature in stage 15 is somehow varied sinusoidally between 30 and 60°C. The solution starts with Eq. (46), which is a three-mode controller with $K_i = K_d = N = 0.0$. The value for the monitored variable (m) is varying between 30 and 60; but since we would like a variation about zero, S_m is set to 45. Thus, $m - S_m$ will vary from -15 to 15. The proportional gain (K_p) is used to scale the ± 15 to the desired $\pm 5\%$ of 2.5 L/s, so $K_p = 0.008$. The set point for the controlled variable (S_c) is the nominal flow rate. The final equation is

$$C = 2.5 + 0.008(m - 45) . \quad (48)$$

When the value of the monitored variable varies from 30 to 60°C, the value of the controlled variable (the flow rate) will vary between 2.38 and 2.62 L/s. The cards to do this are shown here.

```

7 1 3.0 300.0 3.0 0.0 0.0 0.0 60.0 2.5 1 1 FEED STREAM CARD
8 15 1 7 45.0 0.008 0.0 0.0 2.5 0.0 2.62 2.37 0 CONTROLLER CARD

```

7.2.3 Random walk errors

Random walk errors are entirely different from the random errors discussed in Sect. 7.2.1. With a random walk the controlled variable wanders within an interval rather than constantly jumping within the interval. The walk uses a mechanism whereby the new value for the controlled variable is only slightly changed from its previous value. This is accomplished by having the controller monitor itself so that the value of the monitored variable (m) is also the previous value of the controlled variable (C). Starting with Eq. (45) and again setting $K_i = K_d = 0.0$ on the input card, but allowing for noise, results in

$$C = \left[S_c + K_p (m - S_m) \right] \left(1 + \frac{N}{100} r \right) . \quad (49)$$

The expression in brackets is simplified by setting $K_p = 1.0$ and $S_c = S_m = 0.0$ to give

$$C = m \left(1 + \frac{N}{100} r \right) . \quad (50)$$

Thus the new value of the controlled variable will be changed only slightly from its previous value if the noise is reasonably small. For the example of the flow rate, the error interval is from 2.37 to 2.63 L/s. To make the flow rate wander rather than jump around within the interval, the noise band (N) is set to a small fraction of the interval width. In this case the largest flow rate change from one time increment to the next is 0.021 L/s or 8% of the width of the interval ($N = 0.84\%$). The cards used for this example are presented here.

```

7 1 3.0 300.0 3.0 0.0 0.0 0.0 50.0 2.5 1 1 FEED STREAM CAPD
8 7 3 8 0.0 1.0 0.0 0.0 0.0 0.84 2.63 2.37 0 CONTROLLER CARD

```

The random walk is limited by the maximum and minimum values specified (with some allowance for the noise band since the noise is imposed after the maximum/minimum test). This method has a slight bias toward the minimum value because the size of a step is smaller in that region. This would be especially noticeable if the minimum were zero. If the value of the controlled variable ever became zero, Eq. (50) would then produce only zero. These biases can be limited or changed by manipulating S_c and S_m or by including some amount of derivative control.

7.2.4 Results from the example errors

The differences between these types of errors are shown in Fig. 6. With random errors, the flow rate jumps around within the specified range. With square-wave errors, a periodic shift between the "on" and "off" values is produced. The sinusoidal variation in temperature was converted to a sinusoidal error in the flow rate in the third example. Finally, the flow rate with the random walk errors wanders within the given interval without jumping around too much. The CONCEPT program can produce other forms of similar errors by properly setting the constants for the controllers.

7.3 General Mathematics Using Controllers

At times it will be useful to have the program perform mathematical operations automatically to obtain a result that is subsequently used for

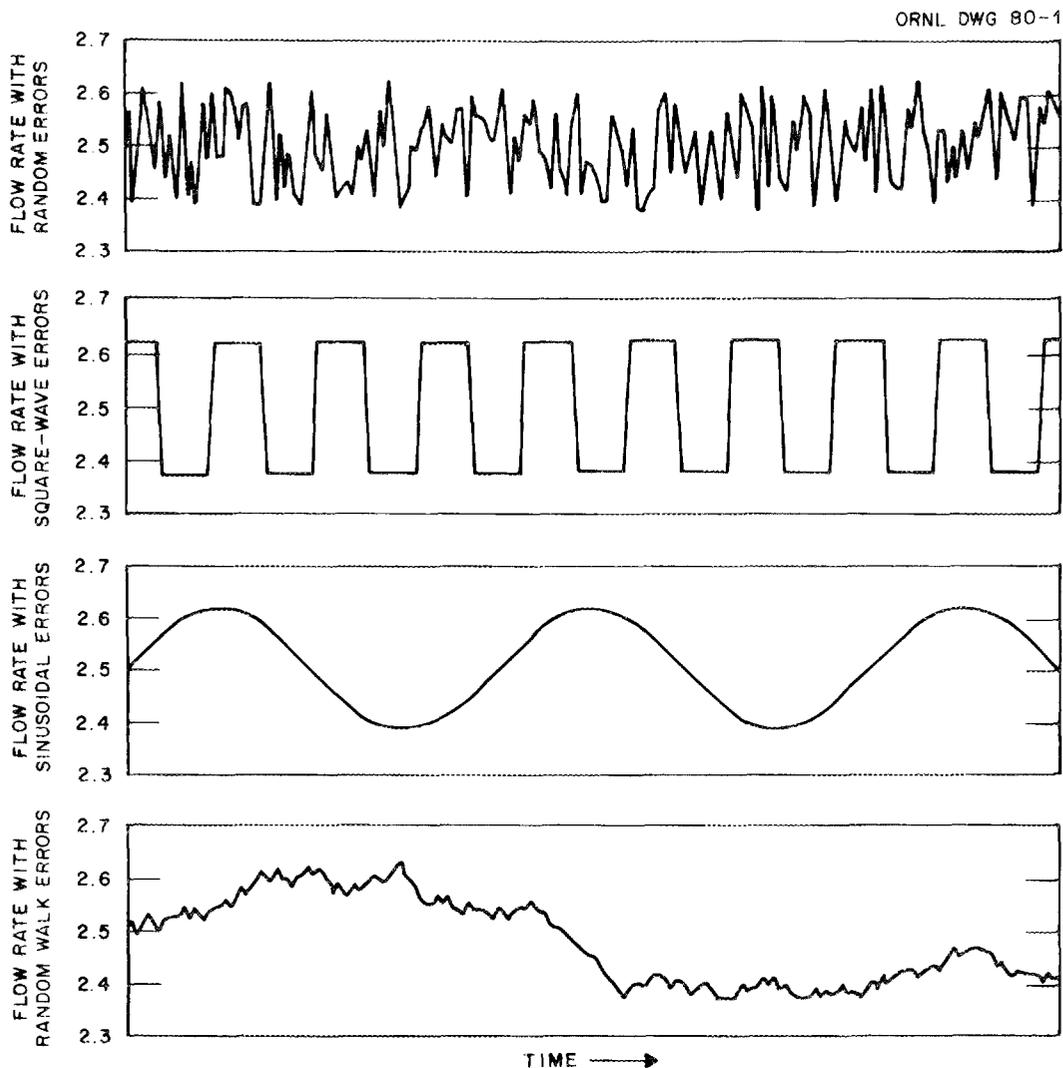


Fig. 6. Results from the errors used as examples.

controlling the process. Examples of this are plutonium reoxidation (adding), estimating uranium concentrations (subtracting), measuring inventories (multiplication), and calculating plutonium contents (division). These operations are all examples of indirect monitoring or controlling in which pseudo-stages are created exclusively to do the given operation. A large degree of careful consideration is required to construct the solutions to these problems.

7.3.1 Addition

Using the program to add two or more variables is relatively easy. In this example the problem is to reoxidize any plutonium(III) leaving stage 14. This involves only the addition of the plutonium(III) concentration to the plutonium(IV) concentration. The final result will be used as the plutonium(IV) concentration in the feed to stage 15.

One easy way to perform addition is with flow rates as shown in Fig. 7. If, for example, the flow rate of the aqueous feed stream to

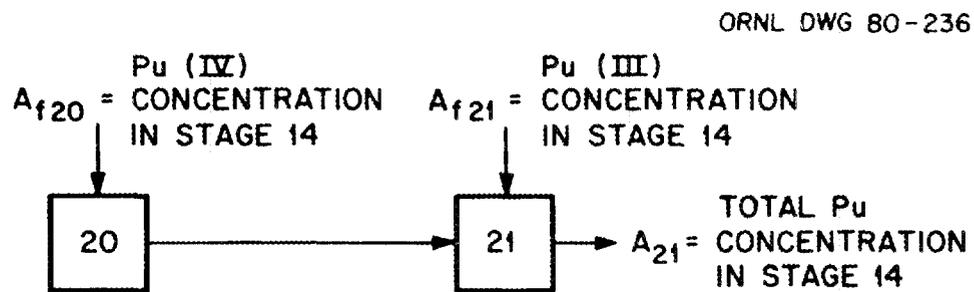


Fig. 7. An example using flow rates to add concentrations.

stage 20 (A_{f20}) is set equal to the plutonium(IV) concentration and the flow rate to stage 21 (A_{f21}) is set equal to the plutonium(III) concentration, then the flow rate out of stage 21 (A_{21}) will be the sum of the two concentrations with some amount of time delay. Equating the feed flow rates to the concentrations is done in exactly the same manner as is discussed in Sect. 7.1 where the feed acidity was set equal to the acid concentration in another stage. The cards required to perform this addition and to transfer the resulting solution to stage 15 are reproduced here.

15	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1	1	FEED STREAM CARD
1	14	1	1	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	5.0	0.0	1	1	CONTROLLER CARDS
2	14	1	2	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	200.0	0.0	1	1		
3	21	1	3	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	1	1		
7	14	1	7	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	70.0	20.0	1	1		
9	14	1	8	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	10.0	0.0	0	0	CONTROLLER CARDS	
20	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1	1		
9	14	1	3	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0	0	FEED STREAM CARD	
21	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0	1	CONTROLLER CARD	
8	14	1	4	0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	100.0	0.0	0	0	CONTROLLER CARD	
14	1	1000.0	0													PRODUCT STREAM CARD	

This idea can be extended to weighting the variables by changing the proportional gain. Averaging two numbers uses 0.5 as the proportionality.

7.3.2 Subtraction

Although subtraction is merely addition of a negative number, the program will not allow the same solution as for addition. The program will not allow a negative concentration or flow rate; however, the program will allow negative temperatures, and these can be used for subtraction. Considering only one phase, the temperature resulting from the addition of two streams would be a flow rate weighted average. The averaging must be considered when determining the proportional gains.

For this example we would like to estimate the aqueous uranium concentration in stage 4 by using the density and temperature in the stage. The equation used for the estimate is

$$U = 1000(\rho - 0.9 - 0.0013T) .^* \quad (51)$$

We can reorganize this to

$$U = 1000(\rho - 0.9) - 1.3T . \quad (52)$$

Employing Eq. (46) for two separate temperature controllers, the 0.9 becomes the set point for the monitored density (S_m). The 1000 and -1.3 are the proportional gains (K_p), but because we are employing temperature as the mechanism for the subtraction, we must consider the impact of Eq. (16) for calculating temperatures. For this example Eq. (16) can be reduced to

$$T = \frac{A_1 T_1 + A_2 T_2}{A_1 + A_2} . \quad (53)$$

Using equivalent flow rates,

$$T = 0.5(T_1 + T_2) . \quad (54)$$

Thus, to obtain the proper sum (or difference, in this example), the proportional gain is doubled as shown in the final solution in Fig. 8.

* This equation is not based on data and is given only for the sake of example.

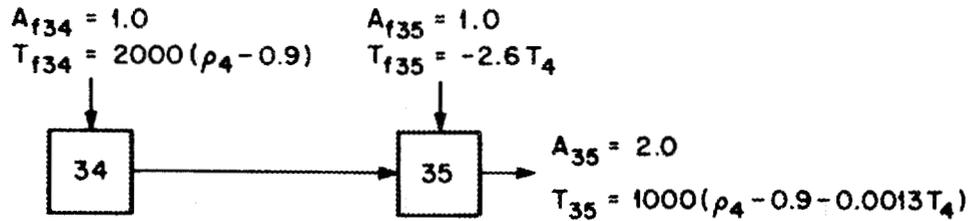


Fig. 8. An example using temperatures in subtraction.

The controllers are specified by the following cards. The estimate of uranium concentration is the resulting temperature in stage 35.

```

34 1 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 1.0 1 1 FEED STREAM CARD
7 4 110 0.0 2000.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 500.0 0.0 0 CONTROLLER CARD
35 1 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 1.0 0 1 FEED STREAM CARD
7 4 17 0.0 -2.6 0.0 0.0 0.0 0.0 0.0 0.0 0.0 -500.0 0 CONTROLLER CARD

```

This method can also be used for addition. In fact, each concentration in stage 35 could have been used for a separate addition problem (keeping in mind that plutonium and the reductant will react if both are present in the stage). These methods will result in terrible answers for the phase density, or for the distribution coefficients if both phases are present in the stage. However, since these pseudo stages are being used exclusively for ulterior motives, a second phase should not be present and the density should be ignored.

7.3.3 Multiplication and division

Multiplication and division in the CONCEPT program exploit the components with distribution coefficients equal to zero: plutonium(III), reductant, and inextractable nitrates. To multiply or divide, an organic feed stream containing one of these components is contacted with an aqueous stream. All of the solute must transfer to the aqueous phase, so the steady-state mass balance being exploited is

$$x = Oy/A \quad (55)$$

For multiplication, the aqueous flow rate can be unity. For division, the organic flow rate or concentration can be unity. An important added

consideration is that extreme flow ratios will not work as described [see Eqs. (17) and (18)].

An example of multiplication is the inventory in a stage. The volume is multiplied by the concentration. The following cards will calculate the aqueous uranium inventory in stage 7 according to the scheme shown in Fig. 9. The product of the multiplication is the aqueous reductant concentration in stage 23.

```

23 1 0.0 0.0 0.0 0.0 0.0 0.0 40.0 1.0 1 0 FEED STREAM CARD
23 2 0.0 0.0 0.0 0.0 0.0 0.0 40.0 0.0 0 1 FEED STREAM CARD
5 7 1 2 0.0 1.0 0.0 0.0 0.0 0.0 300.0 0.0 1 CONTROLLER CARD
8 7 1 9 0.0 1.0 0.0 0.0 0.0 0.0 100.0 0.0 0 CONTROLLER CARD
    
```

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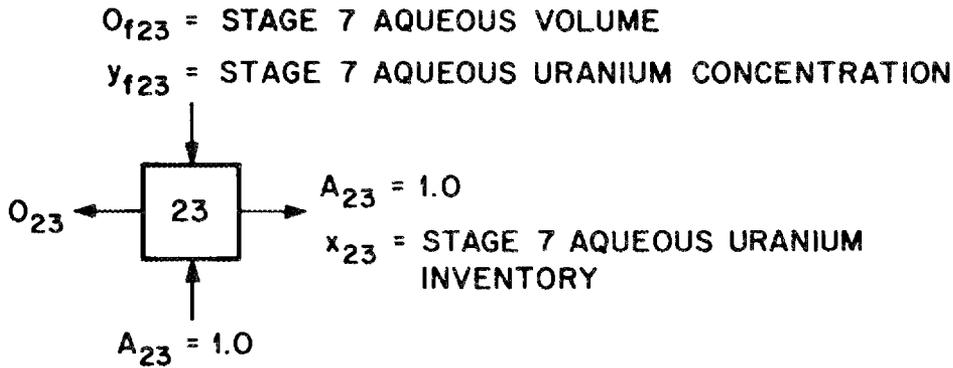


Fig. 9. An example using the reductant concentration to multiply.

For an example of division, we will determine the plutonium as a percent of heavy metal leaving the system at stage 18. The solution to this problem is shown in Fig. 10. The flow rate for the aqueous feed

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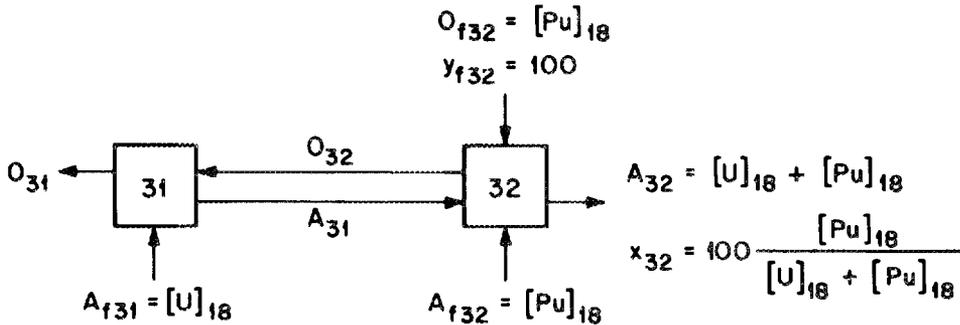


Fig. 10. An example using the reductant concentration to divide.

stream to stage 31 is the uranium concentration in stage 18. The flow rate for the aqueous and organic feed streams to stage 32 is the plutonium(IV) concentration in stage 18. A reductant concentration of 100 is used to obtain the percentage as opposed to the fraction. The cards for this example are shown here.

31	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	40.0	0.0	1	1	FEED STREAM CARD
9	18	1	2	0.0	1.0	0.0	0.0	0.0	0.0	300.0	0.0	0	CONTROLLER CARD
32	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	40.0	0.0	1	1	FEED STREAM CARD
9	18	1	3	0.0	1.0	0.0	0.0	0.0	0.0	100.0	0.0	0	CONTROLLER CARD
32	2	0.0	0.0	0.0	0.0	0.0	100.0	0.0	40.0	0.0	0	1	FEED STREAM CARD
9	18	1	2	0.0	1.0	0.0	0.0	0.0	0.0	100.0	0.0	0	CONTROLLER CARD

7.4 Batch Operations

The equations in the CONCEPT program are written for continuous operations, but semicontinuous or batch operations can be performed with careful use of the controllers. Batch processing, in this context, is the filling and draining of tanks with intermediate solutions. An example of this type of operation is the semicontinuous concentrator shown in Fig. 11. The entering stream is continuous, but the product stream is

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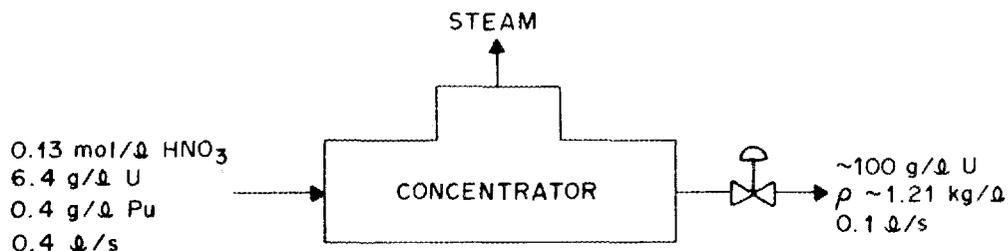


Fig. 11. A semicontinuous concentrator.

removed only when the density of the solution is within a prescribed range. Because of the low concentration of the entering stream and the concentration factor desired, the product cannot be drained continuously at the required flow rate. Thus, a method must be found to open a valve on the product stream only when the proper density is achieved. To maintain proper mass balances in the system, the solutions must accumulate when the product is not being removed, and drain when the product is being removed.

A solution to this problem is shown in Fig. 12. Stage 28 merely provides the entrance for the feed stream and is not necessary if the

ORNL DWG 80-3

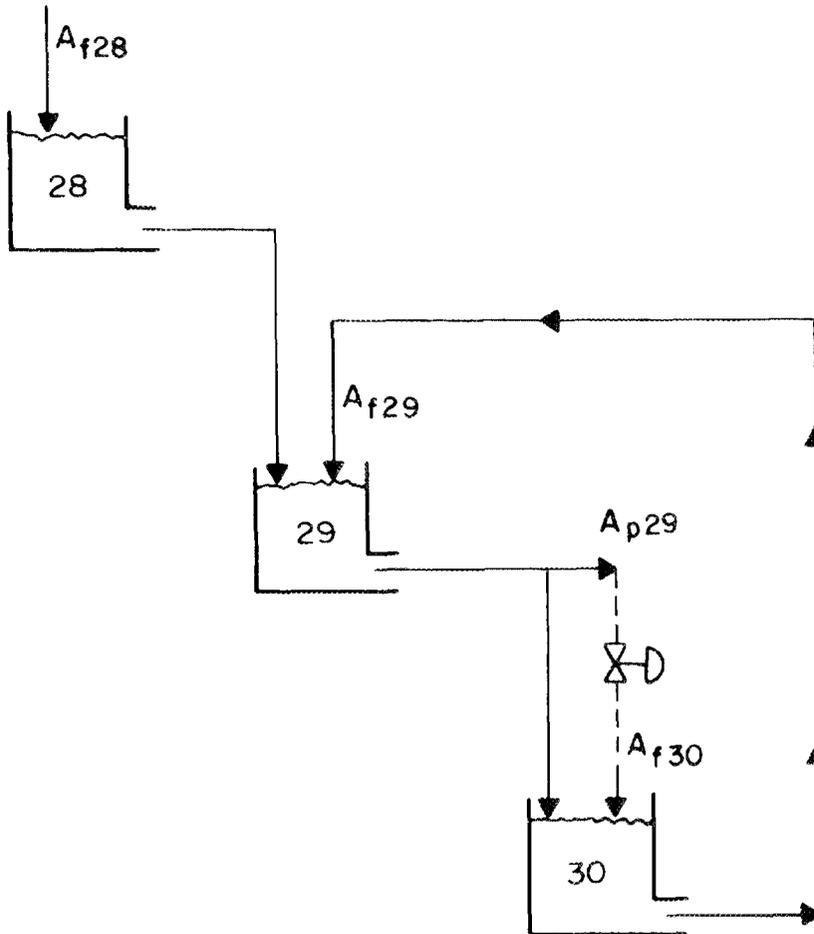


Fig. 12. A solution to the semicontinuous concentrator problem.

feed to the concentrator ordinarily flows from the previous stage. The feed stream to stage 29 is the recirculated product from stage 30. This provides the tank action since any solution flowing out of the bottom of the tank (stage 30) is simply put back into the top (stage 29). In this example, the recirculation stream also provides the concentrating action due to the specification of the proportional gains.

Given the tank action described above, the product stream leaving stage 29 is the only way that solutes can leave the concentrator. This

product stream, in conjunction with the feed stream to stage 30, provides the valve action that makes this a semicontinuous process. The product stream is constantly draining the concentrator at its given flow rate (0.1 L/s), but the feed stream to stage 30 acts to counter the draining. The concentrations of the feed stream to stage 30 are controlled to be equal to the concentrations of the product stream. The flow rate of the feed stream is controlled by an on/off controller. When this feed stream is turned on, the effect is simply to reinsert the product stream that was removed from stage 29. Conversely, when this feed stream is turned off, the product stream is not reinserted and the concentrator drains. The following cards describe this solution.

29	1	0.13	6.4	0.4	0.0	0.0	0.0	0.0	40.0	0.4	1	0	FEED STREAM CARD
29	1	4.03	190.4	15.1	0.0	0.0	0.0	0.0	60.0	0.391	1	1	FEED STREAM CARD
1	30	1	1	0.0	2.0	0.0	0.0	0.0	0.0	6.0	0.0	1	CONTROLLER CARDS
2	30	1	2	0.0	2.0	0.0	0.0	0.0	0.0	300.0	0.0	1	
3	30	1	3	0.0	2.0	0.0	0.0	0.0	0.0	300.0	0.0	1	
9	30	1	8	0.0	0.5	0.0	0.0	0.0	0.0	1000.0	0.0	0	
30	1	2.02	95.8	7.61	0.0	0.0	0.0	0.0	35.9	0.1	0	1	FEED STREAM CARD
1	29	1	1	0.0	1.0	0.0	0.0	0.0	0.0	6.0	0.0	1	CONTROLLER CARDS
2	29	1	2	0.0	1.0	0.0	0.0	0.0	0.0	300.0	0.0	1	
3	29	1	3	0.0	1.0	0.0	0.0	0.0	0.0	200.0	0.0	1	
7	29	1	7	0.0	1.0	0.0	0.0	0.0	0.0	60.0	10.0	1	
8	-29	110	1.22	1.20	0.0	0.0	0.0	0.0	0.0	0.1	0	0	

A consequence of recirculation of the solutes is that errors in the calculations are also recirculated. This accumulation of errors may lead to significant overall deviations from ideal mass balances if special care is not given to the selection of a suitably small value for DTHETA.

8. SAMPLE CALCULATIONS USING THE CONCEPT PROGRAM

The following examples demonstrate how the CONCEPT program can be applied to specific problems. In each case the input cards for the program are given with the resulting computer output. The examples illustrate several uses of the program and contain several solutions from Sect. 7.

8.1 Sample Calculation for a Simple Flowsheet

In this example, nothing complicated is being done, no controllers are being used, and no tricks are required. The user will merely be introduced to the program by following the progress of a calculation.

The system being modeled, a uranium stripping column (Fig. 13), is the same example as was used to demonstrate SEPHIS-MOD4.¹ The volume parameters are set arbitrarily so that each stage has a 1-min residence time. Due to the use of SI-metric units, the flow rates in the figure have been converted to those found in the output (Table 9). The cards used to produce this output are reproduced here.

2	6	0.3	35.0	0	0							START A NEW CASE
SECTION 8.1 AN EXAMPLE CALCULATION FOR A SIMPLE FLOWSHEET												TITLE CARD
THIS EXAMPLE IS A URANIUM STRIPPING COLUMN.												TITLE CARD
12.5	100.0	400.0	0.0001	1	0	1	0	0				START A TIME PERIOD
1	1	0.15	0.0	0.0	0.0	0.0	0.0	0.0	25.0	0.25	1	FEED STREAM CARD
6	2	0.25	50.0	0.0	0.0	0.0	0.0	0.0	55.0	0.1667	0	FEED STREAM CARD
1	20.0	5.0	0.025	0.0333	0							VOLUME CONSTANT CARD
12.5	10000.0	10000.0	0.0001	0	0	0	0	0				START A TIME PERIOD
0.0	0.0											END OF THIS CASE

Notice in the output that at the start of the calculations (elapsed time = 0.0 s), only the feed streams are printed in the profile. This occurs because the program will not list a stage with zero volume, and at the start of this calculation, the system is empty. The volume gradually builds with the progression of time and more stages are listed in the profile. In the final, steady-state profile, the changes in concentrations, temperatures, flow rates, and volumes have fallen below the convergence tolerance.

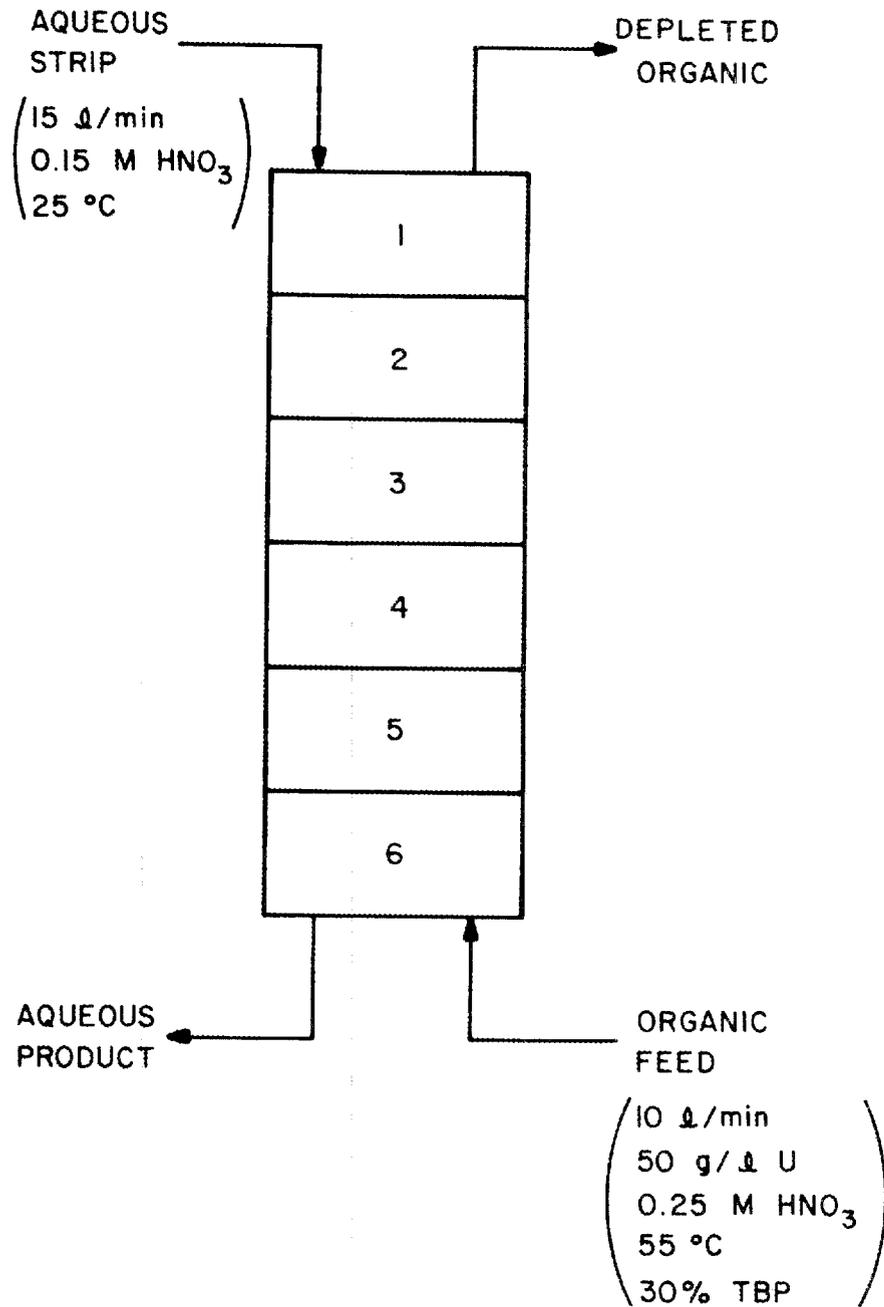


Fig. 13. A six-stage uranium stripping column.

Table 9. Sample calculation for a simple flowsheet

CONCEPT CONTROLLER-PUN SOLVENT EXTRACTION PROCESS TESTING PROGRAM DECEMBER 1979 VERSION
 PUFEX PROCESS USING 30.0 % TBP

SECTION 8.1 AN EXAMPLE CALCULATION FOR A SIMPLE FLOWSHEET
 THIS EXAMPLE IS A URANIUM STRIPPING COLUMN.

DTHETA = 1.250E+01 S, DPRINT = 1.00E+02 S, TSTOP = 4.00E+02 S, CONVERGENCE TOLERANCE = 1.00E-04 % / S
 NEWIN = 1 NEW FEED STREAMS WILL BE SPECIFIED
 NEWOUT = 0 THE PRESENT PRODUCT STREAMS WILL BE USED
 IVCL = 1 NEW VOLUME CONSTANTS WILL BE SPECIFIED
 IPFO = 0 THE PRESENT BANK PROFILE WILL BE CONTINUED
 IPNCH = 0 THE FINAL PROFILE WILL NOT BE PUNCHED
 IRXN = 0 NO REDUCTION OF PLUTONIUM

FEED STREAM DATA

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	
1	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	2.500E-01	AQUEOUS
6	2.500E-01	5.000E+01	0.0	0.0	0.0	0.0	5.500E+01	1.667E-01	ORGANIC

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PROCESS CONTROLLER INFORMATION

FEED STREAM VARIABLE BEING CONTROLLED	VARIABLE BEING USED AS CONTROLLER INPUT	CONTROL TYPE	SET POINT	PROP GAIN	INTEGRAL TIME	DERIVATIVE TIME	SET POINT FOR CNTRL	ERROR BAND	MAX VALUE OR ON VALUE	MIN VALUE OR OFF VALUE
STG	VARIABLE	STG	VARIABLE	SET POINT	SET POINT		VARIABLE			
1										

VOLUME CONSTANTS

STAGE	TOTAL VOLUME	AQ SET POINT	AQ CONSTANT	OR CONSTANT
1	2.000E+01	5.000E+00	2.500E-02	3.330E-02
2	2.000E+01	5.000E+00	2.500E-02	3.330E-02
3	2.000E+01	5.000E+00	2.500E-02	3.330E-02
4	2.000E+01	5.000E+00	2.500E-02	3.330E-02
5	2.000E+01	5.000E+00	2.500E-02	3.330E-02
6	2.000E+01	5.000E+00	2.500E-02	3.330E-02

ELAPSED TIME = 0.0 S SECTION 8.1 AN EXAMPLE CALCULATION FOR A SIMPLE FLOWSHEET

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)
1	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	2.500E-01			FEED STREAM

Table 9 (continued)

ORGANIC PHASE												
STAGE NC.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)	
6	2.500E-01	5.000E+01	0.0	0.0	0.0	0.0	5.500E+01	1.667E-01	FEED STREAM			

ELAPSED TIME = 100.0 S SECTION 8.1 AN EXAMPLE CALCULATION FOR A SIMPLE FLOWSHEET

AQUEOUS PHASE												
STAGE NC.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)	
1	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	2.500E-01	FEED STREAM			
1	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	2.158E-01	1.363E+01	1.0019	4.65E-01	
2	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	1.091E-01	9.366E+00	1.0019	2.71E+00	
3	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	0.0	1.923E+00	1.0019	4.71E+00	

ORGANIC PHASE												
STAGE NC.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)	
6	2.500E-01	5.000E+01	0.0	0.0	0.0	0.0	5.500E+01	0.0	1.667E+01	0.8742	1.00E+00	
6	2.500E-01	5.000E+01	0.0	0.0	0.0	0.0	5.500E+01	1.667E-01	FEED STREAM			

ELAPSED TIME = 200.0 S SECTION 8.1 AN EXAMPLE CALCULATION FOR A SIMPLE FLOWSHEET

AQUEOUS PHASE												
STAGE NC.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)	
1	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	2.500E-01	FEED STREAM			
1	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	2.472E-01	1.489E+01	1.0019	3.33E-02	
2	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	2.314E-01	1.425E+01	1.0019	1.95E-01	
3	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	1.827E-01	1.231E+01	1.0019	7.39E-01	
4	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	6.614E-02	7.646E+00	1.0019	4.82E+00	
5	8.332E-01	2.112E+01	0.0	0.0	0.0	0.0	4.579E+01	0.0	7.422E-01	1.0455	6.23E+00	

ORGANIC PHASE												
STAGE NC.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)	
5	1.930E-01	4.817E+01	0.0	0.0	0.0	0.0	4.579E+01	0.0	8.632E+00	0.8755	1.76E+00	
6	2.500E-01	5.000E+01	0.0	0.0	0.0	0.0	5.500E+01	1.549E-01	2.465E+01	0.8742	3.15E-01	
6	2.500E-01	5.000E+01	0.0	0.0	0.0	0.0	5.500E+01	1.667E-01	FEED STREAM			

Table 9 (continued)

ELAPSED TIME = 300.0 S SECTION 8.1 AN EXAMPLE CALCULATION FOR A SIMPLE FLOWSHEET

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)
1	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	2.500E-01	FEED STREAM		
1	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	2.498E-01	1.499E+01	1.0019	2.70E-03
2	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	2.479E-01	1.492E+01	1.0019	2.18E-02
3	1.505E-01	7.859E-01	0.0	0.0	0.0	0.0	2.505E+01	2.399E-01	1.460E+01	1.0030	8.00E+00
4	1.924E-01	1.084E+01	0.0	0.0	0.0	0.0	2.685E+01	2.156E-01	1.362E+01	1.0175	1.39E+00
5	4.019E-01	2.288E+01	0.0	0.0	0.0	0.0	3.278E+01	1.543E-01	1.117E+01	1.0387	1.09E+00
6	7.169E-01	2.554E+01	0.0	0.0	0.0	0.0	4.362E+01	1.015E-02	5.406E+00	1.0486	9.00E+00

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)
3	1.318E-02	5.376E+00	0.0	0.0	0.0	0.0	2.505E+01	0.0	8.871E-01	0.8238	1.81E+01
4	2.118E-02	1.878E+01	0.0	0.0	0.0	0.0	2.685E+01	1.078E-01	9.614E+00	0.8414	5.73E+00
5	8.368E-02	3.823E+01	0.0	0.0	0.0	0.0	3.278E+01	2.686E-01	1.689E+01	0.8664	8.40E-01
6	1.946E-01	4.929E+01	0.0	0.0	0.0	0.0	4.362E+01	2.615E-01	2.245E+01	0.8784	6.94E-01
6	2.500E-01	5.000E+01	0.0	0.0	0.0	0.0	5.500E+01	1.667E-01	FEED STREAM		

ELAPSED TIME = 400.0 S SECTION 8.1 AN EXAMPLE CALCULATION FOR A SIMPLE FLOWSHEET

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)
1	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	2.500E-01	FEED STREAM		
1	1.502E-01	4.103E-01	0.0	0.0	0.0	0.0	2.501E+01	2.500E-01	1.500E+01	1.0025	4.58E+00
2	1.511E-01	3.751E+00	0.0	0.0	0.0	0.0	2.512E+01	2.498E-01	1.499E+01	1.0070	1.66E+00
3	1.559E-01	1.115E+01	0.0	0.0	0.0	0.0	2.562E+01	2.487E-01	1.495E+01	1.0170	7.04E-01
4	1.949E-01	2.038E+01	0.0	0.0	0.0	0.0	2.698E+01	2.445E-01	1.478E+01	1.0304	2.92E-01
5	3.273E-01	2.692E+01	0.0	0.0	0.0	0.0	2.987E+01	2.320E-01	1.428E+01	1.0427	3.04E-01
6	5.406E-01	2.814E+01	0.0	0.0	0.0	0.0	3.599E+01	1.992E-01	1.297E+01	1.0493	4.52E-01

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)
1	1.002E-02	5.053E-01	0.0	0.0	0.0	0.0	2.501E+01	0.0	2.869E+00	0.8171	4.63E+00
2	1.161E-02	3.560E+00	0.0	0.0	0.0	0.0	2.512E+01	1.576E-01	9.743E+00	0.8212	2.51E+00
3	1.389E-02	1.188E+01	0.0	0.0	0.0	0.0	2.562E+01	2.593E-01	1.284E+01	0.8325	4.71E-01
4	1.904E-02	2.481E+01	0.0	0.0	0.0	0.0	2.698E+01	2.814E-01	1.367E+01	0.8496	1.82E-01
5	4.176E-02	3.825E+01	0.0	0.0	0.0	0.0	2.987E+01	2.611E-01	1.356E+01	0.8670	6.31E-01
6	1.080E-01	4.736E+01	0.0	0.0	0.0	0.0	3.599E+01	2.204E-01	1.365E+01	0.8778	6.87E-01
6	2.500E-01	5.000E+01	0.0	0.0	0.0	0.0	5.500E+01	1.667E-01	FEED STREAM		

Table 9 (continued)

DTFFTA = 1.250E+01 S, DPRINT = 1.00E+04 S, TSTOP = 1.00E+04 S, CONVERGENCE TOLERANCE = 1.00E-04 % / S

ELAPSED TIME = 5987.5 S

SECTION 8.1 AN EXAMPLE CALCULATION FOR A SIMPLE FLOWSHEET

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)
1	1.500E-01	0.0	0.0	0.0	0.0	0.0	2.500E+01	2.500E-01	FEED STREAM		
1	1.510E-01	2.086E+00	0.0	0.0	0.0	0.0	2.500E+01	2.500E-01	1.500E+01	1.0048	9.51E-05
2	1.519E-01	6.410E+00	0.0	0.0	0.0	0.0	2.502E+01	2.500E-01	1.500E+01	1.0107	6.67E-05
3	1.524E-01	1.268E+01	0.0	0.0	0.0	0.0	2.508E+01	2.500E-01	1.500E+01	1.0191	4.03E-05
4	1.531E-01	2.007E+01	0.0	0.0	0.0	0.0	2.536E+01	2.500E-01	1.500E+01	1.0291	2.43E-05
5	1.633E-01	2.814E+01	0.0	0.0	0.0	0.0	2.658E+01	2.500E-01	1.500E+01	1.0400	1.30E-05
6	3.097E-01	3.265E+01	0.0	0.0	0.0	0.0	3.189E+01	2.500E-01	1.500E+01	1.0492	7.42E-06

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)
1	1.043E-02	1.042E+00	0.0	0.0	0.0	0.0	2.500E+01	1.667E-01	1.001E+01	0.8178	9.52E-05
2	1.188E-02	4.170E+00	0.0	0.0	0.0	0.0	2.502E+01	1.667E-01	1.001E+01	0.8222	8.96E-05
3	1.324E-02	1.065E+01	0.0	0.0	0.0	0.0	2.508E+01	1.667E-01	1.001E+01	0.8311	6.66E-05
4	1.400E-02	2.006E+01	0.0	0.0	0.0	0.0	2.536E+01	1.667E-01	1.001E+01	0.8439	3.65E-05
5	1.509E-02	3.113E+01	0.0	0.0	0.0	0.0	2.658E+01	1.667E-01	1.001E+01	0.8584	1.57E-05
6	3.037E-02	4.325E+01	0.0	0.0	0.0	0.0	3.189E+01	1.667E-01	1.001E+01	0.8722	5.65E-06
6	2.500E-01	5.000E+01	0.0	0.0	0.0	0.0	5.590E+01	1.667E-01	FEED STREAM		

8.2 Sample Calculation for Flowsheet Design

This example is a partial partitioning column using hydroxylamine nitrate as the reductant. The system being modeled is shown in Fig. 14. The flow rate of the organic backscrub is to be controlled based on the uranium concentration in the aqueous product. The controller is set to achieve a 30-g/L concentration in the aqueous product. The constants in

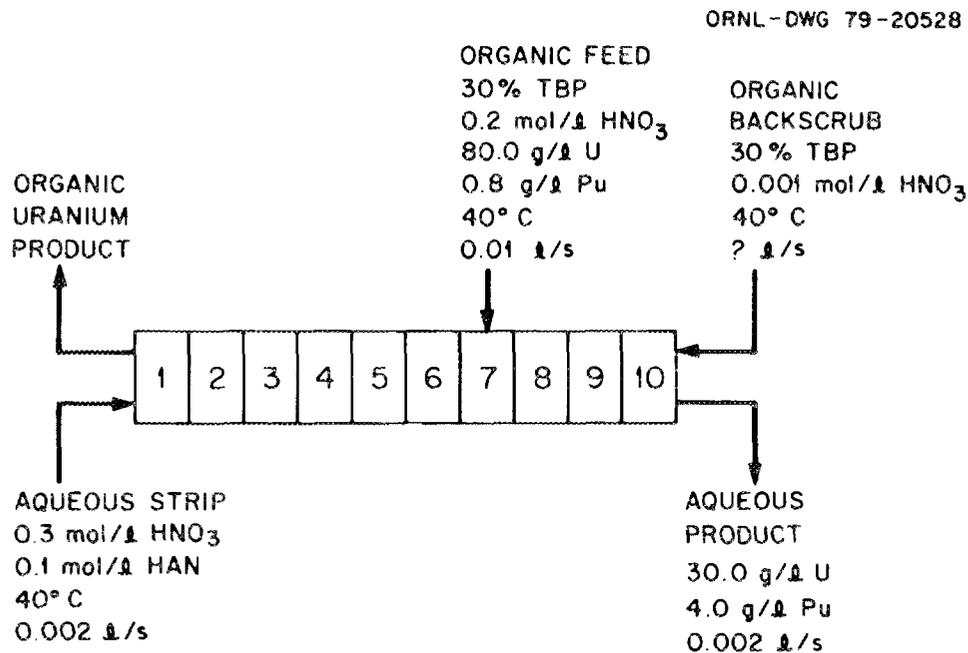


Fig. 14. A ten-stage partial partitioning column.

the three-mode controller equation were chosen by considering how a change in the flow rate would affect the concentration and how long the system would require to change the concentration. The initial profile was previously calculated by the program. Because the goal of this computation is flowsheet design rather than transient simulation, the volume constants are set arbitrarily to give a residence time of ~ 1.00 s for each stage.

The results indicate that the flow rate of the organic backscrub required to achieve a 30-g/L uranium concentration in the product stream is 0.4 mL/s for the given system. Figure 15 shows how the uranium concentration and the backscrub flow rate changed with time. The input

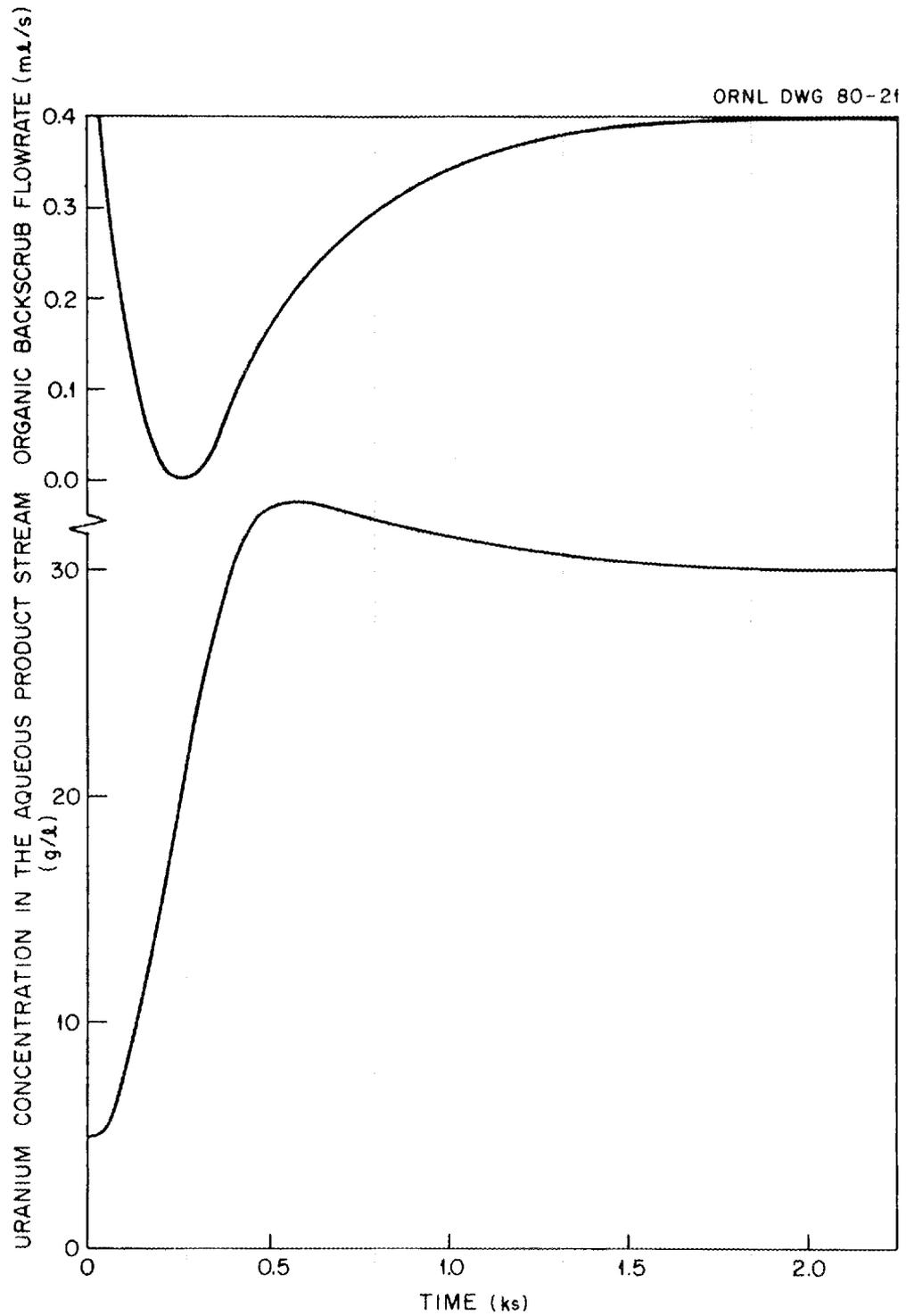


Fig. 15. The uranium concentration and backscrub flow rate response in the partial partitioning column.

Table 10. Sample calculation for flowsheet design

CONCEPT CONTROLLER-RUN SOLVENT EXTRACTION PROCESS TESTING PROGRAM DECEMBER 1979 VERSION
 PUFEX PROCESS USING 30.0 % TBP

SECTION 8.2 AN EXAMPLE CALCULATION FOR FLOWSHEET DESIGN
 THIS EXAMPLE IS A PARTIAL PARTITIONING COLUMN. THE URANIUM
 CONCENTRATION IN STAGE 10 IS USED TO CONTROL THE FLOWRATE
 OF THE ORGANIC BACKSCRUB ENTERING STAGE 10.

DTHEA = 2.500E+01 S, DPRINT = 1.00E+04 S, TSTOP = 1.00E+04 S, CONVERGENCE TOLERANCE = 1.00E-04 % / S
 NEWIN = 1 NEW FEED STREAMS WILL BE SPECIFIED
 NEWOUT = 0 THE PRESENT PRODUCT STREAMS WILL BE USED
 IVCL = 1 NEW VOLUME CONSTANTS WILL BE SPECIFIED
 IFR0 = 1 A NEW BANK PROFILE WILL BE SPECIFIED
 IFNCH = 0 THE FINAL PROFILE WILL NOT BE PUNCHED
 IRRN = 3 REDUCTION OF PLUTONIUM BY HYDROXYLAMINE

FEED STREAM DATA

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	
1	2.000E-01	0.0	0.0	0.0	1.000E-01	1.000E-01	4.000E+01	2.000E-03	AQUEOUS
7	2.000E-01	8.000E+01	8.000E-01	0.0	0.0	0.0	4.000E+01	1.000E-02	ORGANIC
10	1.000E-03	0.0	0.0	0.0	0.0	0.0	4.000E+01	1.000E-03	ORGANIC

PROCESS CONTROLLER INFORMATION

FEED STREAM VARIABLE BEING CONTROLLED	VARIABLE	STG	VARIABLE	STG	CONTROL TYPE	SET POINT	PROP GAIN	INTEGRAL TIME	DERIVATIVE TIME	SET POINT FOR CNTRL	ERROR BAND	MAX VALUE	MIN VALUE	OR	OR
10	ORG FEED FLOWRATE	10	AQUEOUS URANIUM	10	3-MODE	3.00E+01	2.00E-05	1.25E+02	0.0	1.00E-03	0.0	3.00E-03	0.0		

VOLUME CONSTANTS

STAGE	TOTAL VOLUME	AQ SET POINT	AQ CONSTANT	OR CONSTANT
1	2.200E-01	0.0	1.000E-02	1.000E-02
2	2.200E-01	0.0	1.000E-02	1.000E-02
3	2.200E-01	0.0	1.000E-02	1.000E-02
4	2.200E-01	0.0	1.000E-02	1.000E-02
5	2.200E-01	0.0	1.000E-02	1.000E-02
6	2.200E-01	0.0	1.000E-02	1.000E-02
7	2.200E-01	0.0	1.000E-02	1.000E-02
8	2.200E-01	0.0	1.000E-02	1.000E-02
9	2.200E-01	0.0	1.000E-02	1.000E-02
10	2.200E-01	0.0	1.000E-02	1.000E-02

Table 10 (continued)

ELAPSED TIME = 0.0 S SECTION 8.2 AN EXAMPLE CALCULATION FOR FLOWSHEET DESIGN											
AQUEOUS PHASE											
STAGE	NITRIC ACID	URANIUM	PU (IV)	PU (III)	REDUCTANT	NITRATE ION	TEMPERATURE	FLOW RATE	VOLUME	DENSITY	MAX CHNGE
NO.	{MOL/L}	{G/L}	{G/L}	{G/L}	{MOL/L}	{MOL/L}	{DEGREES C}	{L/S}	{LITERS}	{KG/L}	{% / S}
1	3.000E-01	0.0	0.0	0.0	1.000E-01	1.000E-01	4.000E+01	2.000E-03	FEED STREAM		
1	2.810E-01	6.390E+01	0.0	1.910E-07	1.000E-01	1.000E-01	4.000E+01	2.000E-03	2.000E-01	1.1061	2.00E+02
2	2.790E-01	8.360E+01	9.310E-08	1.030E-05	1.000E-01	1.000E-01	4.000E+01	2.000E-03	2.000E-01	1.1327	2.00E+02
3	2.900E-01	9.050E+01	5.290E-06	5.630E-04	1.000E-01	1.000E-01	4.000E+01	2.000E-03	2.000E-01	1.1424	2.00E+02
4	3.270E-01	9.130E+01	2.880E-04	3.060E-02	9.990E-02	9.990E-02	4.000E+01	2.000E-03	2.000E-01	1.1447	2.00E+02
5	4.370E-01	8.610E+01	1.440E-02	8.600E-01	9.640E-02	9.640E-02	4.000E+01	2.000E-03	2.000E-01	1.1418	2.00E+02
6	7.140E-01	7.090E+01	3.200E-01	3.050E+00	8.720E-02	8.720E-02	4.000E+01	2.000E-03	2.000E-01	1.1323	2.00E+02
7	1.260E+00	4.450E+01	7.160E-01	3.610E+00	8.490E-02	8.490E-02	4.000E+01	2.000E-03	2.000E-01	1.1153	2.00E+02
8	1.280E+00	3.560E+01	6.460E-01	3.720E+00	8.440E-02	8.440E-02	4.000E+01	2.000E-03	2.000E-01	1.1029	2.00E+02
9	1.310E+00	1.820E+01	4.640E-01	3.780E+00	8.420E-02	8.420E-02	4.000E+01	2.000E-03	2.000E-01	1.0811	2.00E+02
10	1.210E+00	4.890E+00	1.920E-01	3.810E+00	8.410E-02	8.410E-02	4.000E+01	2.000E-03	2.000E-01	1.0594	2.00E+02
ORGANIC PHASE											
STAGE	NITRIC ACID	URANIUM	PU (IV)	PU (III)	REDUCTANT	NITRATE ION	TEMPERATURE	FLOW RATE	VOLUME	DENSITY	MAX CHNGE
NO.	{MOL/L}	{G/L}	{G/L}	{G/L}	{MOL/L}	{MOL/L}	{DEGREES C}	{L/S}	{LITERS}	{KG/L}	{% / S}
1	2.230E-02	7.180E+01	0.0	0.0	0.0	0.0	4.000E+01	1.100E-02	1.120E+00	0.9052	2.00E+02
2	1.880E-02	8.350E+01	3.480E-08	0.0	0.0	0.0	4.000E+01	1.100E-02	1.120E+00	0.9222	2.00E+02
3	1.850E-02	8.700E+01	1.880E-05	0.0	0.0	0.0	4.000E+01	1.100E-02	1.120E+00	0.9270	2.00E+02
4	2.050E-02	8.830E+01	1.030E-04	0.0	0.0	0.0	4.000E+01	1.100E-02	1.120E+00	0.9288	2.00E+02
5	2.720E-02	8.840E+01	5.620E-03	0.0	0.0	0.0	4.000E+01	1.100E-02	1.120E+00	0.9292	2.00E+02
6	4.590E-02	8.750E+01	1.590E-01	0.0	0.0	0.0	4.000E+01	1.100E-02	1.120E+00	0.9288	2.00E+02
7	9.290E-02	8.470E+01	6.120E-01	0.0	0.0	0.0	4.000E+01	1.100E-02	1.120E+00	0.9272	2.00E+02
7	2.000E-01	8.000E+01	8.000E-01	0.0	0.0	0.0	4.000E+01	1.000E-02	FEED STREAM		
8	1.060E-01	7.930E+01	6.460E-01	0.0	0.0	0.0	4.000E+01	1.000E-03	1.200E-01	0.9202	2.00E+02
9	1.480E-01	6.140E+01	7.230E-01	0.0	0.0	0.0	4.000E+01	1.000E-03	1.200E-01	0.8971	2.00E+02
10	2.100E-01	2.660E+01	4.910E-01	0.0	0.0	0.0	4.000E+01	1.000E-03	1.200E-01	0.8508	2.00E+02
10	1.000E-03	0.0	0.0	0.0	0.0	0.0	4.000E+01	1.000E-03	FEED STREAM		

Table 10 (continued)

ELAPSED TIME = 10000.0 S SECTION 9.2 AN EXAMPLE CALCULATION FOR FLOWSHEET DESIGN

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)
1	3.000E-01	0.0	0.0	0.0	1.000E-01	1.000E-01	4.000E+01	2.000E-03	FEED STREAM		
1	2.805E-01	6.298E+01	0.0	8.788E-08	1.000E-01	1.000E-01	4.000E+01	2.000E-03	2.000E-01	1.1048	0.0
2	2.770E-01	8.339E+01	4.524E-08	4.803E-06	1.000E-01	1.000E-01	4.000E+01	2.000E-03	2.000E-01	1.1323	7.57E-07
3	2.842E-01	9.120E+01	2.642E-06	2.700E-04	1.000E-01	1.000E-01	4.000E+01	2.000E-03	2.000E-01	1.1431	2.20E-05
4	3.133E-01	9.302E+01	1.490E-04	1.520E-02	9.994E-02	9.994E-02	4.000E+01	2.000E-03	2.000E-01	1.1465	0.0
5	4.060E-01	8.900E+01	7.858E-03	5.786E-01	9.758E-02	9.758E-02	4.000E+01	2.000E-03	2.000E-01	1.1445	2.09E-05
6	6.665E-01	7.492E+01	2.413E-01	2.729E+00	8.858E-02	8.858E-02	4.000E+01	2.000E-03	2.000E-01	1.1359	0.0
7	1.229E+00	4.795E+01	7.045E-01	3.388E+00	8.582E-02	8.582E-02	4.000E+01	2.000E-03	2.000E-01	1.1176	3.38E-06
8	1.230E+00	4.682E+01	5.994E-01	3.486E+00	8.541E-02	8.541E-02	4.000E+01	2.000E-03	2.000E-01	1.1172	1.54E-03
9	1.235E+00	4.458E+01	5.256E-01	3.558E+00	8.511E-02	8.511E-02	4.000E+01	2.000E-03	2.000E-01	1.1143	1.46E-04
10	1.213E+00	3.000E+01	3.915E-01	3.608E+00	8.490E-02	8.490E-02	4.000E+01	2.000E-03	2.000E-01	1.0937	9.74E-06

ORGANIC PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)
1	2.250E-02	7.117E+01	0.0	0.0	0.0	0.0	4.000E+01	1.040E-02	1.060E+00	0.9053	0.0
2	1.876E-02	8.329E+01	1.691E-08	0.0	0.0	0.0	4.000E+01	1.040E-02	1.060E+00	0.9219	0.0
3	1.807E-02	8.721E+01	9.327E-07	0.0	0.0	0.0	4.000E+01	1.040E-02	1.060E+00	0.9272	0.0
4	1.947E-02	8.871E+01	5.245E-05	0.0	0.0	0.0	4.000E+01	1.040E-02	1.060E+00	0.9294	0.0
5	2.504E-02	8.906E+01	2.952E-03	0.0	0.0	0.0	4.000E+01	1.040E-02	1.060E+00	0.9300	1.51E-05
6	4.197E-02	8.829E+01	1.128E-01	0.0	0.0	0.0	4.000E+01	1.040E-02	1.060E+00	0.9297	0.0
7	8.861E-02	8.558E+01	5.714E-01	0.0	0.0	0.0	4.000E+01	1.040E-02	1.060E+00	0.9282	3.34E-06
7	2.000E-01	8.000E+01	8.000E-01	0.0	0.0	0.0	4.000E+01	1.000E-02	FEED STREAM		
8	8.907E-02	8.579E+01	4.674E-01	0.0	0.0	0.0	4.000E+01	3.975E-04	5.975E-02	0.9283	1.43E-03
9	9.180E-02	8.463E+01	4.292E-01	0.0	0.0	0.0	4.000E+01	3.975E-04	5.975E-02	0.9268	1.02E-04
10	1.116E-01	7.333E+01	4.199E-01	0.0	0.0	0.0	4.000E+01	3.975E-04	5.975E-02	0.9118	6.25E-06
10	1.000E-03	0.0	0.0	0.0	0.0	0.0	4.000E+01	3.975E-04	FEED STREAM		

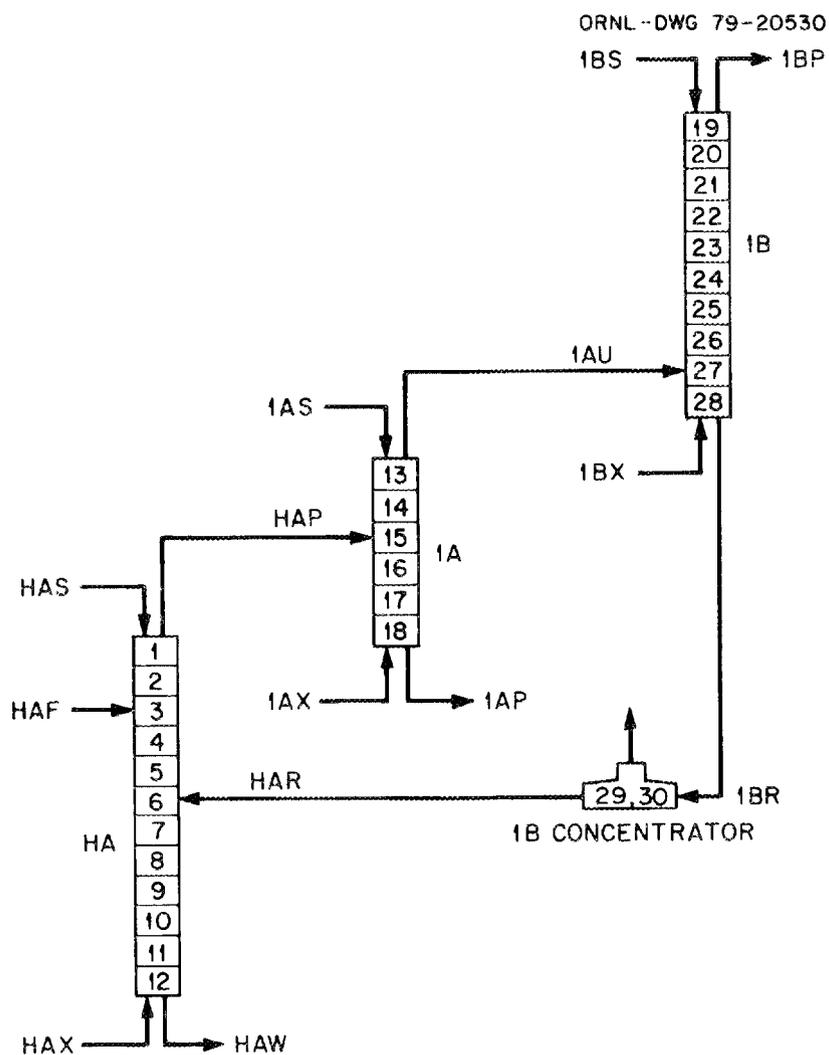


Fig. 16. A coprocessing flowsheet.

varies randomly about two points, providing a positive bias on the error. The recycle stream (HAR) enters at stage 6. This stream comes from the concentrator so the concentrations are controlled accordingly. The flow rate provides the batch operation since this stream is turned on only when the density in the concentrator is in the proper range. The scrub stream (HAS) enters stage 1 and randomly varies about its nominal flow rate. The organic extractant (HAX) enters stage 12. The flow rate and acidity vary randomly.

The 1A column is a partial partitioning column. The organic product from the HA column is the feed to the 1A column and enters at stage 15.

The transfer is performed as described in Sect. 7.1. The aqueous strip (1AS) enters at stage 13. The organic backscrub (1AX) enters stage 18. Its flow rate is regulated by a three-mode controller used as a controller. The controller is trying to produce a coprocessed product with 20% plutonium.

The 1B column provides uranium purification. The organic stream leaving the 1A column is transferred to stage 27 (near the bottom of the 1B column). The aqueous strip stream (1BS) is intended to remove the plutonium from the organic phase while leaving a large fraction of the uranium. The 1BS flow rate uses a random walk error. The organic backscrub (1BX) enters at stage 28 and is constant. The aqueous product leaving the column after stage 28 is concentrated in stages 29 and 30 and recycled to the HA column.

Several pseudo-stages (some not shown in Fig. 16) were used for specific purposes. Stages 29 and 30, which make up a semicontinuous concentrator as described in Sect. 7.4, concentrate the 1BR stream to the concentration level required in the HAR recycle stream. Stages 31 and 32 are used to calculate the ratio $\text{Pu}/(\text{U} + \text{Pu})$ for the coprocessed product (1AP) as described in Sect. 7.3.3. Stage 33 is an aqueous tank collecting the coprocessed product stream leaving the 1A column at stage 18. Similarly, stage 34 is an organic tank catching the uranium product stream leaving the 1B column at stage 19.

The $\text{Pu}/(\text{U} + \text{Pu})$ ratio produced in stages 31 and 32 is used to control the flow rates in the 1A column. The 1AS flow rate is controlled by an on/off controller. If the ratio in stage 32 (reflecting the ratio in the aqueous product leaving stage 18) becomes too high, the 1AS flow rate will be switched to its high value, thus stripping more uranium into the coprocessed product. The 1AX flow rate uses a three-mode controller, which monitors the ratio and adjusts the backscrub flow rate accordingly.

The following cards produced the computer output that is given in Table 11. The number of cards could have been reduced by rearranging the stages. Many of the cards serve only to transfer streams within the system; rearranging the stages can reduce the number of transfers.

10 34 0.3 30.0 0 0

SECTION 8.3 TESTING AN EXAMPLE OF PLANT OPERATION

THIS EXAMPLE IS OF A REPROCESSING PLANT PRODUCING A COPROCESSED PRODUCT. THE EXAMPLE ILLUSTRATES MANY OF THE IDEAS IN SECTION 7. SEVERAL STREAMS ARE MOVED FROM PLACE TO PLACE IN ORDER TO GIVE THE RECYCLE STREAMS AND THE INTER-COLUMN STREAMS. THE CONCENTRATOR IN THIS CALCULATION IS A SEMI-BATCH OPERATION IN STAGES 29 AND 30. SEVERAL TYPES OF ERRORS ARE APPLIED TO THE FEED STREAMS. THESE ARE OF THE TYPE DESCRIBED IN SECTION 7, BUT THERE ARE ALSO SOME ERRORS IMPOSED IN MANNERS NOT DESCRIBED. THE GENERAL MATH IS USED IN CONTROLLING A FLOWRATE ACCORDING TO THE PU/(U+PU) RATIO.

START A NEW CASE

10.0 2500.0 5000.0 0.0001 1 1 1 1 0

1	1	3.0	0.0	0.0	0.0	0.0	0.0	0.0	35.0	0.035	1	1	START A TIME PERIOD
1	3	8	0.035	0.0	0.0	0.0	0.0	0.035	5.0	0.04	0.03	0	FEED STREAM (HAS)
3	1	3.4	315.0	2.95	0.0	0.0	0.0	0.0	35.0	0.054	1	1	CONTROLLER CARD
1	-3	3	1	3.7365	3.3665	0.0	0.0	0.0	1.0	3.40	3.70	1	FEED STREAM (HAF)
2	-3	3	1	3.6	3.5	0.0	0.0	0.0	1.0	275.0	315.0	1	CONTROLLER CARDS
3	-3	3	1	3.6	3.5	0.0	0.0	0.0	1.0	2.59	2.950	1	
9	-3	3	9	0.055	0.048	0.0	0.0	0.0	5.0	0.049	0.052	0	
6	1	5.2	95.8	76.1	0.0	0.0	0.0	0.0	35.9	0.0	0.0	1	FEED STREAM (HAR)
2	29	1	2	0.0	1.0	0.0	0.0	0.0	0.0	300.0	0.0	1	
3	29	1	3	0.0	1.0	0.0	0.0	0.0	0.0	300.0	0.0	1	CONTROLLER CARDS
7	29	1	7	0.0	1.0	0.0	0.0	0.0	0.0	60.0	10.0	1	
8	-29	110	1.22	1.2	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0	
12	2	0.18	0.0	0.0	0.0	0.0	0.0	0.0	35.0	0.3	0.3	1	FEED STREAM (HAX)
1	12	4	1	0.18	0.0	0.0	0.0	0.18	20.0	0.3	0.0	1	CONTROLLER CARD
8	12	4	8	0.3	0.0	0.0	0.0	0.3	3.5	0.5	0.0	0	CONTROLLER CARD
13	1	0.8	0.0	0.0	0.0	0.0	0.0	0.0	20.0	0.255	0.255	1	FEED STREAM (IAS)
8	-32	1	4	0.23	0.17	0.0	0.0	0.0	1.0	0.255	0.245	0	CONTROLLER CARD
15	2	0.399	58.0	0.549	0.0	0.0	0.0	0.0	35.0	0.284	0.284	1	FEED STREAM (HAP)
1	1	2	1	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1	
2	1	2	2	0.0	1.0	0.0	0.0	0.0	0.0	200.0	0.0	1	
3	1	2	3	0.0	1.0	0.0	0.0	0.0	0.0	20.0	0.0	1	CONTROLLER CARDS
7	1	2	7	0.0	1.0	0.0	0.0	0.0	0.0	50.0	30.0	1	
9	1	2	8	0.0	1.0	0.0	0.0	0.0	0.0	0.5	0.0	0	
18	2	0.01	0.0	0.0	0.0	0.0	0.0	0.0	20.0	0.0825	0.0825	1	FEED STREAM (IAX)
8	32	1	4	0.20	-0.05	150.0	0.0	0.0825	0.0	0.0925	0.0825	0	CONTROLLER CARD
19	1	0.05	0.0	0.0	0.0	0.0	0.0	0.0	10.0	0.375	0.375	1	FEED STREAM (IBS)
8	19	3	8	0.0	1.0	0.0	6.5	0.0	0.3	0.43	0.37	0	CONTROLLER CARD
27	2	0.092	47.1	0.445	0.0	0.0	0.0	0.0	20.8	0.354	0.354	1	FEED STREAM (IAU)
1	13	2	1	0.0	1.0	0.0	0.0	0.0	0.0	1.0	0.0	1	
2	13	2	2	0.0	1.0	0.0	0.0	0.0	0.0	200.0	0.0	1	
3	13	2	3	0.0	1.0	0.0	0.0	0.0	0.0	20.0	0.0	1	CONTROLLER CARDS
7	13	2	7	0.0	1.0	0.0	0.0	0.0	0.0	40.0	10.0	1	
9	13	2	8	0.0	1.0	0.0	0.0	0.0	0.0	0.5	0.0	0	
28	2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	10.0	0.9	0.9	1	FEED STREAM (IBX)
29	1	4.03	190.4	15.1	0.0	0.0	0.0	0.0	60.0	0.391	0.391	1	FEED STREAM CARD
1	30	1	1	0.0	2.0	0.0	0.0	0.0	0.0	6.0	0.0	1	
2	30	1	2	0.0	2.0	0.0	0.0	0.0	0.0	300.0	0.0	1	
3	30	1	3	0.0	2.0	0.0	0.0	0.0	0.0	300.0	0.0	1	CONTROLLER CARDS
8	30	1	8	0.0	0.5	0.0	0.0	0.0	0.0	1000.0	0.0	0	
30	1	2.02	95.9	7.61	0.0	0.0	0.0	0.0	35.9	0.1	0.1	1	FEED STREAM CARD
1	29	1	1	0.0	1.0	0.0	0.0	0.0	0.0	6.0	0.0	1	
2	29	1	2	0.0	1.0	0.0	0.0	0.0	0.0	300.0	0.0	1	
3	29	1	3	0.0	1.0	0.0	0.0	0.0	0.0	300.0	0.0	1	CONTROLLER CARDS
7	29	1	7	0.0	1.0	0.0	0.0	0.0	0.0	60.0	10.0	1	
9	-6	3	8	0.09	0.01	0.0	0.0	0.0	0.0	0.0	0.1	0	
31	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	3.77	3.77	1	FEED STREAM (IAP U)
8	18	1	2	0.0	1.0	0.0	0.0	0.0	0.0	200.0	0.0	0	CONTROLLER CARD
32	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.772	0.772	1	FEED STREAM (IAP PU)
8	18	1	3	0.0	1.0	0.0	0.0	0.0	0.0	20.0	0.0	0	CONTROLLER CARD
32	2	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.772	0.772	1	FEED STREAM (IAP PU)
8	18	1	3	0.0	1.0	0.0	0.0	0.0	0.0	20.0	0.0	0	CONTROLLER CARD
33	1	1.05	3.77	0.772	0.0	0.0	0.0	0.0	0.0	0.255	0.255	1	FEED STREAM (IAP)
1	18	1	1	0.0	1.0	0.0	0.0	0.0	0.0	10.0	0.0	1	
2	18	1	2	0.0	1.0	0.0	0.0	0.0	0.0	10.0	0.0	1	
3	18	1	3	0.0	1.0	0.0	0.0	0.0	0.0	10.0	0.0	1	CONTROLLER CARDS
8	18	1	8	0.0	1.0	0.0	0.0	0.0	0.0	10.0	0.0	0	
34	2	0.004	14.2	0.009	0.0	0.0	0.0	0.0	0.0	1.14	1.14	0	FEED STREAM (IBP)
1	19	2	1	0.0	1.0	0.0	0.0	0.0	0.0	200.0	0.0	1	
2	19	2	2	0.0	1.0	0.0	0.0	0.0	0.0	200.0	0.0	1	
3	19	2	3	0.0	1.0	0.0	0.0	0.0	0.0	200.0	0.0	1	CONTROLLER CARDS
8	19	2	8	0.0	1.0	0.0	0.0	0.0	0.0	200.0	0.0	0	
12	1	1000.0	1										PRODUCT STREAM (HAW)
13	2	1000.0	1										PRODUCT STREAM (IAU)
18	1	1000.0	1										PRODUCT STREAM (IAP)
19	2	1000.0	1										PRODUCT STREAM (IBP)
29	1	0.1	1										
30	1	1000.0	1										
31	2	1000.0	1										
32	1	1000.0	1										
33	1	1000.0	1										
34	2	1000.0	0										

TITLE CARDS

START A TIME PERIOD

FEED STREAM (HAS)

CONTROLLER CARD

FEED STREAM (HAF)

CONTROLLER CARDS

FEED STREAM (HAR)

CONTROLLER CARDS

FEED STREAM (HAX)

CONTROLLER CARD

CONTROLLER CARD

FEED STREAM (IAS)

CONTROLLER CARD

FEED STREAM (HAP)

CONTROLLER CARDS

FEED STREAM (IAX)

CONTROLLER CARD

FEED STREAM (IBS)

CONTROLLER CARD

FEED STREAM (IAU)

CONTROLLER CARDS

FEED STREAM (IBX)

FEED STREAM CARD

CONTROLLER CARDS

FEED STREAM CARD

CONTROLLER CARDS

FEED STREAM (IAP U)

CONTROLLER CARD

FEED STREAM (IAP PU)

CONTROLLER CARD

FEED STREAM (IAP PU)

CONTROLLER CARD

FEED STREAM (IAP)

CONTROLLER CARDS

FEED STREAM (IBP)

CONTROLLER CARDS

PRODUCT STREAM (HAW)

PRODUCT STREAM (IAU)

PRODUCT STREAM (IAP)

PRODUCT STREAM (IBP)

PRODUCT STREAM CARDS

Table 11. Sample simulation of plant operations

CONCEPT CONTROLLER-RUN SOLVENT EXTRACTION PROCESS TESTING PROGRAM DECEMBER 1979 VERSION
 PUREX PROCESS USING 30.0 % TBP

SECTION 8.3 TESTING AN EXAMPLE OF PLANT OPERATION

THIS EXAMPLE IS OF A REPROCESSING PLANT PRODUCING A COPROCESSED PRODUCT. THE EXAMPLE ILLUSTRATES MANY OF THE IDEAS IN SECTION 7. SEVERAL STREAMS ARE MOVED FROM PLACE TO PLACE IN ORDER TO GIVE THE RECYCLE STREAMS AND THE INTER-COLUMN STREAMS. THE CONCENTRATOR IN THIS CALCULATION IS A SEMI-BATCH OPERATION IN STAGES 29 AND 30. SEVERAL TYPES OF ERRORS ARE APPLIED TO THE FEED STREAMS. THESE ARE OF THE TYPE DESCRIBED IN SECTION 7, BUT THERE ARE ALSO SOME ERRORS IMPOSED IN MANNERS NOT DESCRIBED. THE GENERAL MATH IS USED IN CONTROLLING A FLOWRATE ACCORDING TO THE $PU/(U+PU)$ RATIO.

DTHETA = 1.000E+01 S, DPRINT = 2.50E+03 S, TSTOP = 5.00E+03 S, CONVERGENCE TOLERANCE = 1.00E-04 % / S
 NEWIN = 1 NEW FEED STREAMS WILL BE SPECIFIED
 NEWOUT = 1 NEW PRODUCT STREAMS WILL BE SPECIFIED
 IVCL = 1 NEW VOLUME CONSTANTS WILL BE SPECIFIED
 IFFO = 1 A NEW BANK PROFILE WILL BE SPECIFIED
 IFNCH = 0 THE FINAL PROFILE WILL NOT BE PUNCHED
 IRIN = 0 NO REDUCTION OF PLUTONIUM

FEED STREAM DATA

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	
1	3.000E+00	0.0	0.0	0.0	0.0	0.0	3.500E+01	3.500E-02	AQUEOUS
3	3.400E+00	3.150E+02	2.950E+00	0.0	0.0	0.0	3.500E+01	5.400E-02	AQUEOUS
6	5.200E+00	9.580E+01	7.610E+01	0.0	0.0	0.0	3.590E+01	0.0	AQUEOUS
12	1.800E-01	0.0	0.0	0.0	0.0	0.0	3.500E+01	3.000E-01	ORGANIC
13	8.000E-01	0.0	0.0	0.0	0.0	0.0	2.000E+01	2.550E-01	AQUEOUS
15	3.990E-01	5.800E+01	5.450E-01	0.0	0.0	0.0	3.500E+01	2.840E-01	ORGANIC
18	1.000E-02	0.0	0.0	0.0	0.0	0.0	2.000E+01	8.250E-02	ORGANIC
19	5.000E-02	0.0	0.0	0.0	0.0	0.0	1.000E+01	3.750E-01	AQUEOUS
27	9.200E-02	4.710E+01	4.450E-01	0.0	0.0	0.0	2.080E+01	3.540E-01	ORGANIC
28	0.0	0.0	0.0	0.0	0.0	0.0	1.000E+01	8.000E-01	ORGANIC
29	4.030E+00	1.904E+02	1.510E+01	0.0	0.0	0.0	6.000E+01	3.910E-01	AQUEOUS
30	2.020E+00	9.580E+01	7.610E+00	0.0	0.0	0.0	3.590E+01	1.000E-01	AQUEOUS
31	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	3.770E+00	AQUEOUS
32	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	7.720E-01	AQUEOUS
32	0.0	0.0	0.0	1.000E+00	0.0	0.0	3.000E+01	7.720E-01	ORGANIC
33	1.050E+00	3.770E+00	7.720E-01	0.0	0.0	0.0	3.000E+01	2.550E-01	AQUEOUS
34	4.000E-03	1.420E+01	9.000E-03	0.0	0.0	0.0	3.000E+01	1.140E+00	ORGANIC

Table 11 (continued)

PRODUCT STREAMS ARE REMOVED AT	STAGE	PHASE	RATE
	1	ORGANIC	1.000E+20
	12	AQUEOUS	1.000E+03
	13	ORGANIC	1.000E+03
	18	AQUEOUS	1.000E+03
	19	ORGANIC	1.000E+03
	29	AQUEOUS	1.000E-01
	30	AQUEOUS	1.000E+03
	31	ORGANIC	1.000E+03
	32	AQUEOUS	1.000E+03
	33	AQUEOUS	1.000E+03
	34	AQUEOUS	1.000E+20
	34	ORGANIC	1.000E+03

VOLUME CONSTANTS	STAGE	TOTAL VOLUME	AQ SET POINT	AQ CONSTANT	OR CONSTANT
	1	8.000E+00	0.0	2.000E-02	4.000E-02
	2	8.000E+00	0.0	2.000E-02	4.000E-02
	3	8.000E+00	0.0	2.000E-02	4.000E-02
	4	8.000E+00	0.0	2.000E-02	4.000E-02
	5	8.000E+00	0.0	2.000E-02	4.000E-02
	6	8.000E+00	0.0	2.000E-02	4.000E-02
	7	8.000E+00	0.0	2.000E-02	4.000E-02
	8	8.000E+00	0.0	2.000E-02	4.000E-02
	9	8.000E+00	0.0	2.000E-02	4.000E-02
	10	8.000E+00	0.0	2.000E-02	4.000E-02
	11	8.000E+00	0.0	2.000E-02	4.000E-02
	12	8.000E+00	0.0	2.000E-02	4.000E-02
	13	1.500E+01	0.0	2.000E-02	2.000E-02
	14	1.500E+01	0.0	2.000E-02	2.000E-02
	15	1.500E+01	0.0	2.000E-02	2.000E-02
	16	1.500E+01	0.0	2.000E-02	2.000E-02
	17	1.500E+01	0.0	2.000E-02	2.000E-02
	18	1.500E+01	0.0	2.000E-02	2.000E-02
	19	1.500E+01	0.0	5.000E-02	3.500E-02
	20	1.500E+01	0.0	5.000E-02	3.500E-02
	21	1.500E+01	0.0	5.000E-02	3.500E-02
	22	1.500E+01	0.0	5.000E-02	3.500E-02
	23	1.500E+01	0.0	5.000E-02	3.500E-02
	24	1.500E+01	0.0	5.000E-02	3.500E-02
	25	1.500E+01	0.0	5.000E-02	3.500E-02
	26	1.500E+01	0.0	5.000E-02	3.500E-02
	27	1.500E+01	0.0	5.000E-02	3.500E-02
	28	1.500E+01	0.0	5.000E-02	3.500E-02
	29	1.000E+03	0.0	1.000E-02	1.000E-02
	30	1.000E+03	0.0	1.000E-02	1.000E-02
	31	1.000E+01	0.0	1.000E-01	1.000E-01
	32	1.000E+01	0.0	1.000E-01	1.000E-01
	33	1.000E+04	9.000E+03	1.000E-02	1.000E-02
	34	1.000E+04	9.000E+03	1.000E-02	1.000E-02

Table 11 (continued)

PROCESS CONTROLLER INFORMATION

FEED STREAM VARIABLE BEING CONTROLLED		VARIABLE BEING USED AS CONTROLLER INPUT		CONTROL TYPE	SET POINT OR UPPER	PROP GAIN OR LOWER	INTEGRAL TIME	DERIVATIVE TIME	SET POINT FOR CNTRL	ERROR BAND	MAX VALUE OR	MIN VALUE OR
STG	VARIABLE	STG	VARIABLE		SET POINT	SET POINT			VARIABLE		ON VALUE	OFF VALUE
1	AQ FEED FLOWRATE	1	AQ FEED FLOWRATE	3-MODE	3.50E-02	0.0	1.00E+40	0.0	3.50E-02	5.00E+00	4.00E-02	3.00E-02
2	AQ FEED HNO3	3	AQ FEED HNO3	ON/OFF	3.74E+00	3.37E+00	1.00E+40	0.0	0.0	1.00E+00	3.40E+00	3.70E+00
3	AQ FEED URANIUM	3	AQ FEED HNO3	ON/OFF	3.60E+00	3.50E+00	1.00E+40	0.0	0.0	1.00E+00	2.75E+02	3.15E+02
3	AQ FEED PU (IV)	3	AQ FEED HNO3	ON/OFF	3.60E+00	3.50E+00	1.00E+40	0.0	0.0	1.00E+00	2.59E+00	2.95E+00
3	AQ FEED FLOWRATE	3	AQ FEED FLOWRATE	ON/OFF	5.50E-02	4.80E-02	1.00E+40	0.0	0.0	5.00E+00	4.90E-02	5.20E-02
6	AQ FEED URANIUM	29	AQUEOUS URANIUM	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	3.00E+02	0.0
6	AQ FEED PU (IV)	29	AQUEOUS PU (IV)	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	3.00E+02	0.0
6	AQ FEED TEMP	29	AQUEOUS TEMP	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	6.00E+01	1.00E+01
6	AQ FEED FLOWRATE	29	AQUEOUS DENSITY	ON/OFF	1.22E+00	1.20E+00	1.00E+40	0.0	0.0	0.0	1.00E-01	0.0
12	ORG FEED HNO3	12	ORG FEED HNO3	3-MODE	1.80E-01	0.0	1.00E+40	0.0	1.80E-01	2.00E+01	3.00E-01	0.0
12	ORG FEED FLOWRATE	12	ORG FEED FLOWRATE	3-MODE	3.00E-01	0.0	1.00E+40	0.0	3.00E-01	3.50E+00	5.00E-01	0.0
13	AQ FEED FLOWRATE	32	AQUEOUS PU (III)	ON/OFF	2.30E-01	1.70E-01	1.00E+40	0.0	0.0	1.00E+00	2.55E-01	2.45E-01
15	ORG FEED HNO3	1	ORGANIC HNO3	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	1.00E+00	0.0
15	ORG FEED URANIUM	1	ORGANIC URANIUM	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	2.00E+02	0.0
15	ORG FEED PU (IV)	1	ORGANIC PU (IV)	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	2.00E+01	0.0
15	ORG FEED TEMP	1	ORGANIC TEMP	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	5.00E+01	3.00E+01
15	ORG FEED FLOWRATE	1	ORGANIC FLOWRATE	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	5.00E-01	0.0
18	ORG FEED FLOWRATE	32	AQUEOUS PU (III)	3-MODE	2.00E-01	-5.00E-02	1.50E+02	0.0	8.25E-02	0.0	9.25E-02	8.25E-02
19	AQ FEED FLOWRATE	19	AQ FEED FLOWRATE	3-MODE	0.0	1.00E+00	1.00E+40	6.50E+00	0.0	3.00E-01	4.30E-01	3.70E-01
27	ORG FEED HNO3	13	ORGANIC HNO3	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	1.00E+00	0.0
27	ORG FEED URANIUM	13	ORGANIC URANIUM	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	2.00E+02	0.0
27	ORG FEED PU (IV)	13	ORGANIC PU (IV)	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	2.00E+01	0.0
27	ORG FEED TEMP	13	ORGANIC TEMP	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	4.00E+01	1.00E+01
27	ORG FEED FLOWRATE	13	ORGANIC FLOWRATE	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	5.00E-01	0.0
29	AQ FEED HNO3	30	AQUEOUS HNO3	3-MODE	0.0	2.00E+00	1.00E+40	0.0	0.0	0.0	6.00E+00	0.0
29	AQ FEED URANIUM	30	AQUEOUS URANIUM	3-MODE	0.0	2.00E+00	1.00E+40	0.0	0.0	0.0	3.00E+02	0.0
29	AQ FEED PU (IV)	30	AQUEOUS PU (IV)	3-MODE	0.0	2.00E+00	1.00E+40	0.0	0.0	0.0	3.00E+02	0.0
29	AQ FEED FLOWRATE	30	AQUEOUS FLOWRATE	3-MODE	0.0	5.00E-01	1.00E+40	0.0	0.0	0.0	1.00E+03	0.0
30	AQ FEED HNO3	29	AQUEOUS HNO3	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	6.00E+00	0.0
30	AQ FEED URANIUM	29	AQUEOUS URANIUM	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	3.00E+02	0.0
30	AQ FEED PU (IV)	29	AQUEOUS PU (IV)	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	3.00E+02	0.0
30	AQ FEED TEMP	29	AQUEOUS TEMP	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	6.00E+01	1.00E+01
30	AQ FEED FLOWRATE	6	AQ FEED FLOWRATE	ON/OFF	9.00E-02	1.00E-02	1.00E+40	0.0	0.0	0.0	0.0	1.00E-01
31	AQ FEED FLOWRATE	18	AQUEOUS URANIUM	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	2.00E+02	0.0
32	AQ FEED FLOWRATE	18	AQUEOUS PU (IV)	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	2.00E+01	0.0
32	ORG FEED FLOWRATE	18	AQUEOUS PU (IV)	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	2.00E+01	0.0
33	AQ FEED HNO3	18	AQUEOUS HNO3	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	1.00E+01	0.0
33	AQ FEED URANIUM	18	AQUEOUS URANIUM	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	1.00E+01	0.0
33	AQ FEED PU (IV)	18	AQUEOUS PU (IV)	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	1.00E+01	0.0
33	AQ FEED FLOWRATE	18	AQUEOUS FLOWRATE	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	1.00E+01	0.0
34	ORG FEED HNO3	19	ORGANIC HNO3	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	2.00E+02	0.0
34	ORG FEED URANIUM	19	ORGANIC URANIUM	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	2.00E+02	0.0
34	ORG FEED PU (IV)	19	ORGANIC PU (IV)	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	2.00E+02	0.0
34	ORG FEED FLOWRATE	19	ORGANIC FLOWRATE	3-MODE	0.0	1.00E+00	1.00E+40	0.0	0.0	0.0	2.00E+02	0.0

Table 11 (continued)

ELAPSED TIME =		SECTION 8.3 TESTING AN EXAMPLE OF PLANT OPERATION										
AQUEOUS PHASE												
STAGE	{NITRIC ACID}	{URANIUM}	{PU (IV)}	{PU (III)}	{REDUCTANT}	{NITRATE ION}	{TEMPERATURE}	{FLOW RATE}	{VOLUME}	{DENSITY}	{MAX CHNGE}	
NC.	{(MOL/L)}	{(G/L)}	{(G/L)}	{(G/L)}	{(MOL/L)}	{(MOL/L)}	{(DEGREES C)}	{(L/S)}	{(LITERS)}	{(KG/L)}	{(% / S)}	
1	3.000E+00	0.0	0.0	0.0	0.0	0.0	3.500E+01	3.500E-02	FEED STREAM			
1	3.300E+00	6.030E+00	1.030E-01	0.0	0.0	0.0	3.500E+01	3.460E-02	1.730E+00	1.1089	2.00E+02	
2	3.800E+00	5.530E+00	8.690E-02	0.0	0.0	0.0	3.500E+01	3.480E-02	1.740E+00	1.1244	2.00E+02	
3	3.400E+00	3.150E+02	2.950E+00	0.0	0.0	0.0	3.500E+01	5.400E-02	FEED STREAM			
3	4.930E+00	5.490E+00	6.820E-02	0.0	0.0	0.0	3.500E+01	8.590E-02	4.300E+00	1.1608	2.00E+02	
4	4.960E+00	5.420E-02	9.040E-04	0.0	0.0	0.0	3.500E+01	8.580E-02	4.290E+00	1.1543	2.00E+02	
5	4.950E+00	5.460E-04	1.320E-05	0.0	0.0	0.0	3.500E+01	8.600E-02	4.300E+00	1.1539	2.00E+02	
6	5.200E+00	9.580E+01	7.610E+01	0.0	0.0	0.0	3.590E+01	0.0	FEED STREAM			
6	4.950E+00	8.600E-06	5.390E-07	0.0	0.0	0.0	3.500E+01	8.620E-02	4.310E+00	1.1539	2.00E+02	
7	4.950E+00	4.660E-07	5.830E-08	0.0	0.0	0.0	3.500E+01	8.630E-02	4.320E+00	1.1539	2.00E+02	
8	4.950E+00	3.190E-08	5.170E-09	0.0	0.0	0.0	3.500E+01	8.640E-02	4.320E+00	1.1539	2.00E+02	
9	4.910E+00	1.720E-09	3.390E-10	0.0	0.0	0.0	3.500E+01	8.640E-02	4.320E+00	1.1526	2.00E+02	
10	4.680E+00	0.0	0.0	0.0	0.0	0.0	3.500E+01	8.650E-02	4.320E+00	1.1452	2.00E+02	
11	3.950E+00	0.0	0.0	0.0	0.0	0.0	3.500E+01	8.670E-02	4.330E+00	1.1216	2.00E+02	
12	2.620E+00	3.0	0.0	0.0	0.0	0.0	3.500E+01	8.710E-02	4.360E+00	1.0787	2.00E+02	
12	2.620E+00	0.0	0.0	0.0	0.0	0.0	3.500E+01	8.710E-02	AQUEOUS PRODUCT			
13	8.000E-01	0.0	0.0	0.0	0.0	0.0	2.000E+01	2.550E-01	FEED STREAM			
13	7.880E-01	1.550E+01	4.420E-01	0.0	0.0	0.0	2.080E+01	2.550E-01	1.270E+01	1.0451	2.00E+02	
14	8.280E-01	2.180E+01	7.990E-01	0.0	0.0	0.0	2.240E+01	2.550E-01	1.270E+01	1.0551	2.00E+02	
15	1.120E+00	1.930E+01	7.580E-01	0.0	0.0	0.0	2.580E+01	2.550E-01	1.270E+01	1.0602	2.00E+02	
16	1.110E+00	1.620E+01	1.060E+00	0.0	0.0	0.0	2.580E+01	2.550E-01	1.280E+01	1.0562	2.00E+02	
17	1.110E+00	1.000E+01	1.150E+00	0.0	0.0	0.0	2.570E+01	2.550E-01	1.280E+01	1.0479	2.00E+02	
18	1.050E+00	3.770E+00	7.710E-01	0.0	0.0	0.0	2.510E+01	2.550E-01	1.280E+01	1.0372	2.00E+02	
18	1.050E+00	3.770E+00	7.710E-01	0.0	0.0	0.0	2.510E+01	2.550E-01	AQUEOUS PRODUCT			
19	5.000E-02	0.0	0.0	0.0	0.0	0.0	1.000E+01	3.750E-01	FEED STREAM			
19	5.060E-02	1.750E+01	4.110E-02	0.0	0.0	0.0	1.060E+01	3.740E-01	7.480E+00	1.0255	2.00E+02	
20	5.080E-02	2.140E+01	9.190E-02	0.0	0.0	0.0	1.120E+01	3.740E-01	7.490E+00	1.0308	2.00E+02	
21	5.080E-02	2.220E+01	1.570E-01	0.0	0.0	0.0	1.180E+01	3.780E-01	7.550E+00	1.0319	2.00E+02	
22	5.100E-02	2.230E+01	2.420E-01	0.0	0.0	0.0	1.230E+01	3.840E-01	7.680E+00	1.0321	2.00E+02	
23	5.130E-02	2.230E+01	3.500E-01	0.0	0.0	0.0	1.280E+01	3.920E-01	7.850E+00	1.0321	2.00E+02	
24	5.240E-02	2.210E+01	4.840E-01	0.0	0.0	0.0	1.330E+01	4.010E-01	8.020E+00	1.0320	2.00E+02	
25	5.650E-02	2.170E+01	6.350E-01	0.0	0.0	0.0	1.380E+01	4.090E-01	8.170E+00	1.0317	2.00E+02	
26	7.320E-02	2.060E+01	7.660E-01	0.0	0.0	0.0	1.430E+01	4.130E-01	8.270E+00	1.0309	2.00E+02	
27	1.350E-01	1.710E+01	7.370E-01	0.0	0.0	0.0	1.480E+01	4.160E-01	8.320E+00	1.0280	2.00E+02	
28	1.180E-01	6.980E+00	5.310E-01	0.0	0.0	0.0	1.290E+01	4.160E-01	8.320E+00	1.0138	2.00E+02	
29	4.030E+00	1.904E+02	1.510E+01	0.0	0.0	0.0	6.000E+01	3.910E-01	FEED STREAM			
29	2.020E+00	9.580E+01	7.610E+00	0.0	0.0	0.0	3.590E+01	7.920E-01	7.920E+01	1.2002	2.00E+02	
29	2.020E+00	9.580E+01	7.610E+00	0.0	0.0	0.0	3.590E+01	1.000E-01	AQUEOUS PRODUCT			
30	2.020E+00	9.580E+01	7.610E+00	0.0	0.0	0.0	3.590E+01	1.000E-01	FEED STREAM			
30	2.020E+00	9.520E+01	7.560E+00	0.0	0.0	0.0	3.610E+01	7.920E-01	7.920E+01	1.1952	2.00E+02	
30	2.020E+00	9.520E+01	7.560E+00	0.0	0.0	0.0	3.610E+01	7.920E-01	AQUEOUS PRODUCT			

Table 11 (continued)

31	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	3.770E+00	FEED STREAM		
31	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	3.770E+00	9.500E+00	0.9957	2.00E+02
32	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	7.720E-01	FEED STREAM		
32	0.0	0.0	0.0	1.710E-01	0.0	0.0	3.000E+01	4.560E+00	9.500E+00	0.9959	2.00E+02
32	0.0	0.0	0.0	1.710E-01	0.0	0.0	3.000E+01	4.560E+00	AQUEOUS PRODUCT		
33	1.050E+00	3.770E+00	7.720E-01	0.0	0.0	0.0	3.000E+01	2.550E-01	FEED STREAM		
ORGANIC PHASE											
STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)
1	3.990E-01	5.800E+01	5.490E-01	0.0	0.0	0.0	3.500E+01	2.840E-01	ORGANIC PRODUCT		
1	3.990E-01	5.800E+01	5.490E-01	0.0	0.0	0.0	3.500E+01	2.840E-01	1.340E+01	0.9033	2.00E+02
2	4.460E-01	5.750E+01	5.470E-01	0.0	0.0	0.0	3.500E+01	2.870E-01	1.340E+01	0.9041	2.00E+02
3	5.160E-01	5.660E+01	5.350E-01	0.0	0.0	0.0	3.500E+01	2.890E-01	1.090E+01	0.9051	2.00E+02
4	9.280E-01	1.680E+00	2.100E-02	0.0	0.0	0.0	3.500E+01	2.910E-01	1.100E+01	0.8418	2.00E+02
5	9.290E-01	1.710E-02	2.960E-04	0.0	0.0	0.0	3.500E+01	2.920E-01	1.100E+01	0.8399	2.00E+02
6	9.290E-01	1.930E-04	6.440E-06	0.0	0.0	0.0	3.500E+01	2.940E-01	1.100E+01	0.8398	2.00E+02
7	9.390E-01	6.170E-06	5.660E-07	0.0	0.0	0.0	3.500E+01	2.950E-01	1.110E+01	0.8398	2.00E+02
8	9.390E-01	4.520E-07	5.890E-08	0.0	0.0	0.0	3.500E+01	2.960E-01	1.110E+01	0.8398	2.00E+02
9	9.350E-01	2.790E-08	4.420E-09	0.0	0.0	0.0	3.500E+01	2.980E-01	1.110E+01	0.8397	2.00E+02
10	9.150E-01	1.280E-09	2.340E-10	0.0	0.0	0.0	3.500E+01	2.990E-01	1.110E+01	0.8391	2.00E+02
11	8.290E-01	0.0	0.0	0.0	0.0	0.0	3.500E+01	3.000E-01	1.120E+01	0.8363	2.00E+02
12	5.900E-01	0.0	0.0	0.0	0.0	0.0	3.500E+01	3.000E-01	1.110E+01	0.8286	2.00E+02
12	1.800E-01	0.0	0.0	0.0	0.0	0.0	3.500E+01	3.000E-01	FEED STREAM		
13	9.220E-02	4.710E+01	4.450E-01	0.0	0.0	0.0	2.080E+01	3.540E-01	ORGANIC PRODUCT		
13	9.220E-02	4.710E+01	4.450E-01	0.0	0.0	0.0	2.080E+01	3.540E-01	2.000E+01	0.8873	2.00E+02
14	8.510E-02	5.770E+01	7.070E-01	0.0	0.0	0.0	2.240E+01	3.580E-01	2.010E+01	0.9010	2.00E+02
15	1.170E-01	6.110E+01	3.690E-01	0.0	0.0	0.0	2.580E+01	3.620E-01	2.040E+01	0.9348	2.00E+02
15	3.990E-01	5.800E+01	5.490E-01	0.0	0.0	0.0	3.500E+01	2.840E-01	FEED STREAM		
16	1.230E-01	5.610E+01	1.370E+00	0.0	0.0	0.0	2.580E+01	8.320E-02	6.410E+00	0.8950	2.00E+02
17	1.460E-01	4.290E+01	1.870E+00	0.0	0.0	0.0	2.570E+01	8.300E-02	6.390E+00	0.8824	2.00E+02
18	1.760E-01	2.080E+01	1.610E+00	0.0	0.0	0.0	2.510E+01	8.270E-02	6.380E+00	0.8529	2.00E+02
18	1.000E-02	0.0	0.0	0.0	0.0	0.0	2.000E+01	8.250E-02	FEED STREAM		
19	3.640E-03	1.420E+01	8.850E-03	0.0	0.0	0.0	1.060E+01	1.140E+00	ORGANIC PRODUCT		
19	3.640E-03	1.420E+01	8.850E-03	0.0	0.0	0.0	1.060E+01	1.140E+00	4.020E+01	0.8450	2.00E+02
20	3.840E-03	1.980E+01	2.240E-02	0.0	0.0	0.0	1.120E+01	1.140E+00	4.010E+01	0.8523	2.00E+02
21	3.880E-03	2.080E+01	3.920E-02	0.0	0.0	0.0	1.180E+01	1.140E+00	4.010E+01	0.8534	2.00E+02
22	3.900E-03	2.080E+01	6.080E-02	0.0	0.0	0.0	1.230E+01	1.140E+00	4.000E+01	0.8531	2.00E+02
23	3.940E-03	2.960E+01	8.840E-02	0.0	0.0	0.0	1.280E+01	1.150E+00	3.990E+01	0.8525	2.00E+02
24	4.040E-03	2.030E+01	1.230E-01	0.0	0.0	0.0	1.330E+01	1.150E+00	3.990E+01	0.8518	2.00E+02
25	4.400E-03	2.010E+01	1.640E-01	0.0	0.0	0.0	1.380E+01	1.150E+00	3.980E+01	0.8513	2.00E+02
26	5.850E-03	1.980E+01	2.100E-01	0.0	0.0	0.0	1.430E+01	1.160E+00	3.970E+01	0.8507	2.00E+02
27	1.180E-02	1.930E+01	2.440E-01	0.0	0.0	0.0	1.480E+01	1.160E+00	3.970E+01	0.8499	2.00E+02
27	9.200E-02	4.710E+01	4.450E-01	0.0	0.0	0.0	2.080E+01	3.540E-01	FEED STREAM		
28	8.700E-03	5.230E+00	1.180E-01	0.0	0.0	0.0	1.290E+01	8.030E-01	2.960E+01	0.8315	2.00E+02
28	0.0	0.0	0.0	0.0	0.0	0.0	1.000E+01	8.000E-01	FEED STREAM		

Table 11 (continued)

31	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	8.120E-01	ORGANIC PRODUCT
31	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	8.120E-01	8.620E+00 0.8129 2.00E+02
32	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	7.970E-01	8.470E+00 0.8129 2.00E+02
32	0.0	0.0	0.0	1.000E+00	0.0	0.0	3.000E+01	7.720E-01	FEED STREAM

24	4.000E-03	1.420E+01	9.000E-03	0.0	0.0	0.0	3.000E+01	1.140E+00	FEED STREAM
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ELAPSED TIME = 2500.0 S SECTION 8.3 TESTING AN EXAMPLE OF PLANT OPERATION

AQUEOUS PHASE

STAGE NC.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PU (IV) (G/L)	PU (III) (G/L)	REDUCTANT (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)
1	3.000E+00	0.0	0.0	0.0	0.0	0.0	3.500E+01	3.452E-02	FEED STREAM		
2	3.419E+00	3.781E+00	6.298E-02	0.0	0.0	0.0	3.500E+01	3.508E-02	1.754E+00	1.1097	1.79E-01
2	3.959E+00	3.618E+00	5.511E-02	0.0	0.0	0.0	3.500E+01	3.525E-02	1.762E+00	1.1269	1.88E-02
3	3.720E+00	2.768E+02	2.587E+00	0.0	0.0	0.0	3.500E+01	5.119E-02	FEED STREAM		
3	5.029E+00	3.695E+00	4.518E-02	0.0	0.0	0.0	3.500E+01	8.726E-02	4.363E+00	1.1615	1.48E-01
4	5.055E+00	3.408E-02	5.427E-04	0.0	0.0	0.0	3.500E+01	8.740E-02	4.370E+00	1.1574	1.65E-02
5	5.054E+00	3.047E-04	6.323E-06	0.0	0.0	0.0	3.500E+01	8.723E-02	4.361E+00	1.1573	1.78E-02
6	5.200E+00	1.042E+02	8.406E+00	0.0	0.0	0.0	3.646E+01	0.0	FEED STREAM		
6	5.050E+00	2.695E-06	7.302E-08	0.0	0.0	0.0	3.500E+01	8.697E-02	4.348E+00	1.1571	3.29E-02
7	5.038E+00	2.374E-05	8.426E-10	0.0	0.0	0.0	3.500E+01	8.673E-02	4.336E+00	1.1567	5.38E-03
8	4.998E+00	2.065E-10	0.0	0.0	0.0	0.0	3.500E+01	8.651E-02	4.326E+00	1.1555	4.95E-03
9	4.863E+00	0.0	0.0	0.0	0.0	0.0	3.500E+01	8.632E-02	4.316E+00	1.1511	4.51E-03
10	4.460E+00	0.0	0.0	0.0	0.0	0.0	3.500E+01	8.617E-02	4.308E+00	1.1321	3.32E-03
11	3.605E+00	0.0	0.0	0.0	0.0	0.0	3.500E+01	8.610E-02	4.305E+00	1.1105	2.99E-03
12	2.358E+00	0.0	0.0	0.0	0.0	0.0	3.500E+01	8.612E-02	4.306E+00	1.0702	1.04E-02
12	2.358E+00	0.0	0.0	0.0	0.0	0.0	3.500E+01	8.612E-02	AQUEOUS PRODUCT		
13	8.000E-01	0.0	0.0	0.0	0.0	0.0	2.000E+01	2.468E-01	FEED STREAM		
13	8.090E-01	1.083E+01	2.889E-01	0.0	0.0	0.0	2.106E+01	2.459E-01	1.229E+01	1.0392	9.78E-02
14	9.013E-01	1.288E+01	4.333E-01	0.0	0.0	0.0	2.300E+01	2.458E-01	1.229E+01	1.0447	2.46E-02
15	1.282E+00	9.465E+00	3.301E-01	0.0	0.0	0.0	2.655E+01	2.457E-01	1.228E+01	1.0513	1.09E-02
16	1.294E+00	4.331E+00	3.185E-01	0.0	0.0	0.0	2.654E+01	2.455E-01	1.228E+01	1.0447	6.64E-02
17	1.293E+00	1.527E+00	2.237E-01	0.0	0.0	0.0	2.645E+01	2.454E-01	1.227E+01	1.0408	1.16E-01
18	1.204E+00	4.143E-01	1.122E-01	0.0	0.0	0.0	2.573E+01	2.453E-01	1.227E+01	1.0364	1.41E-01
18	1.204E+00	4.143E-01	1.122E-01	0.0	0.0	0.0	2.573E+01	2.453E-01	AQUEOUS PRODUCT		
19	5.000E-02	0.0	0.0	0.0	0.0	0.0	1.000E+01	3.695E-01	FEED STREAM		
19	5.075E-02	1.580E+01	3.890E-02	0.0	0.0	0.0	1.074E+01	3.715E-01	7.430E+00	1.0232	3.10E-02
20	5.092E-02	1.941E+01	8.550E-02	0.0	0.0	0.0	1.142E+01	3.729E-01	7.458E+00	1.0281	3.58E-02
21	5.103E-02	2.025E+01	1.428E-01	0.0	0.0	0.0	1.206E+01	3.742E-01	7.485E+00	1.0292	3.60E-02
22	5.120E-02	2.048E+01	2.138E-01	0.0	0.0	0.0	1.265E+01	3.755E-01	7.510E+00	1.0295	3.40E-02
23	5.171E-02	2.054E+01	3.014E-01	0.0	0.0	0.0	1.322E+01	3.767E-01	7.534E+00	1.0296	2.89E-02
24	5.357E-02	2.047E+01	4.074E-01	0.0	0.0	0.0	1.376E+01	3.778E-01	7.557E+00	1.0297	2.37E-02
25	6.069E-02	2.004E+01	5.264E-01	0.0	0.0	0.0	1.427E+01	3.789E-01	7.578E+00	1.0294	1.86E-02
26	8.695E-02	1.842E+01	6.167E-01	0.0	0.0	0.0	1.476E+01	3.798E-01	7.597E+00	1.0281	1.64E-02
27	1.703E-01	1.394E+01	5.482E-01	0.0	0.0	0.0	1.522E+01	3.806E-01	7.613E+00	1.0245	1.97E-02
28	1.460E-01	5.115E+00	3.650E-01	0.0	0.0	0.0	1.303E+01	3.813E-01	7.627E+00	1.0119	2.65E-02
29	4.415E+00	2.062E+02	1.665E+01	0.0	0.0	0.0	6.000E+01	3.810E-01	FEED STREAM		
29	2.240E+00	1.042E+02	8.406E+00	0.0	0.0	0.0	3.646E+01	7.629E-01	7.629E+01	1.2198	1.61E-02
29	2.240E+00	1.042E+02	8.406E+00	0.0	0.0	0.0	3.646E+01	1.000E-01	AQUEOUS PRODUCT		

Table 11 (continued)

30	2.240E+00	1.042E+02	8.406E+00	0.0	0.0	0.0	3.646E+01	1.000E-01	FEED STREAM		
30	2.208E+00	1.031E+02	8.326E+00	0.0	0.0	0.0	3.642E+01	7.621E-01	7.621E+01 1.2171 1.61E-02		
30	2.208E+00	1.031E+02	8.326E+00	0.0	0.0	0.0	3.642E+01	7.621E-01	AQUEOUS PRODUCT		
31	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	4.143E-01	FEED STREAM		
31	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	4.265E-01	4.265E+00 0.9957 1.52E-C1		
32	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	1.122E-01	FEED STREAM		
32	0.0	0.0	0.0	2.096E-01	0.0	0.0	3.000E+01	5.480E-01	5.480E+00 0.9960 1.49E-01		
32	0.0	0.0	0.0	2.096E-01	0.0	0.0	3.000E+01	5.480E-01	AQUEOUS PRODUCT		
33	1.204E+00	4.143E-01	1.122E-01	0.0	0.0	0.0	3.000E+01	2.453E-01	FEED STREAM		
33	1.112E+00	2.216E+00	5.338E-01	0.0	0.0	0.0	3.000E+01	0.0	6.238E+02 1.0353 1.41E-01		
ORGANIC PHASE											
STAGE	NITRIC ACID	URANIUM	PU (IV)	PU (III)	REDUCTANT	NITRATE ION	TEMPERATURE	FLOW RATE	VOLUME	DENSITY	WAT. CHNGE
NO.	(MOL/L)	(G/L)	(G/L)	(G/L)	(MOL/L)	(MOL/L)	(DEGREES C)	(L/S)	(LITERS)	(KG/L)	(% / S)
1	4.715E-01	4.772E+01	4.486E-01	0.0	0.0	0.0	3.500E+01	3.000E-01	ORGANIC PRODUCT		
1	4.715E-01	4.772E+01	4.486E-01	0.0	0.0	0.0	3.500E+01	3.000E-01	1.375E+01	0.8913	1.33E-C2
2	5.201E-01	4.820E+01	4.564E-01	0.0	0.0	0.0	3.500E+01	2.998E-01	1.373E+01	0.8935	1.04E-02
3	5.853E-01	4.794E+01	4.532E-01	0.0	0.0	0.0	3.500E+01	2.996E-01	1.113E+01	0.8953	2.09E-02
4	9.390E-01	1.086E+00	1.328E-02	0.0	0.0	0.0	3.500E+01	2.999E-01	1.113E+01	0.8414	2.54E-C2
5	9.465E-01	9.895E-03	1.576E-04	0.0	0.0	0.0	3.500E+01	3.000E-01	1.114E+01	0.8401	1.40E-02
6	9.467E-01	8.758E-05	1.819E-06	0.0	0.0	0.0	3.500E+01	2.999E-01	1.115E+01	0.8401	3.37E-C2
7	9.460E-01	7.720E-07	2.094E-08	0.0	0.0	0.0	3.500E+01	2.999E-01	1.116E+01	0.8401	1.85E-02
8	9.433E-01	6.728E-09	2.385E-10	0.0	0.0	0.0	3.500E+01	2.995E-01	1.116E+01	0.8400	1.69E-03
9	9.328E-01	0.0	0.0	0.0	0.0	0.0	3.500E+01	2.994E-01	1.117E+01	0.8396	3.51E-C3
10	8.552E-01	0.0	0.0	0.0	0.0	0.0	3.500E+01	2.995E-01	1.118E+01	0.8384	3.01E-03
11	7.811E-01	0.0	0.0	0.0	0.0	0.0	3.500E+01	2.993E-01	1.118E+01	0.8348	1.57E-02
12	5.359E-01	0.0	0.0	0.0	0.0	0.0	3.500E+01	2.975E-01	1.113E+01	0.8269	6.80E-01
12	1.596E-01	0.0	0.0	0.0	0.0	0.0	3.500E+01	2.945E-01	FEED STREAM		
13	1.063E-01	3.808E+01	3.389E-01	0.0	0.0	0.0	2.106E+01	3.894E-01	ORGANIC PRODUCT		
13	1.063E-01	3.808E+01	3.389E-01	0.0	0.0	0.0	2.106E+01	3.894E-01	2.217E+01	0.8750	1.20E-C2
14	1.126E-01	4.461E+01	5.167E-01	0.0	0.0	0.0	2.300E+01	3.897E-01	2.220E+01	0.8832	1.61E-02
15	1.717E-01	4.559E+01	5.998E-01	0.0	0.0	0.0	2.655E+01	3.898E-01	2.221E+01	0.8843	1.64E-02
15	4.715E-01	4.772E+01	4.486E-01	0.0	0.0	0.0	3.500E+01	3.000E-01	FEED STREAM		
16	2.129E-01	2.835E+01	7.911E-01	0.0	0.0	0.0	2.654E+01	9.943E-02	7.192E+00	0.8622	5.20E-02
17	2.503E-01	1.266E+01	7.013E-01	0.0	0.0	0.0	2.645E+01	8.921E-02	7.186E+00	0.8417	1.08E-01
18	2.511E-01	3.588E+00	3.603E-01	0.0	0.0	0.0	2.573E+01	8.891E-02	7.179E+00	0.8292	1.49E-C1
18	1.000E-02	0.0	0.0	0.0	0.0	0.0	2.000E+01	8.848E-02	FEED STREAM		

Table 11 (continued)

19	3.538E-03	1.180E+01	7.877E-03	0.0	0.0	0.0	1.074E+01	1.180E+00	ORGANIC PRODUCT		
19	3.538E-03	1.180E+01	7.877E-03	0.0	0.0	0.0	1.074E+01	1.180E+00	4.129E+01	0.8416	3.94E-02
20	3.771E-03	1.669E+01	1.987E-02	0.0	0.0	0.0	1.142E+01	1.181E+00	4.129E+01	0.8479	4.23E-02
21	3.825E-03	1.773E+01	3.404E-02	0.0	0.0	0.0	1.206E+01	1.182E+00	4.129E+01	0.8450	4.25E-02
22	3.857E-03	1.788E+01	5.128E-02	0.0	0.0	0.0	1.265E+01	1.183E+00	4.130E+01	0.8498	4.01E-02
23	3.911E-03	1.785E+01	7.253E-02	0.0	0.0	0.0	1.322E+01	1.184E+00	4.130E+01	0.8484	3.61E-02
24	4.075E-03	1.777E+01	9.880E-02	0.0	0.0	0.0	1.376E+01	1.185E+00	4.130E+01	0.8480	2.95E-02
25	4.677E-03	1.767E+01	1.309E-01	0.0	0.0	0.0	1.427E+01	1.186E+00	4.131E+01	0.8476	2.26E-02
26	6.983E-03	1.745E+01	1.671E-01	0.0	0.0	0.0	1.476E+01	1.187E+00	4.132E+01	0.8471	1.65E-02
27	1.550E-02	1.685E+01	1.943E-01	0.0	0.0	0.0	1.522E+01	1.188E+00	4.133E+01	0.8463	1.25E-02
27	1.063E-01	3.808E+01	3.389E-01	0.0	0.0	0.0	2.106E+01	3.894E-01	FEED STREAM		
28	1.128E-02	4.245E+00	8.855E-02	0.0	0.0	0.0	1.303E+01	7.994E-01	3.021E+01	0.8301	1.83E-02
28	0.0	0.0	0.0	0.0	0.0	0.0	1.000E+01	8.000E-01	FEED STREAM		
31	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	1.009E-01	ORGANIC PRODUCT		
31	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	1.009E-01	6.744E+00	0.8129	8.50E-02
32	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	1.065E-01	5.565E+00	0.8129	1.28E-01
32	0.0	0.0	0.0	1.000E+00	0.0	0.0	3.000E+01	1.122E-01	FEED STREAM		
34	3.606E-03	1.327E+01	9.794E-03	0.0	0.0	0.0	3.000E+01	0.0	2.944E+03	0.8313	4.01E-02
34	3.538E-03	1.180E+01	7.877E-03	0.0	0.0	0.0	3.000E+01	1.180E+00	FEED STREAM		

ELAPSED TIME = 5000.0 S

SECTION 8.3 TESTING AN EXAMPLE OF PLANT OPERATION

AQUEOUS PHASE

STAGE NO.	NITRIC ACID (MOL/L)	URANIUM (G/L)	PH (IV) (G/L)	PH (III) (G/L)	REDUCTANI (MOL/L)	NITRATE ION (MOL/L)	TEMPERATURE (DEGREES C)	FLOW RATE (L/S)	VOLUME (LITERS)	DENSITY (KG/L)	MAX CHNGE (% / S)
1	3.000E+00	0.0	0.0	0.0	0.0	0.0	3.500E+01	3.343E-02	FEED STREAM		
1	3.385E+00	5.491E+00	1.458E-01	0.0	0.0	0.0	3.505E+01	3.523E-02	1.761E+00	1.1110	1.04E+00
2	3.902E+00	5.997E+00	1.985E-01	0.0	0.0	0.0	3.509E+01	3.526E-02	1.763E+00	1.1285	1.24E+00
3	3.405E+00	3.171E+02	2.971E+00	0.0	0.0	0.0	3.500E+01	5.348E-02	FEED STREAM		
3	4.995E+00	7.570E+00	2.564E-01	0.0	0.0	0.0	3.515E+01	8.783E-02	4.391E+00	1.1659	1.24E+00
4	5.051E+00	1.028E+00	1.037E-01	0.0	0.0	0.0	3.528E+01	8.764E-02	4.382E+00	1.1586	8.94E-01
5	5.107E+00	1.266E+00	1.324E-01	0.0	0.0	0.0	3.542E+01	8.735E-02	4.368E+00	1.1608	4.16E-01
6	5.290E+00	1.014E+02	8.330E+00	0.0	0.0	0.0	3.547E+01	1.000E-01	FEED STREAM		
6	5.567E+00	1.594E+00	1.503E-01	0.0	0.0	0.0	3.551E+01	1.639E-01	7.600E+00	1.1761	2.86E+00
7	5.488E+00	2.546E-02	2.821E-03	0.0	0.0	0.0	3.543E+01	1.922E-01	7.600E+00	1.1712	5.03E-01
8	5.344E+00	3.584E-04	4.828E-05	0.0	0.0	0.0	3.521E+01	2.157E-01	7.600E+00	1.1665	2.62E+00
9	5.116E+00	3.649E-06	6.268E-07	0.0	0.0	0.0	3.519E+01	1.316E-01	6.581E+00	1.1592	2.62E+00
10	4.617E+00	1.809E-08	4.424E-09	0.0	0.0	0.0	3.508E+01	1.039E-01	5.193E+00	1.1421	4.63E-01
11	3.680E+00	0.0	0.0	0.0	0.0	0.0	3.503E+01	9.226E-02	4.613E+00	1.1129	2.23E-01
12	2.388E+00	0.0	0.0	0.0	0.0	0.0	3.501E+01	8.754E-02	4.377E+00	1.0712	9.41E-02
12	2.388E+00	0.0	0.0	0.0	0.0	0.0	2.501E+01	8.754E-02	AQUEOUS PRODUCT		

Table 11 (continued)

13	0.000E-01	0.0	0.0	0.0	0.0	0.0	2.000E+01	2.556E-01	FEED STREAM
13	8.037E-01	1.156E+01	2.631E-01	0.0	0.0	0.0	2.097E+01	2.550E-01	1.275E+01 1.0400 1.23E-01
14	8.800E-01	1.491E+01	4.379E-01	0.0	0.0	0.0	2.286E+01	2.550E-01	1.275E+01 1.0468 1.14E-01
15	1.277E+00	1.227E+01	4.106E-01	0.0	0.0	0.0	2.651E+01	2.549E-01	1.275E+01 1.0558 2.18E-01
16	1.245E+00	5.847E+00	3.465E-01	0.0	0.0	0.0	2.642E+01	2.550E-01	1.275E+01 1.0454 1.12E-01
17	1.254E+00	2.058E+00	2.332E-01	0.0	0.0	0.0	2.630E+01	2.550E-01	1.275E+01 1.0407 9.23E-02
18	1.182E+00	5.538E-01	1.162E-01	0.0	0.0	0.0	2.564E+01	2.551E-01	1.275E+01 1.0359 1.01E-01
18	1.182E+00	5.538E-01	1.162E-01	0.0	0.0	0.0	2.564E+01	2.551E-01	AQUEOUS PRODUCT
19	5.000E-02	0.0	0.0	0.0	0.0	0.0	1.000E+01	4.113E-01	FEED STREAM
19	5.080E-02	1.447E+01	1.971E-02	0.0	0.0	0.0	1.057E+01	4.127E-01	8.254E+00 1.0214 8.10E-02
20	5.099E-02	1.828E+01	4.622E-02	0.0	0.0	0.0	1.114E+01	4.126E-01	8.252E+00 1.0265 7.70E-02
21	5.109E-02	1.931E+01	8.206E-02	0.0	0.0	0.0	1.171E+01	4.123E-01	8.246E+00 1.0279 7.17E-02
22	5.123E-02	1.969E+01	1.305E-01	0.0	0.0	0.0	1.228E+01	4.119E-01	8.236E+00 1.0294 6.60E-02
23	5.163E-02	1.990E+01	1.951E-01	0.0	0.0	0.0	1.284E+01	4.111E-01	8.222E+00 1.0297 6.03E-02
24	5.312E-02	2.002E+01	2.798E-01	0.0	0.0	0.0	1.340E+01	4.103E-01	8.206E+00 1.0289 5.33E-02
25	5.901E-02	1.987E+01	3.831E-01	0.0	0.0	0.0	1.395E+01	4.096E-01	8.191E+00 1.0289 4.73E-02
26	8.194E-02	1.866E+01	4.775E-01	0.0	0.0	0.0	1.450E+01	4.089E-01	8.178E+00 1.0281 3.87E-02
27	1.598E-01	1.461E+01	4.563E-01	0.0	0.0	0.0	1.505E+01	4.084E-01	8.168E+00 1.0250 2.85E-02
28	1.393E-01	5.631E+00	3.138E-01	0.0	0.0	0.0	1.301E+01	4.079E-01	8.158E+00 1.0123 3.32E-02
29	4.573E+00	2.045E+02	1.686E+01	0.0	0.0	0.0	6.000E+01	3.589E-01	FEED STREAM
29	2.272E+00	1.014E+02	8.330E+00	0.0	0.0	0.0	3.547E+01	7.838E-01	7.838E+01 1.2172 4.87E-02
29	2.272E+00	1.014E+02	8.330E+00	0.0	0.0	0.0	3.547E+01	1.000E-01	AQUEOUS PRODUCT
30	2.272E+00	1.014E+02	8.330E+00	0.0	0.0	0.0	3.547E+01	0.0	FEED STREAM
30	2.286E+00	1.022E+02	8.432E+00	0.0	0.0	0.0	3.586E+01	7.178E-01	7.178E+01 1.2188 4.87E-02
30	2.286E+00	1.022E+02	8.432E+00	0.0	0.0	0.0	3.586E+01	7.178E-01	AQUEOUS PRODUCT
31	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	5.539E-01	FEED STREAM
31	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	5.427E-01	5.427E+00 0.9957 1.01E-01
32	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	1.162E-01	FEED STREAM
32	0.0	0.0	0.0	1.763E-01	0.0	0.0	3.000E+01	6.522E-01	6.522E+00 0.9959 9.17E-02
32	0.0	0.0	0.0	1.763E-01	0.0	0.0	3.000E+01	6.522E-01	AQUEOUS PRODUCT
33	1.182E+00	5.538E-01	1.162E-01	0.0	0.0	0.0	3.000E+01	2.551E-01	FEED STREAM
33	1.132E+00	1.796E+00	4.620E-01	0.0	0.0	0.0	3.000E+01	0.0	1.255E+03 1.0353 1.01E-01

Table 11 (continued)

ORGANIC PHASE											
STAGE	NITRIC ACID	URANIUM	PU (IV)	PU (III)	REDUCTANT	NITRATE ION	TEMPERATURE	FLOW RATE	VOLUME	DENSITY	MAX CHNGR
NO.	(MOL/L)	(G/L)	(G/L)	(G/L)	(MOL/L)	(MOL/L)	(DEGREES C)	(L/S)	(LITERS)	(KG/L)	(% / S)
1	4.157E-01	5.625E+01	8.592E-01	0.0	0.0	0.0	3.505E+01	3.358E-01	ORGANIC PRODUCT		
1	4.157E-01	5.625E+01	8.592E-01	0.0	0.0	0.0	3.505E+01	3.358E-01	1.463E+01	0.9019	9.17E-C1
2	4.373E-01	5.941E+01	1.236E+00	0.0	0.0	0.0	3.509E+01	3.457E-01	1.486E+01	0.9075	9.56E-C1
3	4.546E-01	6.380E+01	1.760E+00	0.0	0.0	0.0	3.515E+01	3.537E-01	1.245E+01	0.9149	7.55E-C1
4	7.571E-01	2.370E+01	1.855E+00	0.0	0.0	0.0	3.528E+01	3.580E-01	1.257E+01	0.8695	5.87E-C1
5	7.360E-01	2.659E+01	2.186E+00	0.0	0.0	0.0	3.542E+01	3.589E-01	1.261E+01	0.8733	2.27E-01
6	7.387E-01	2.856E+01	2.354E+00	0.0	0.0	0.0	3.551E+01	3.581E-01	9.353E+00	0.8763	2.23E-02
7	9.682E-01	8.058E-01	7.610E-02	0.0	0.0	0.0	3.543E+01	3.579E-01	9.347E+00	0.8417	1.36E-C1
8	9.668E-01	1.197E-02	1.334E-03	0.0	0.0	0.0	3.531E+01	3.549E-01	9.273E+00	0.8406	6.41E-01
9	9.518E-01	1.218E-04	1.658E-05	0.0	0.0	0.0	3.519E+01	3.485E-01	1.013E+01	0.8401	2.43E+00
10	9.120E-01	6.483E-07	1.139E-07	0.0	0.0	0.0	3.508E+01	3.183E-01	1.076E+01	0.8389	1.72E-C1
11	7.950E-01	2.222E-09	5.070E-10	0.0	0.0	0.0	3.503E+01	3.071E-01	1.106E+01	0.8352	1.17E-C1
12	5.444E-01	0.0	0.0	0.0	0.0	0.0	3.501E+01	3.056E-01	1.126E+01	0.8272	3.09E-01
12	1.719E-01	0.0	0.0	0.0	0.0	0.0	3.500E+01	3.069E-01	FEED STREAM		
13	1.037E-01	3.953E+01	2.995E-01	0.0	0.0	0.0	2.097E+01	3.868E-01	ORGANIC PRODUCT		
13	1.037E-01	3.953E+01	2.995E-01	0.0	0.0	0.0	2.097E+01	3.868E-01	2.159E+01	0.8769	2.99E-C2
14	1.049E-01	4.791E+01	4.805E-01	0.0	0.0	0.0	2.286E+01	3.906E-01	2.178E+01	0.8875	8.29E-C2
15	1.526E-01	5.117E+01	6.363E-01	0.0	0.0	0.0	2.651E+01	3.986E-01	2.219E+01	0.8915	9.17E-C1
15	4.157E-01	5.625E+01	8.592E-01	0.0	0.0	0.0	3.505E+01	3.358E-01	FEED STREAM		
16	1.946E-01	3.275E+01	7.368E-01	0.0	0.0	0.0	2.642E+01	8.234E-02	6.369E+00	0.8677	6.53E-C2
17	2.371E-01	1.491E+01	6.490E-01	0.0	0.0	0.0	2.630E+01	8.240E-02	6.369E+00	0.8444	6.86E-C2
18	2.451E-01	4.287E+00	3.421E-01	0.0	0.0	0.0	2.564E+01	8.246E-02	6.370E+00	0.8300	8.18E-C2
18	1.000E-02	0.0	0.0	0.0	0.0	0.0	2.000E+01	8.250E-02	FEED STREAM		
19	3.438E-03	1.011E+01	3.770E-03	0.0	0.0	0.0	1.057E+01	1.188E+00	ORGANIC PRODUCT		
19	3.438E-03	1.011E+01	3.770E-03	0.0	0.0	0.0	1.057E+01	1.188E+00	4.070E+01	0.8394	8.59E-C2
20	3.714E-03	1.511E+01	1.039E-02	0.0	0.0	0.0	1.114E+01	1.188E+00	4.070E+01	0.8455	7.95E-C2
21	3.780E-03	1.642E+01	1.906E-02	0.0	0.0	0.0	1.171E+01	1.188E+00	4.071E+01	0.8474	7.26E-C2
22	3.816E-03	1.678E+01	3.062E-02	0.0	0.0	0.0	1.228E+01	1.188E+00	4.071E+01	0.8475	6.50E-C2
23	3.867E-03	1.695E+01	4.612E-02	0.0	0.0	0.0	1.284E+01	1.188E+00	4.071E+01	0.8474	5.72E-C2
24	4.007E-03	1.709E+01	6.681E-02	0.0	0.0	0.0	1.340E+01	1.187E+00	4.072E+01	0.8473	5.06E-C2
25	4.516E-03	1.723E+01	9.389E-02	0.0	0.0	0.0	1.395E+01	1.187E+00	4.072E+01	0.8472	4.34E-C2
26	6.530E-03	1.731E+01	1.269E-01	0.0	0.0	0.0	1.450E+01	1.187E+00	4.072E+01	0.8470	3.66E-02
27	1.436E-02	1.706E+01	1.566E-01	0.0	0.0	0.0	1.505E+01	1.187E+00	4.073E+01	0.8467	2.99E-02
27	1.037E-01	3.953E+01	2.995E-01	0.0	0.0	0.0	2.097E+01	3.868E-01	FEED STREAM		
28	1.066E-02	4.513E+00	7.416E-02	0.0	0.0	0.0	1.301E+01	8.006E-01	2.972E+01	0.8304	3.12E-02
28	0.0	0.0	0.0	0.0	0.0	0.0	1.000E+01	8.000E-01	FEED STREAM		

Table 11 (continued)

31	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	1.256E-01	ORGANIC PRODUCT
31	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	1.256E-01	5.829E+00 0.8129 8.07E-02
32	0.0	0.0	0.0	0.0	0.0	0.0	3.000E+01	1.209E-01	4.687E+00 0.8129 1.13E-01
32	0.0	0.0	0.0	1.000E+00	0.0	0.0	3.000E+01	1.162E-01	FEED STREAM
34	3.571E-03	1.255E+01	8.903E-03	0.0	0.0	0.0	3.000E+01	0.0	5.912E+03 0.8303 8.59E-02
34	3.436E-03	1.011E+01	3.770E-03	0.0	0.0	0.0	3.000E+01	1.188E+00	FEED STREAM

Several controllers were used to impose errors in the feed-stream variables. Figure 17 shows the responses of four such controllers. The controller for the HAS flow rate imposed a simple random error on it,

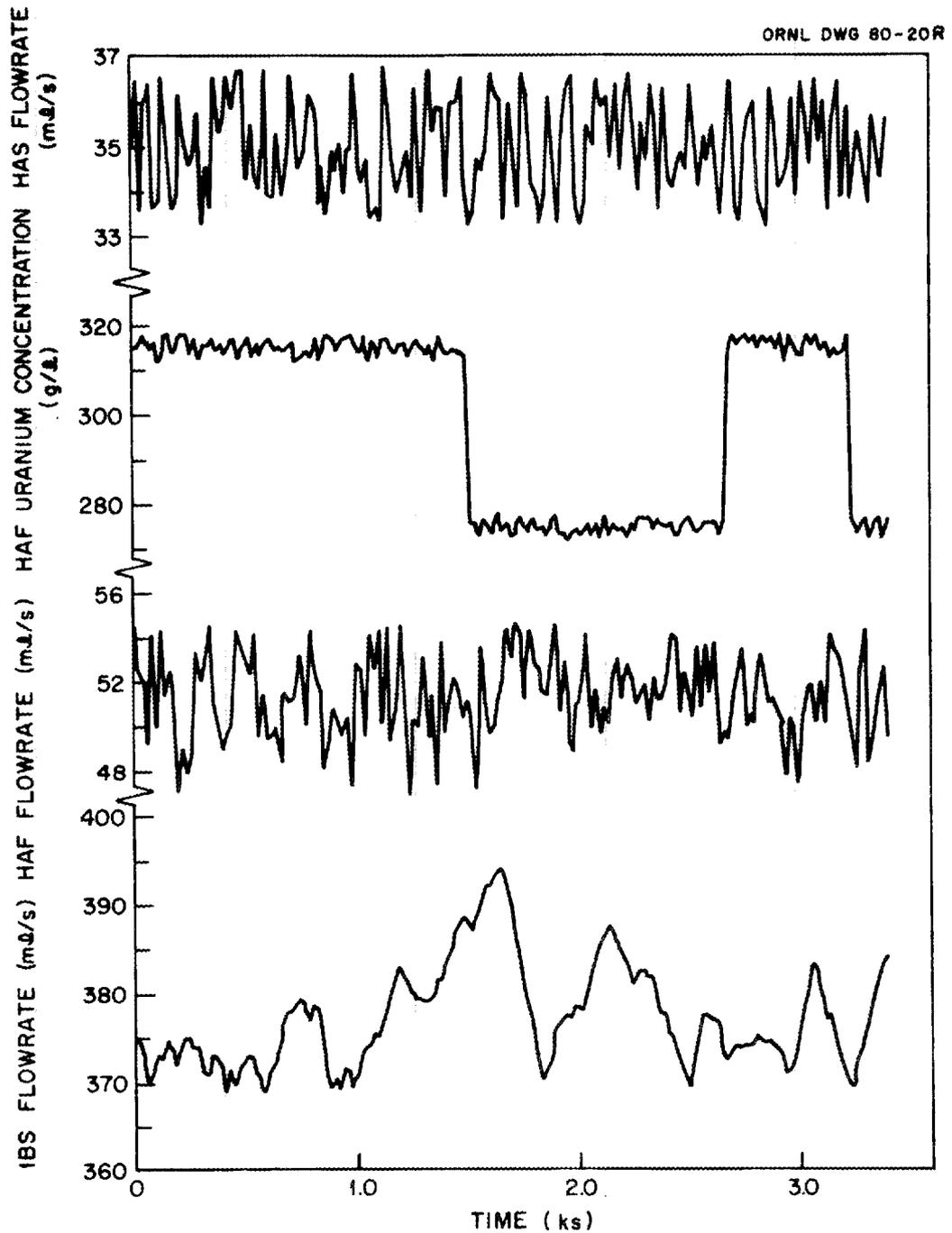


Fig. 17. Responses of various error forms in the sample calculation.

and the results show such a random variation.

The controllers on the HAF concentrations are used to illustrate the effect of having two batch-feed concentrations on the extraction system response. The major changes in the HAF concentrations are the step changes formed by the on/off controller, with more minor variations due to the setting of the error band. In contrast to the regularly spaced square waves in Sect. 7.2, these step changes occur as dictated by the probability that a random number will fall within a given interval.

The controller for the HAF flow rate was set to produce random variations with a slight positive bias. If the variations were totally random, the average would have been 50.5 mL/s. However, in this case the average was 51.4 mL/s due to the specification of the controller.

The LBS flow rate was allowed to wander randomly in the interval 370 to 430 mL/s. In this case, a positive value was given for the derivative time. Weighting the derivative with this type of error increases the chance that if the controlled variable is increasing, it will continue to increase. Its influence can be seen by comparing Fig. 17 with the random walk in Fig. 6.

The response of the semibatchwise concentrator is shown in Fig. 18. A product is withdrawn from the concentrator only after the density exceeds 1.22 kg/L. The product is taken until the density falls below 1.20 kg/L. The top curve shows the rise and fall in the density as the solutes flow into and out of the concentrator. The flow rate of the product being removed from the concentrator is shown by the middle curve. The lower curve shows the liquid volume in the concentrator. As the product is removed, the volume and density decrease as fluid flows out of the concentrator, and the remaining solution is diluted by the low-concentration, entering stream (1BR). After the density falls below 1.20 kg/L, the product is turned off and the volume and density begin to rise again.

The product streams leaving the system are the 1AP stream, which is the coprocessed product, and the 1BP stream, which is the uranium product. The goal of this flowsheet is to produce a 20% plutonium coprocessed

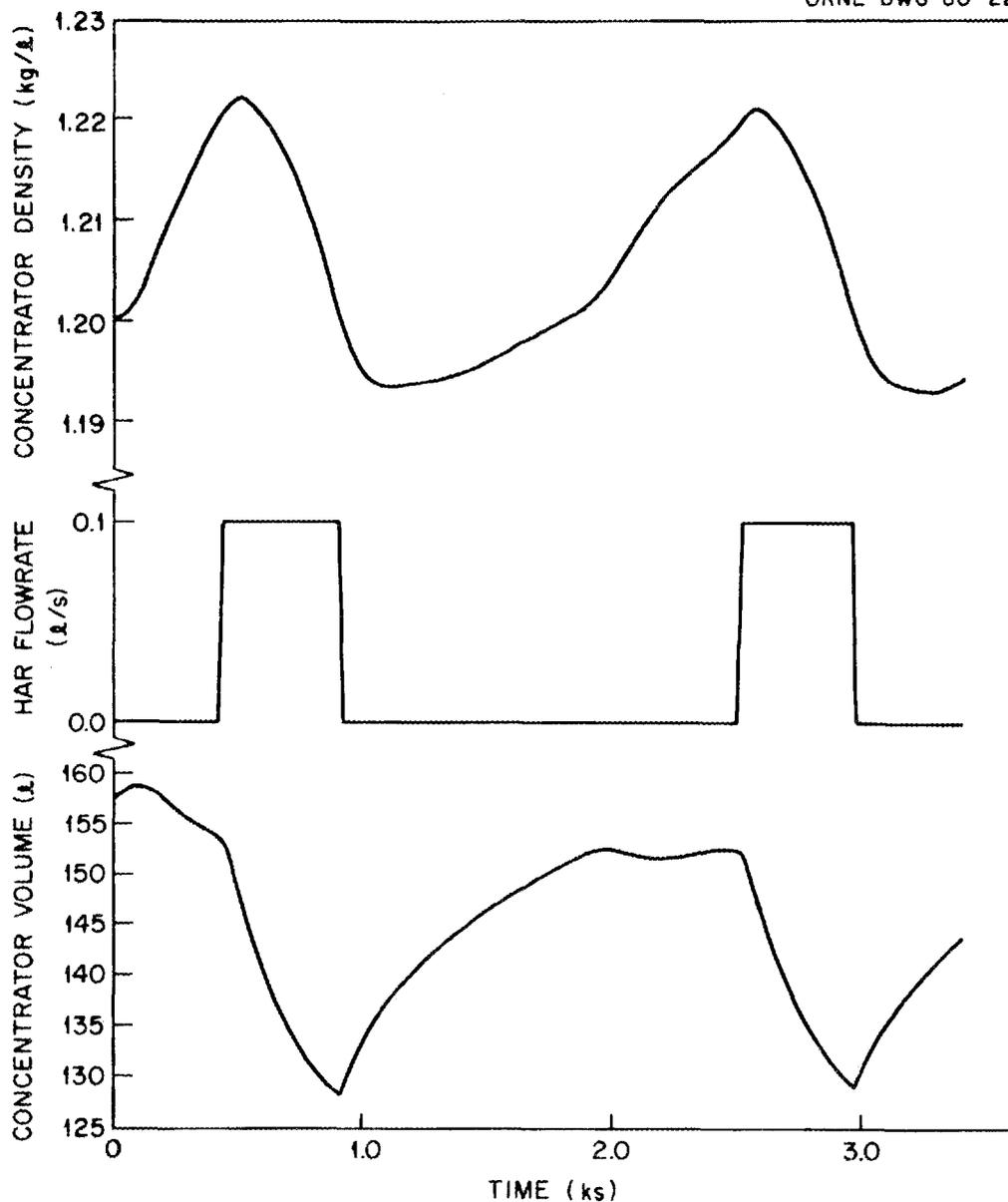


Fig. 18. Concentrator responses for the sample calculation.

product and a decontaminated uranium product. Figure 19 shows the product stream responses to the other changes in the system. The LAP uranium and plutonium concentrations begin to increase shortly after the HAR recycle stream turns on, and they subsequently decrease when the recycle is turned off. The Pu/(U + Pu) ratio varies as the controller attempts to produce the desired 20% product. The efforts of the controller are thwarted when the recycle stream is turned on, and the ratio

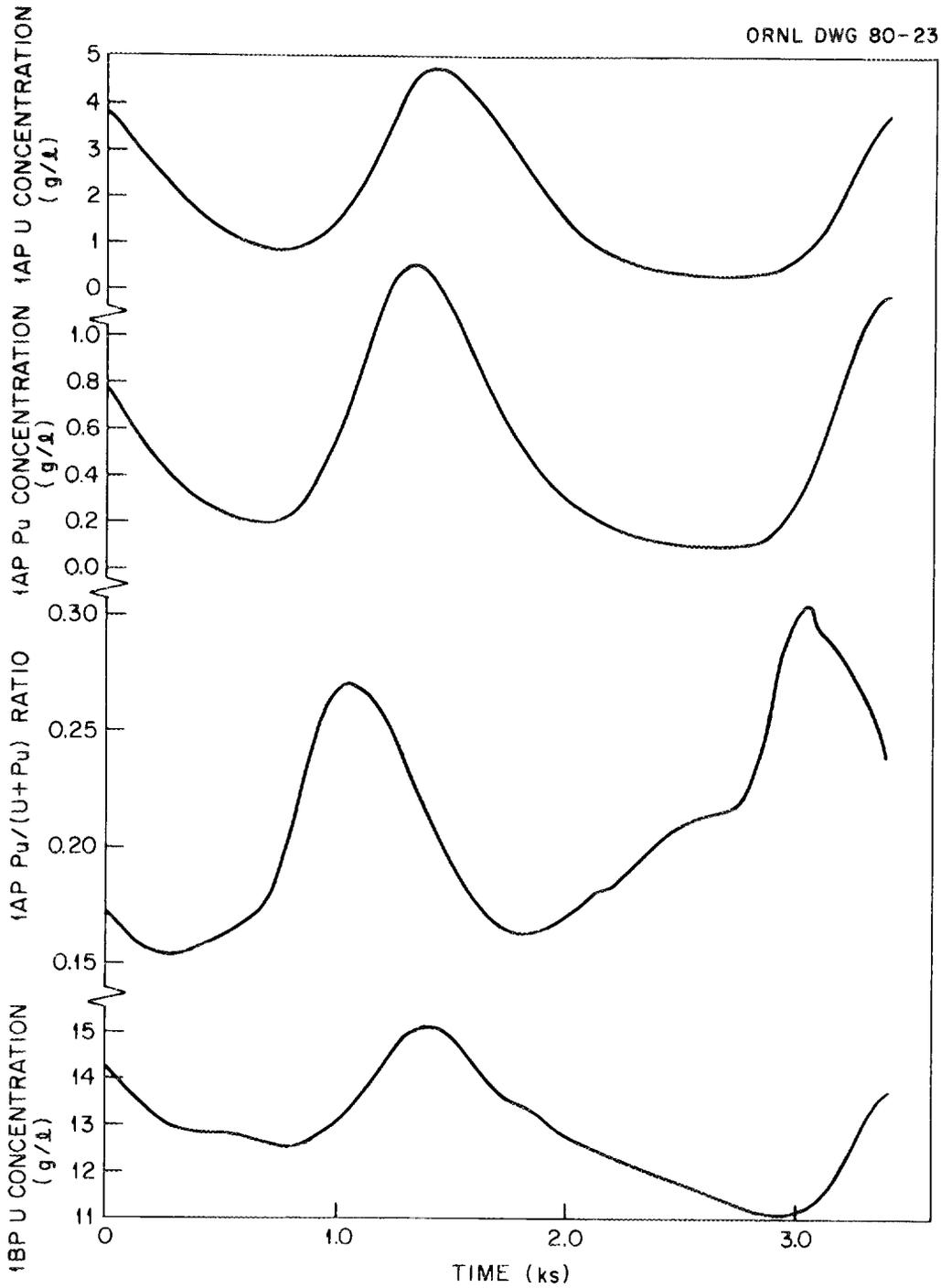


Fig. 19. Product stream responses for the sample calculation.

changes more quickly than the controller can handle. The 1BP uranium concentration also rises and falls with the recycle flow. The 1BP plutonium concentration is generally below 0.02 g/L.

The responses of the controllers that adjust the 1AP composition are shown in Fig. 20. The variable being monitored is the $\text{Pu}/(\text{U} + \text{Pu})$ ratio, which is calculated by the program in stages 31 and 32 and shown in the top curve. The second curve is the ratio in the storage tank where the 1AP is held (stage 33). This ratio is low initially but gradually builds to the desired level. The third curve is the response of the controller on the 1AX flow rate. Initially, the flow rate is increasing because the ratio is below 20%. This increase gradually causes the ratio to increase (0.3-0.7 ks). The HAR recycle stream causes the ratio to increase rapidly, and the controller responds by decreasing the 1AX flow rate. Decreasing the 1AX flow rate should allow more uranium to leave in the 1AP stream, thereby decreasing the ratio. When the recycle stream turns off, the ratio declines and the controller responds by increasing the 1AX flow rate. This control is gradually effective until the recycle stream turns on again.

The 1AS flow rate, shown by the bottom curve, varies between a high and low value. When the 1AP ratio exceeds 0.23, the 1AS flow rate switches to the high value to encourage a higher uranium concentration in the product and thereby reduces the ratio. Conversely, when the 1AP ratio falls below 0.17, the flow rate switches to the low value. The small variations in the the 1AS flow rate are due to the noise band.

This example shows how information produced by the program can be instructive in flowsheet evaluation. In general, this flowsheet seems to produce the desired products despite the errors inserted by the controllers. It should be noted that although this flowsheet employs a column (1B) operating at 10 to 15°C, the calculated distribution coefficients in this region should not be trusted too implicitly due to a sparsity of data in this region.

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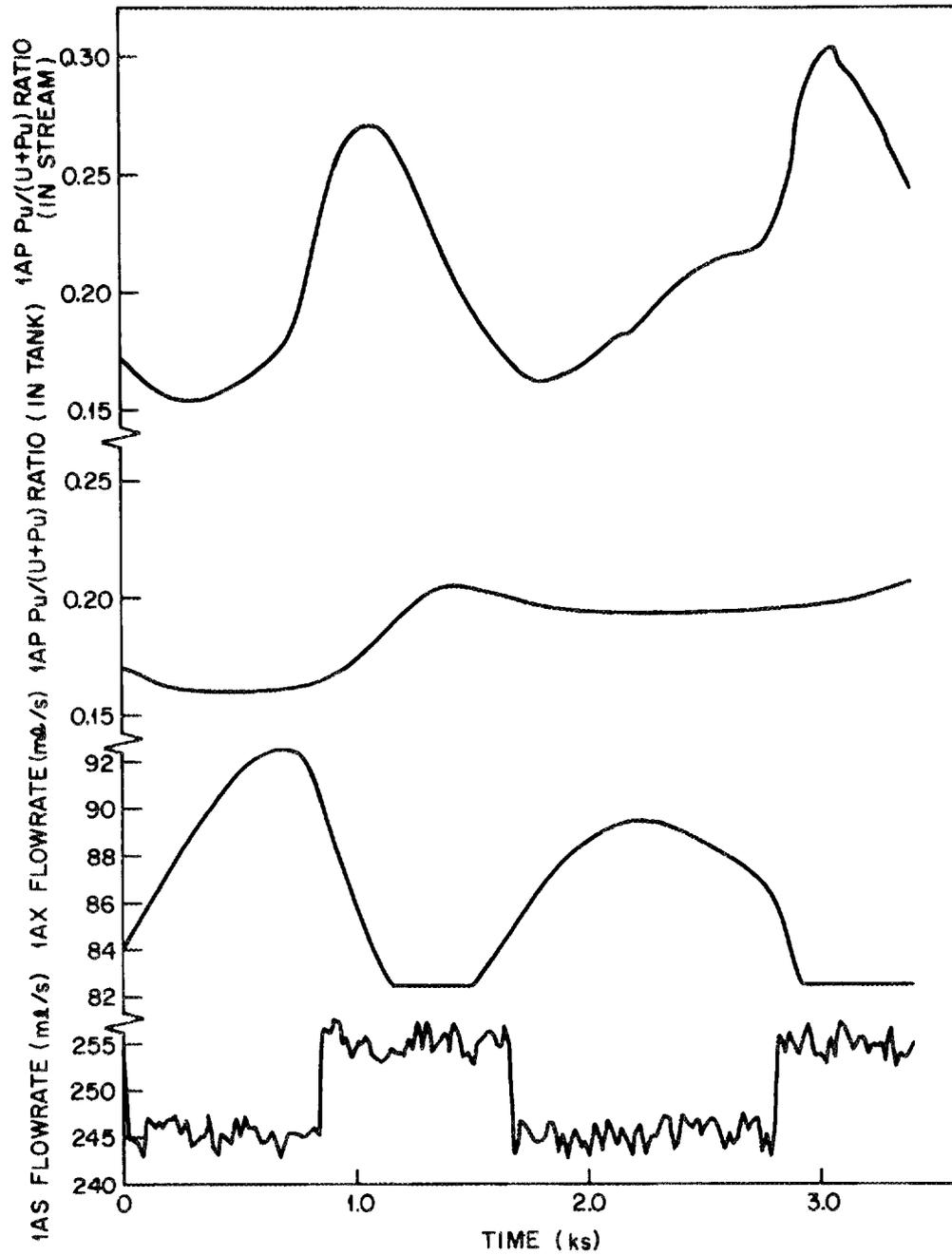


Fig. 20. The 1A column controller responses for the sample calculation.

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REFERENCES

1. A. D. Mitchell, *SEPHIS-MOD4: A User's Manual to a Revised Model of the Purex Solvent Extraction System*, ORNL-5471 (May 1979).
2. A. D. Mitchell, *A Comparison Between SEPHIS-MOD4 and Previous Models of the Purex Solvent Extraction System*, ORNL/TM-6565 (February 1979).
3. A. D. Mitchell, *Modification of the SEPHIS-MOD4 Computer Program to Simulate the Thorex Solvent Extraction Process*, ORNL/TM-6825 (December 1979).
4. R. T. Jubin, *A Modified Mathematical Model for Calculating Distribution Coefficients for U(VI), Pu(IV), and Nitric Acid in the Uranyl Nitrate-Plutonium(IV) Nitrate-Nitric Acid-Water/TBP System*, ORNL/TM-7217 (April 1980).
5. D. W. Tedder, ORNL, personal communication with A. D. Mitchell, 1978.

APPENDIXES

Appendix A. NOMENCLATURE

c,c'	Output of the controller, Fig. 3
e	Error in the monitored variable, Fig. 3
k	Volume proportionality constant, Eqs. (3)-(4)
m	Value of the variable being monitored by a controller, Fig. 3
r	Random number ($-1 \leq r \leq 1$)
t	Time
x	Aqueous concentration
y	Organic concentration
z	Variable of integration, Eq. (25)
A	Aqueous flow rate
C	Constant of integration, Eq. (24), or output of the controller, Fig. 3
D	Distribution coefficient, Eq. (15)
G	Generation term, Eq. (20)
K_d	Derivative time, Fig. 3
K_i	Integral time, Fig. 3
K_p	Proportional gain, Fig. 3
N	Noise band, Fig. 3
O	Organic flow rate
P	Function of time, Eq. (26)
Q	Function of time, Eq. (27)
S_c	Set point for the controlled variable, Fig. 3
S_m	Set point for the monitored variable, Fig. 3
S_U	Upper set point for on/off controllers, Fig. 4
S_L	Lower set point for on/off controllers, Fig. 4
T	Temperature
U	Estimate of uranium concentration, Eq. (45)
V	Volume
V_S	Aqueous volume set point, Fig. 1
V_T	Total stage volume, Fig. 1
ρ	Density

Subscripts (excluding those defined above)

a	Aqueous phase
f	Feed stream
j	Stage number
m	Pertaining to the mixer, see Sect. 2.1
o	Organic phase
p	Product stream
t	Time

Appendix B. PROGRAM LISTING

CCCCC

```

C
C CONCEPT CONTROLLER-RUN SOLVENT EXTRACTION PROCESS TESTING PROGRAM
C THIS VARIANT OF THE SEPHIS PROGRAM ALLOWS FOR TIME DEPENDENT
C FLOWRATES, VOLUMES, AND CONCENTRATIONS. PROCESS CONTROLLERS
C CAN AUTOMATICALLY ADJUST ANY DESIRED FEED STREAM. BY PROPER
C USE OF THE VOLUMES AND CONTROLLERS, MANY MORE FUNCTIONS OF A
C REPROCESSING PLANT CAN BE SIMULATED SIMULTANEOUSLY.
C
C
C THE MAJOR VARIABLES USED BY THE PROGRAM ARE FEED(J,K,L,M) & BANK(J,K,L,M)
C FOR FEED
C J = STAGE NUMBER
C K = PHASE K = 1 AQUEOUS
C = 2 ORGANIC
C L = VARIABLE L = 1 NITRIC ACID CONCENTRATION (M)
C = 2 URANUM CONCENTRATION (G/L)
C = 3 PU (IV) CONCENTRATION (G/L)
C = 4 PU(III) CONCENTRATION (G/L)
C = 5 PU REDUCTANT CONCENTRATION (M)
C = 6 NITRATE CONCENTRATION (M)
C = 7 TEMPERATURE (C)
C = 8 FLOWRATE (L/S)
C FOR THE THOREX PROCESS, L=3 TO 5 CHANGE TO:
C = 3 THORIUM CONCENTRATION (G/L)
C = 4 NOT DEFINED
C = 5 NOT DEFINED
C M = VALUE M = 1 VALUE AT T
C = 2 VALUE AT T PLUS DELTA T
C
C THE REMAINING VALUES OF M DESCRIBE THE CONTROLLERS
C M = 3 NUMBER OF STAGE BEING MONITORED
C > 0 FOR 3-MODE CONTROL
C = 0 FOR NO CONTROL
C < 0 FOR ON/OFF CONTROL
C M = 4 NUMBER OF PHASE BEING MONITORED
C = 1 AQUEOUS BANK
C = 2 ORGANIC BANK
C = 3 AQUEOUS FEED
C = 4 ORGANIC FEED
C M = 5 NUMBER OF VARIABLE BEING MONITORED
C = 1 TO 9 SAME AS 'L' ABOVE
C = 0 VOLUME (LITERS)
C = 10 DENSITY (KG/L)
C
C FOR 3-MODE CONTROL
C M = 6 SET POINT FOR MONITORED VARIABLE
C = 7 PROPORTIONAL GAIN
C = 9 INTEGRAL TIME
C = 9 DERIVATIVE TIME
C =10 SET POINT FOR CONTROLLED VARIABLE
C =11 % ERROR BAND ON OUTGOING VALUE
C =12 MAXIMUM VALUE ALLOWED
C =13 MINIMUM VALUE ALLOWED
C =14 INTEGRATED ERROR
C
C FOR ON/OFF CONTROL
C M = 6 UPPER SET POINT FOR MONITORED VARIABLE
C = 7 LOWER SET POINT FOR MONITORED VARIABLE
C = 8 NOT DEFINED
C = 9 NOT DEFINED
C =10 NOT DEFINED
C =11 % ERROR BAND ON OUTGOING VALUE
C =12 OUTGOING VALUE AFTER #6 VALUE EXCEEDED
C =13 OUTGOING VALUE AFTER #7 VALUE PASSED
C =14 NOT DEFINED
C
C FOR BANK
C J = STAGE NUMBER
C K = PHASE K = 1 AQUEOUS
C = 2 ORGANIC
C L = VARIABLE L = 1 TO 8 SAME AS 'L' ABOVE
C = 9 VOLUME (LITERS)
C =10 DENSITY (KG/L)
C M = VALUE M = 1 VALUE AT T
C = 2 VALUE AT T PLUS DELTA T

```

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C     FIVE ARRAYS DESCRIBE 'THE EQUIPMENT'
C     VT(J)          TOTAL VOLUME OF THE STAGE (LITERS)
C     VS(J)          AQUEOUS VOLUME SET POINT (LITERS)
C     VKA(J)         AQUEOUS PROPORTIONALITY CONSTANT (1.0/S)
C     VKO(J)         ORGANIC PROPORTIONALITY CONSTANT (1.0/S)
C     THE AQUEOUS FLOWRATE OUT OF STAGE J IS GIVEN BY
C     VKA(J)*(AQ VOLUME-VS(J))
C     SIMILARLY, THE ORGANIC FLOWRATE IS
C     VKO(J)*(AQ VOL+OR VOL-VT(J))
C     PROD(J,K)     PRODUCT STREAMS
C                   J = STAGE NUMBER
C                   K = PHASE      K = 1 AQUEOUS
C                                     = 2 ORGANIC
C     THE VALUE OF PROD IS THE MAXIMUM FLOWRATE OF THE
C     PRODUCT STREAM REMOVED FROM THE STAGE. IF
C     NO PRODUCT STREAM IS REMOVED, THE VALUE IS 0.0.
C
C     OTHER MISCELLANEOUS VARIABLES.
C     NSOLU          HIGHEST NUMBERED SOLUTE FOUND IN THE SYSTEM.
C                   NSOLU IS USED TO AVOID UNNECESSARY CALCULATIONS
C                   BY BYPASSING CALCULATIONS WHEN THERE IS NONE OF
C                   A PARTICULAR SOLUTE IN A SYSTEM.
C     SPH           SPECIFIC HEAT OF THE ORGANIC (APPROX)
C     ISOL          INDICATION OF THE PRESENCE OF NON-ZERO VALUES IN FEED
C     ICNTRL        INDICATION OF THE PRESENCE OF CONTROLLERS IN THE STAGE
C     CONVRG        MEASURE OF THE RATE OF CHANGE BY STAGE BY PHASE
C     TITLE         DESCRIPTIVE TITLE FOR THE CASE (UP TO 10 CARDS)
C
CCCCC
COMMON/VAPS/ BANK(100,2,10,2), FEED(100,2,8,14)
COMMON/SWITCH/ NTOST,NSOLU,CTBP,SPH,NEWIN,NEWOUT,IVOL,IPOO,TEMPI,
.   DTHETA,ISOL(10),CONVRG(100,2),IPXN,IPROCE,ICNTRL(100)
COMMON/SYSTEM/ VT(100),VS(100),VKA(100),VKO(100),PROD(100,2)
FEAL*8 TITLE(10,10)
NDIPEC=1
10 CONTINUE
C
C     READING THE CONTROL CARD FOR THE NEXT CASE
C     NTTL = NUMBER OF TITLE CARDS (UP TO 10)
C     NTOST = NUMBER OF STAGES (UP TO 100)
C     CTBP = VOLUME FRACTION OF TBP IN THE ORGANIC PHASE
C     TEMPI = INITIAL AND DEFAULT TEMPERATURE
C     IPXN = NUMBER OF THE REDUCTION REACTION BEING USED (PUPEX ONLY)
C           IPXN = 0 FOR NO REDUCTION
C                 = 1 FOR INSTANTANEOUS REDUCTION
C                 = 2 FOR REDUCTION BY U (IV)
C                 = 3 FOR REDUCTION BY HYDROXYLAMINE
C     IPROCE= PROCESS NUMBER (0=PUPEX, 1=THOPEX)
C
READ 999,NTTL,NTOST,CTBP,TEMPI,IPXN,IPROCE
DO 11 I=1,NTTL
READ 1000,(TITLE(I,N),N=1,10)
11 CONTINUE
IF(NTOST.LE.0) NTOST=100
NSOLU=6
SPH=0.321+0.078*CTBP
C
C     INITIALIZING VARIABLES
C
DO 14 I=1,10
ISOL(I)=0
14 CONTINUE
DO 20 J=1,NTOST
ICNTRL(J)=0
VT(J)=-1.0
VS(J)=-1.0
VKA(J)=0.0
VKO(J)=0.0
DO 20 K=1,2
CONVRG(J,K)=200.0
DO 16 L=1,8
DO 16 M=1,14
FEED(J,K,L,M)=0.0
16 CONTINUE
PROD(J,K)=0.0
DO 18 L=1,10
DO 19 M=1,2
BANK(J,K,L,M)=0.0
19 CONTINUE

```

```

BANK (J,K,7,1)=TEMPI
BANK (J,K,7,2)=TEMPI
BANK (J,1,10,1)=0.992247-0.0002806*(TEMPI-40.)-0.00000375*(TEMPI
-40.)**2
  BANK (J,1,10,2)=BANK (J,1,10,1)
  BANK (J,2,10,1)=(0.762*(1.-CTBP)*((386.-TEMPI)/366.))**0.29
  +0.9949*(1.-9.6E-4*TEMPI+2.9E-6*TEMPI**2)*CTBP)*(1.
  -0.0174*(3.95-0.0144*TEMPI)*CTBP**1.65)
  BANK (J,2,10,2)=BANK (J,2,10,1)
20 CONTINUE
40 CONTINUE
C
C
C
C READING THE CONTROL CARD FOR THE NEXT TIME PERIOD
C DTHETA = TIME INCREMENT (S)
C DPRINT = TIME BETWEEN SUCCESSIVE PROFILE PRINTINGS (S)
C TSTOP = TIME WHEN THE CALCULATIONS WILL STOP IF THE TOLERANCE IS NOT MET
C TOL = TOLERANCE FOR THE STEADY STATE DETERMINATION (CHANGE IN % / S)
C NEWIN = SWITCH FOR READING NEW FEED STREAMS (0=NO, 1=YES, 2=ONLY REVISED)
C NEWOUT = SWITCH FOR READING NEW PRODUCT STREAMS (VALUE SAME AS FOR NEWIN)
C IVOL = SWITCH FOR READING NEW VOLUME CONSTANTS (VALUE SAME AS FOR NEWIN)
C IPRO = SWITCH FOR READING AN INITIAL PROFILE (1=YES, 0=NO)
C IPNCH = SWITCH FOR PUNCHING THE FINAL PROFILE ONTO CARDS (1=YES, 0=NO)
C
  READ 1001,DTHETA,DPRINT,TSTOP,TOL,NEWIN,NEWOUT,IVOL,IPRO,IPNCH
  IF(DTHETA.EQ.0.0) GO TO 400
  IF(NEWIN+NEWOUT+IVOL+IPRO.NE.0) GO TO 50
  PRTIME=PRTIME+DPRINT
  PRINT 1002,DTHETA,DPRINT,TSTOP,TOL
  GO TO 140
50 CONTINUE
  IF(IPRO.NE.0) IPRO=1
  IF(NEWIN.NE.0.AND.NEWIN.NE.1) NEWIN=2
  IF(NEWOUT.NE.0.AND.NEWOUT.NE.1) NEWOUT=2
  IF(IVOL.NE.0.AND.IVOL.NE.1) IVOL=2
  IF(IPRO.NE.0) IPRO=1
  IF(IPNCH.NE.0) IPNCH=1
  PRINT 1003
  IF(IPRO.EQ.0) PRINT 1021,CTBP
  IF(IPRO.EQ.1) PRINT 1022,CTBP
  DO 60 V=1,NTTL
  PRINT 1020,(TITLE(I,N),V=1,10)
60 CONTINUE
  PRINT 1002,DTHETA,DPRINT,TSTOP,TOL
  IF(NEWIN.EQ.0) PRINT 1004
  IF(NEWIN.EQ.1) PRINT 1005
  IF(NEWIN.EQ.2) PRINT 1105
  IF(NEWOUT.EQ.0) PRINT 1006
  IF(NEWOUT.EQ.1) PRINT 1007
  IF(NEWOUT.EQ.2) PRINT 1107
  IF(IVOL.EQ.0) PRINT 1008
  IF(IVOL.EQ.1) PRINT 1009
  IF(IVOL.EQ.2) PRINT 1109
  IF(IPRO.EQ.0) PRINT 1010
  IF(IPRO.EQ.1) PRINT 1011
  IF(IPNCH.EQ.0) PRINT 1112
  IF(IPNCH.EQ.1) PRINT 1113
  IF(IRXN.EQ.0) PRINT 1115
  IF(IRXN.EQ.1) PRINT 1116
  IF(IRXN.EQ.2) PRINT 1117
  IF(IPKN.EQ.3) PRINT 1119
C
C
C SURROUTINE STARTS DOES ALL THE REMAINING INPTE FUNCTIONS FOR THE PROGRAM.
C IT IS CALLED ONLY IF THE USER HAS INDICATED (WITH THE SWITCHES) THAT
C NEW FEED STREAMS, ETC. ARE TO BE READ OFF CARDS.
C
  CALL STARTS
C
  TOTIME=0.0
  PRTIME=0.0
  GO TO 200
140 CONTINUE
  TOTIME=TOTIME+DTHETA
C
C
C SUBROUTINE STAGES PERFORMS THE STAGE-WISE CALCULATIONS OF FLOWRATES,
C VOLUMES, CONCENTRATIONS, AND TEMPERATURES. STAGES ALSO CHECKS THE
C FEED STREAM CONTROLLERS. NDIRC JUST SWITCHES THE ORDER OF CALCULATION.
C
  CALL STAGES (NDIPEC)
  NDIPEC=-NDIPEC

```

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C
C
C CHECKING CONVERGENCE TO STEADY STATE. CONVRG IS THE MAXIMUM CHANGE
C FOUND IN THE BANK CONCENTRATIONS, TEMPERATURES, OR FLOWRATES, OR
C THE FEED STREAM CONCENTRATIONS, TEMPERATURES, OR FLOWRATES. THE
C CHECK IS MADE BY STAGE, BY PHASE.
C
  DO 150 J=1,NTOST
  DO 150 K=1,2
  IF (CONVRG(J,K).GT.TOL) GO TO 200
150 CONTINUE
  TSTOP=TOTIME
200 CONTINUE
C
C
C THIS 'IF' DETERMINES WHETHER A PROFILE WILL BE PRINTED. THE PROFILE
C IS PRINTED EVERY DPRINT SECONDS, OR IF THE CONVERGENCE TOLERANCE
C HAS BEEN MET, OR IF TSTOP HAS BEEN REACHED.
C
  IF (TOTIME.LT.PRTIME.AND.TOTIME.LT.TSTOP) GO TO 140
  PRTIME=PRTIME+DPRINT
C
C
C PRINTING THE AQUEOUS PROFILE. THE PROGRAM TRIES TO PRINT THE PROFILE
C BY COLUMN, SO A BLANK LINE IS LEFT WHERE A PRODUCT STREAM IS REMOVED,
C AND THE FEED STREAMS ARE PRINTED WHERE THEY ENTER THE BANK.
C A STAGE WILL NOT BE PRINTED IF IT HAS NO VOLUME.
C
  IF (IPROCE.EQ.0) PRINT 1012,TOTIME, (TITLE(1,I),I=1,10)
  IF (IPROCE.EQ.1) PRINT 1023,TOTIME, (TITLE(1,I),I=1,10)
  DO 210 J=1,NTOST
  IF (PROD(J,2).NE.0.0) PRINT 1013
  IF (FEED(J,1,8,2).GT.0.0) ICNTRL(J).EQ.1.OR.ICNTRL(J).EQ.3)
    PRINT 1014,J, (FEED(J,1,I,2),I=1,8)
  IF (BANK(J,1,9,2).GE.1.E-8) PRINT 1015,J, (BANK(J,1,I,2),I=1,10),
    CONVRG(J,1)
  PPLO=AMINI(BANK(J,1,8,2),PROD(J,1))
  IF (PPLO.GE.1.0E-8) PRINT 1016,J, (BANK(J,1,I,2),I=1,7), PPLO
210 CONTINUE
C
C
C PRINTING THE ORGANIC PROFILE.
C
  IF (IPROCE.EQ.0) PRINT 1017
  IF (IPROCE.EQ.1) PRINT 1024
  DO 220 J=1,NTOST
  PPLO=AMINI(BANK(J,2,8,2),PROD(J,2))
  IF (PPLO.GE.1.0E-8) PRINT 1019,J, (BANK(J,2,I,2),I=1,7), PPLO
  IF (IPROCE.EQ.1.AND.BANK(J,2,3,2).GE.232.*(0.0913+6.47E-3)
    *BANK(J,2,7,2)-5.46E-5*BANK(J,2,7,2)**2-0.306*BANK(J,2,1,2))
    .AND.PROD(J,2).NE.0.0) PRINT 1114
  IF (BANK(J,2,9,2).GE.1.E-9) PRINT 1015,J, (BANK(J,2,I,2),I=1,10),
    CONVRG(J,2)
  IF (IPROCE.EQ.1.AND.BANK(J,2,3,2).GE.232.*(0.0913+6.47E-3)
    *BANK(J,2,7,2)-5.46E-5*BANK(J,2,7,2)**2-0.306*BANK(J,2,1,2))
    .AND.BANK(J,2,9,2).GE.1.0E-9) PRINT 1114
  IF (FEED(J,2,8,2).GT.0.0) ICNTRL(J).GE.2) PRINT 1014,
    J, (FEED(J,2,I,2),I=1,8)
  IF (PROD(J,1).NE.0.0) PRINT 1013
220 CONTINUE
  IF (TOTIME.LT.TSTOP) GO TO 140
  IF (IPNCH.EQ.0) GO TO 240
C
C
C PUNCHING THE FINAL PROFILE.
C
  DO 230 J=1,NTOST
  DO 230 K=1,2
  PUNCH 1010, (BANK(J,K,L,2),L=1,9)
230 CONTINUE
240 CONTINUE
  PRTIME=TOTIME
  GO TO 40
400 CONTINUE
  IF (DPRINT.EQ.1.0) GO TO 10
  STOP

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990 FORMAT(12,I4,2F8.0,2I2)
1000 FORMAT(10A8)
1001 FORMAT(4F8.0,5I2)
1002 FORMAT('DTHETA =',1PE10.3,' S, DPRINT =',1PE9.2,' S, TSTOP =',
. 1PE9.2,' S, CONVERGENCE TOLERANCE =',1PE9.2,' % / S')
1003 FORMAT('CONCEPT CONTROLLER-RUN SOLVENT EXTRACTION PROCESS TESTI
NG PROGRAM DECEMBER 1979 VERSION')
1004 FORMAT(' NEWIN = 0 THE PRESENT FEED STREAMS WILL BE CONTINUED')
1005 FORMAT(' NEWIN = 1 NEW FEED STREAMS WILL BE SPECIFIED')
1006 FORMAT(' NEWOUT = 0 THE PRESENT PRODUCT STREAMS WILL BE USED')
1007 FORMAT(' NEWOUT = 1 NEW PRODUCT STREAMS WILL BE SPECIFIED')
1008 FORMAT(' IVOL = 0 THE PRESENT VOLUME CONSTANTS WILL BE CONTINUED')
1009 FORMAT(' IVOL = 1 NEW VOLUME CONSTANTS WILL BE SPECIFIED')
1010 FORMAT(' IPRD = 0 THE PRESENT BANK PROFILE WILL BE CONTINUED')
1011 FORMAT(' IPRD = 1 A NEW BANK PROFILE WILL BE SPECIFIED')
1012 FORMAT('ELAPSED TIME =',F9.1,' S',10X,10A8,/,
. ' AQUEOUS PHASE',/, ' STAGE |NITRIC ACID| URANIUM | PU (I
.V) | PU (III) | REDUCTANT |NITRATE ION|TEMPERATURE| FLOW RATE |
. VOLUME |DENSITY|MAX CHNGE',/, ' NO. | (MOL/L) | (G/L) |
. (G/L) | (G/L) | (MOL/L) | (MOL/L) | (DEGREES C) | (L/S
.) | (LITERS) | (KG/L) | (% / S) ',/,7X,9(' ',11X),',',7X,' ')
1013 FORMAT(' ')
1014 FORMAT(2X,I3,2X,8(' ',1PE10.3,1X),',',1FEED STREAM')
1015 FORMAT(2X,I3,2X,9(' ',1PE10.3,1X),',',1OPF7.4,',',1PE9.2)
1016 FORMAT(2X,I3,2X,8(' ',1PE10.3,1X),',',1AQUEOUS PRODUCT',/, ' ')
1017 FORMAT('ORGANIC PHASE',/, ' STAGE |NITRIC ACID| URANIUM | PU (I
.V) | PU (III) | REDUCTANT |NITRATE ION|TEMPERATURE| FLOW RATE |
. VOLUME |DENSITY|MAX CHNGE',/, ' NO. | (MOL/L) | (G/L) |
. (G/L) | (G/L) | (MOL/L) | (MOL/L) | (DEGREES C) | (L/S
.) | (LITERS) | (KG/L) | (% / S) ',/,7X,9(' ',11X),',',7X,' ')
1018 FORMAT('O ',I3,2X,8(' ',1PE10.3,1X),',',1ORGANIC PRODUCT')
1019 FORMAT(1PE9.2,0PE8.2,0PE8.3,1P2PE8.2)
1020 FORMAT(1X,10A8)
1021 FORMAT(' PUREX PROCESS USING ',2PE6.1,' % TBP',/, ' ')
1022 FORMAT(' THOREX PROCESS USING ',2PE6.1,' % TBP',/, ' ')
1023 FORMAT('ELAPSED TIME =',F9.1,' S',10X,10A8,/,
. ' AQUEOUS PHASE',/, ' STAGE |NITRIC ACID| URANIUM | THORI
UM | SOLUTE 4 | SOLUTE 5 |NITRATE ION|TEMPERATURE| FLOW RATE |
. VOLUME |DENSITY|MAX CHNGE',/, ' NO. | (MOL/L) | (G/L) |
. (G/L) | (MOL/L) | (MOL/L) | (MOL/L) | (DEGREES C) | (L/S
.) | (LITERS) | (KG/L) | (% / S) ',/,7X,9(' ',11X),',',7X,' ')
1024 FORMAT('ORGANIC PHASE ** SIGNALS THE PRESENCE OF THIRD PHASE (WI
THIN A 1% TOLERANCE) ',/, ' STAGE |NITRIC ACID| URANIUM | THORI
UM | SOLUTE 4 | SOLUTE 5 |NITRATE ION|TEMPERATURE| FLOW RATE |
. VOLUME |DENSITY|MAX CHNGE',/, ' NO. | (MOL/L) | (G/L) |
. (G/L) | (MOL/L) | (MOL/L) | (MOL/L) | (DEGREES C) | (L/S
.) | (LITERS) | (KG/L) | (% / S) ',/,7X,9(' ',11X),',',7X,' ')
1105 FORMAT(' NEWIN = 2 THE FEED STREAMS WILL BE REVISED')
1107 FORMAT(' NEWOUT = 2 THE PRODUCT STREAMS WILL BE REVISED')
1109 FORMAT(' IVOL = 2 THE VOLUME CONSTANTS WILL BE REVISED')
1112 FORMAT(' IPNCH = 0 THE FINAL PROFILE WILL NOT BE PUNCHED')
1112 FORMAT(' IPNCH = 1 THE FINAL PROFILE WILL BE PUNCHED ON CARDS')
1114 FORMAT('+ ***')
1115 FORMAT(' IRXN = 0 NO REDUCTION OF PLUTONIUM')
1116 FORMAT(' IRXN = 1 INSTANTANEOUS REDUCTION OF PLUTONIUM')
1117 FORMAT(' IRXN = 2 REDUCTION OF PLUTONIUM BY U(IV)')
1119 FORMAT(' IRXN = 3 REDUCTION OF PLUTONIUM BY HYDROXYLAMINE')
END

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SUBROUTINE STARTS

```

C
C
C SUBROUTINE STARTS DOES THE INPUT DUTIES FOR THE PROGRAM. NEW FEED
C STREAMS, PRODUCT STREAMS, VOLUME CONSTANTS, AND INITIAL PROFILES
C ARE READ IN AS REQUIRED BY THE USER. BEFORE NEW VALUES ARE READ,
C THE OLD VALUES ARE 'ERASED.'
C
COMMON/VARS/ BANK (100,2,10,2), FEED (100,2,8,14)
COMMON/SYSTEM/ VT (100), VS (100), VKA (100), VKO (100), PROD (100,2)
COMMON/SWITCH/ NTOST, NSOLU, CTEP, SPH, NEWIN, NEWOUT, IVOL, IPRO, TEMPI,
.   DTHETA, ISOL (10), CONVRG (100,2), IRXN, IPOCE, ICNTRL (100)
REAL*8 LABPHA (4) /' AQUEOUS', ' ORGANIC', ' AQ FEED', ' ORG FEED' /
REAL*8 LABCON (2) /' 3-MODE ', ' ON/OFF ' /
REAL*8 LABV (2,10) /' HNO3 ', ' HNO3 ',
.   ' URANIUM ', ' URANIUM ',
.   ' PU (IV) ', ' THORIUM ',
.   ' PU (III) ', ' SOLUTE 4 ',
.   ' REDUCTNT ', ' SOLUTE 5 ',
.   ' NITRATE ', ' NITRATE ',
.   ' TEMP ', ' TEMP ',
.   ' FLOWRATE ', ' FLOWRATE ',
.   ' VOLUME ', ' VOLUME ',
.   ' DENSITY ', ' DENSITY ' /
DIMENSION CON (9)
IF (NEWIN.EQ.0) GO TO 40

C
C
C READING NEW FEED STREAMS.
C IN READING NEW INPUT VALUES, THE PROGRAM ALLOWS THE USER TO EITHER
C READ NO NEW VALUES, READ ALL NEW VALUES, OR JUST READ REVISIONS TO
C THE PRESENT VALUES. IF ONLY REVISIONS ARE BEING MADE (NEWIN=2), THE FEED
C STREAM ARRAY IS NOT RE-INITIALIZED. IF ALL NEW VALUES ARE BEING READ
C (NEWIN=1) THE ARRAY IS RE-INITIALIZED BEFORE CARDS ARE READ WHICH
C WIPES OUT ANY PREVIOUS VALUES. IF NO NEW VALUES ARE BEING READ
C (NEWIN=0), THIS SECTION IS SKIPPED.
C
IF (NEWIN.EQ.2) GO TO 15
DO 10 J=1, NTOST
DO 10 K=1, 2
DO 10 L=1, 8
DO 10 M=1, 14
FEED (J, K, L, M) = 0.0
10 CONTINUE
15 CONTINUE
READ (5, 1001) J, K, (CON (I), I=1, 8), INDEX, ICONTR
IF (J.LE.0) J=100
IF (K.NE.1) K=2
IF (CON (7).EQ.0.0) CON (7) = TEMPI
FEED (J, K, 7, 1) = CON (7)
FEED (J, K, 7, 2) = CON (7)
DO 16 L=1, 8
IF (CON (L).GE.0.0) FEED (J, K, L, 1) = CON (L)
IF (CON (L).GE.0.0) FEED (J, K, L, 2) = CON (L)
IF (CON (L).NE.0.0) ISOL (L) = 1
16 CONTINUE
18 CONTINUE
IF (ICONTR.EQ.0.AND.INDEX.EQ.1) GO TO 15
IF (ICONTR.EQ.0) GO TO 20

C
C
C ICNTRL IS SET TO SIGNAL THE PRESENCE OF PROCESS CONTROLLERS FOR
C THE STAGE. ICNTRL = 0 NO CONTROLLERS
C = 1 CONTROLLERS ON THE AQUEOUS FEED
C = 2 CONTROLLERS ON THE ORGANIC FEED
C = 3 CONTROLLERS ON BOTH FEEDS
C
IF (ICNTRL (J).EQ.0) ICNTRL (J) = K
IF (ICNTRL (J).NE.K) ICNTRL (J) = 3

C
C
C THE FEED STREAM HAS ONE OR MORE CONTROLLERS ATTACHED TO IT, SO THEIR
C CONSTANTS NEED TO BE READ IN.
C
READ (5, 1002) L, JM, KM, LM, (CON (I), I=1, 8), ICONTR
ISOL (L) = 1
FEED (J, K, L, 3) = JM
FEED (J, K, L, 4) = KM
FEED (J, K, L, 5) = LM
IF (CON (3).EQ.0.0) CON (3) = 1.0E 40

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DO 19 M=6,13
FEED(J,K,L,M)=CON(M-5)
19 CONTINUE
GO TO 18
20 CONTINUE
C
C
C PRINTING THE FEED STREAM INFORMATION.
C
IF(IPROCE.EQ.0) PRINT 1011
IF(IPROCE.EQ.1) PRINT 1013
DO 25 J=1,NTOST
DO 25 K=1,2
IF(FEED(J,K,8,2).LE.0.0.AND.ICNTRL(J).NE.K.AND.ICNTRL(J).NE.3)
GO TO 25
PRINT 1012,J,(FEED(J,K,L,2),L=1,8),LABPHA(K)
25 CONTINUE
C
C
C PRINTING THE CONTROLLER SPECIFICATIONS.
C
N=IPROCE+1
PRINT 1014
DO 30 J=1,NTOST
IF(ICNTRL(J).EQ.0) GO TO 30
DO 30 K=1,2
IF(ICNTRL(J).NE.K.AND.ICNTRL(J).NE.3) GO TO 30
DO 30 L=1,8
IF(FEED(J,K,L,3).EQ.0.0) GO TO 30
LA=ABS(FEED(J,K,L,3))
LB=FEED(J,K,L,4)
LC=FEED(J,K,L,5)
LD=1
IF(FEED(J,K,L,3).LT.0.0) LD=2
PRINT 1015,J,LABPHA(K+2),LAPV(N,L),LA,LABPHA(LB),LABV(N,LC),
LABCON(LD),(FEED(J,K,L,LE),LE=6,13)
30 CONTINUE
40 CONTINUE
IF(NEWOUT.EQ.0) GO TO 50
C
C
C READING WHERE THE PRODUCT STREAMS ARE REMOVED. PROD=0.0 IF THERE IS
C NO PRODUCT STREAM REMOVED FROM THAT STAGE
C
IF(NEWOUT.EQ.2) GO TO 43
DO 42 J=1,NTOST
DO 42 K=1,2
PROD(J,K)=0.0
42 CONTINUE
43 CONTINUE
PROD(1,2)=1.0E20
PROD(NTOST,1)=1.0E20
45 CONTINUE
READ(5,1004) J,K,PFLO,INDEX
IF(K.NE.1) K=2
PROD(J,K)=AMAX1(0.0,PFLO)
IF(INDEX.EQ.1) GO TO 45
C
C
C PRINTING WHERE PRODUCT STREAMS ARE REMOVED.
C
PRINT 1005
DO 48 J=1,NTOST
DO 48 K=1,2
IF(PROD(J,K).NE.0.0) PRINT 1006,J,LABPHA(K),PROD(J,K)
48 CONTINUE
50 CONTINUE
IF(IVOL.EQ.0) GO TO 60
C
C
C READING NEW VOLUME CONSTANTS. THE CONSTANTS ARE APPLIED ONLY TO ONE
C STAGE. HOWEVER, IF NO CONSTANTS ARE SPECIFIED FOR A STAGE, THE
C CONSTANTS FROM THE PREVIOUS STAGE ARE USED. THE PROPORTIONALITY
C CONSTANTS (VKA & VKO) MUST BE GREATER THAN ZERO. THE TOTAL VOLUME
C OF THE STAGE (VT) SHOULD ALSO BE GREATER THAN ZERO, BUT IS NOT
C REQUIRED TO BE SO.
C
IF(IVOL.EQ.2) GO TO 55

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DO 52 J=1,NTOST
VT(J)=-1.0
VS(J)=-1.0
VKA(J)=0.0
VKO(J)=0.0
52 CONTINUE
55 CONTINUE
READ (5,1007) J,T,S,CA,CO,INDEX
IF(J.LP.0) J=100
VT(J)=T
VS(J)=S
IF(CA.GT.0.0) VKA(J)=CA
IF(CO.GT.0.0) VKO(J)=CO
IF(INDEX.EQ.1) GO TO 55
60 CONTINUE
IF(VKA(1).LP.0.0) VKA(1)=1.0
IF(VKO(1).LE.0.0) VKO(1)=1.0
DO 65 J=2,NTOST
IF(VT(J).LT.0.0) VT(J)=VT(J-1)
IF(VS(J).LT.0.0) VS(J)=VS(J-1)
IF(VKA(J).LE.0.0) VKA(J)=VKA(J-1)
IF(VKO(J).LE.0.0) VKO(J)=VKO(J-1)
65 CONTINUE
C
C
C PRINTING THE VOLUME CONSTANTS.
C
PRINT 1009
DO 70 J=1,NTOST
PRINT 1010,J,VT(J),VS(J),VKA(J),VKO(J)
70 CONTINUE
IF(IPRO.EQ.0) GO TO 80
C
C
C READING THE NEW INITIAL PROFILE.
C REVISIONS ARE NOT ALLOWED WHEN READING INITIAL PROFILES
C
DO 75 J=1,NTOST
DO 72 K=1,2
READ (5,1008) (CON(I),I=1,9)
IF(CON(7).EQ.0.0) CON(7)=TEMP1
DO 72 L=1,9
DO 72 M=1,2
BANK(J,K,L,M)=CON(L)
IF(CON(L).GT.0.0) ISOL(L)=1
72 CONTINUE
C
C
C CALCULATING DENSITIES FOR THE PROFILE.
C
T=BANK(J,1,7,2)
IF(IPROCE.EQ.1) GO TO 73
BANK(J,1,10,2)=(0.992247-0.0003806*(T-40.)-0.00000375*(T-40.)**2)
. * (1.0-0.0200*BANK(J,1,1,2)-0.0724*BANK(J,1,2,2)/239.-0.1?
. * (BANK(J,1,3,2)+BANK(J,1,4,2))/239.-0.021*BANK(J,1,6,2))
. +0.0630*BANK(J,1,1,2)+0.39404*BANK(J,1,2,2)/239.+0.49202
. * (BANK(J,1,3,2)+BANK(J,1,4,2))/239.+0.213*BANK(J,1,6,2)
F=3.65145*CTBP
HS=F*(1.-0.00609*(3.95-0.0144*T)*(CTBP**1.65)/(1.0+0.043*F)
US=238.*F/(2.*(1.+0.046*F))
PS=239.*F/(2.*(1.+0.00*F))
W=((3.95-0.0144*T)*CTBP**1.65)*(1.-0.65*BANK(J,2,1,2)/HS
. -BANK(J,2,2,2)/US-BANK(J,2,3,2)/PS)
BANK(J,2,10,2)=(0.762*(1.-CTBP)*((386.-T)/266.)**0.29+0.0249
. *(1.-2.65-4*T+2.*F-6*T**2)*CTBP)*(1.-0.042*BANK(J,2,1,2)
. -0.097*BANK(J,2,2,2)/239.-0.139*BANK(J,2,3,2)/239.-0.0174*W)
. +0.06301*BANK(J,2,1,2)+0.39404*BANK(J,2,2,2)/239.+0.49202
. *(BANK(J,2,3,2)+BANK(J,2,4,2))/239.
GO TO 74
73 CONTINUE
BANK(J,1,10,2)=1.0348F-0.0012196*T+6.495F-6*T*T
. +0.29291*BANK(J,1,3,2)/232.+0.029322*BANK(J,1,1,2)
. +0.319*BANK(J,1,2,2)/239.
BANK(J,2,10,2)=0.83894-0.0011247*T+3.57F-F*T*T
. +0.370796*BANK(J,2,3,2)/232.+0.028327*BANK(J,2,1,2)
. +0.319*BANK(J,2,2,2)/239.
74 CONTINUE
BANK(J,1,10,1)=BANK(J,1,10,2)
BANK(J,2,10,1)=BANK(J,2,10,2)
75 CONTINUE
80 CONTINUE

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NSOLU=1
DO 85 I=1,6
IF (ISOL(I).EQ.1) NSOLU=I
85 CONTINUE
RETURN
1001 FORMAT (I4,I2,8F8.0,2I2)
1002 FORMAT (I2,I4,2I2,8F8.0,I2)
1004 FORMAT (I4,I2,F8.0,I2)
1005 FORMAT ('-PRODUCT STREAMS ARE REMOVED AT STAGE PHASE',7X,'RATE
.
')
1006 FORMAT (35X,I3,3X,A8,3X,1PE10.3)
1007 FORMAT (I4,4F8.0,I2)
1008 FORMAT (9F8.0)
1009 FORMAT ('-VOLUME CONSTANTS STAGE TOTAL VOLUME AQ SET POINT
. AQ CONSTANT CR CONSTANT',/)
1010 FORMAT (22X,I3,4(5X,1PE10.3))
1011 FORMAT ('-FEED STREAM DATA',/, ' STAGE | NITRIC ACID | URANIUM
. | PU (IV) | PU (III) | REDUCTANT | NITRATE ION | TEMPERA
. TURE | FLOW RATE',/, ' NO. | (MOL/L) | (G/L) | (G/L
. ) | (G/L) | (MOL/L) | (MOL/L) | (DEGREES C) |
. (L/S) ',/,9X,8('|',13X))
1012 FORMAT (2X,I3,2X,8(' | ',1PE10.3),3X,A8)
1013 FORMAT ('-FEED STREAM DATA',/, ' STAGE | NITRIC ACID | URANIUM
. | THORIUM | SOLUTE 4 | SOLUTE 5 | NITRATE ION | TEMPERA
. TURE | FLOW RATE',/, ' NO. | (MOL/L) | (G/L) | (G/L
. ) | (MOL/L) | (MOL/L) | (MOL/L) | (DEGREES C) |
. (L/S) ',/,9X,8('|',13X))
1014 FORMAT ('-PROCESS CONTROLLER INFORMATION ',/, ' FEED STREAM VARIA
. BLE (VARIABLE BEING USED |CONTROL|SET POINT|PROP GAIN|INTEGRAL |D
. ERIVATIVE|SET POINT| FRPROP |MAX VALUE|MIN VALUE',/, ' BEING CONTROLLED
. AS CONTROLLER INPUT | TYPE |OF UPPER |OR LOWER | TIME
. | TIME |FOR CNTRL| BAND | OR | OR ',/, ' STG|
. VARIABLE |STG| VARIABLE | |SET POINT|SET POINT|
. | VARIABLE | |ON VALUE |OFF VALUE',/, '
. |',17X,'| |',17X,'|',7X,8('|',9X))
1015 FORMAT (1X,I3,'|',A8,1X,A9,'|',I3,'|',A8,1X,A8,'|',A8,1PE9.2,
. 7('|',1PE9.2),/, '+',51X,'|')
END

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SUBROUTINE STAGES (NDIPEC)

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C
C
C SUBROUTINE STAGES PERFORMS THE STAGE-WISE CALCULATIONS FOR THE SYSTEM.
C VOLUMES AND FLOWS ARE CALCULATED FIRST. CONCENTRATIONS ARE COMPUTED
C NEXT. FINALLY, THE CONTROLLERS ARE CHECKED TO MODIFY ANY FEED STREAM
C VARIABLE.
C THESE CALCULATIONS ARE BASED ON INTEGRATING THE MASS BALANCES FOR
C THE VARIOUS QUANTITIES. INITIALLY, THE FLOWS AND VOLUMES ARE CALCULATED BY
C INTEGRATING THE VOLUME BALANCE FOR EACH PHASE. THESE ARE CALCULATED FIRST
C SINCE THEY ARE NOT DEPENDENT ON THE CONCENTRATIONS. THE CONCENTRATIONS
C ARE CALCULATED NEXT, TAKING INTO ACCOUNT THE CHANGING FLOWS AND VOLUMES
C IN THE INTEGRATION. THE CONTROLLERS ARE CHECKED LAST SINCE THEY REQUIRE
C VALUES AT TWO POINTS IN TIME, AND THIS IS THE ONLY PLACE WHERE TWO
C POINTS ARE KEPT.
C
COMMON/VARS/ BANK(100,2,10,2), FEED(100,2,8,14)
COMMON/SYSTEM/ VT(100), VS(100), VKA(100), VKO(100), PROD(100,2)
COMMON/SWITCH/ NTOST, NSOLI, CTBP, SPH, NEWIN, NEWOUT, IVOL, IPRO, TEMPI,
. DTHETA, ISOL(10), CONVRG(100,2), IPYN, IPROCE, ICTRL(100)
COMMON/DISTRB/ XTRY(7), DTPY(6), TIN
DIMENSION YTRY(7), ANUMER(7), BNUMBER(7)
CONTROL=0.001
C
C
C CALCULATING AQUEOUS FLOWS AND VOLUMES.
C V = AQUEOUS FLOW INTO THE STAGE AT TIME T.
C D = AQUEOUS FLOW INTO THE STAGE AT TIME T+DTHETA.
C E = EXPONENTIAL FUNCTION.
C
DO 30 J=1,NTOST
V=FEED(J,1,8,1)
D=FEED(J,1,8,2)
IF(J.EQ.1) GO TO 10
V=V+AMAX1(0.0,BANK(J-1,1,8,1)-PROD(J-1,1))
D=D+AMAX1(0.0,BANK(J-1,1,8,2)-PROD(J-1,1))
10 CONTINUE
E=EXP(-DTHETA*VKA(J))
C
C
C THIS EQUATION IS FOR THE REGULAR OPERATION OF A STAGE. AQUEOUS IS
C FLOWING OUT OF THE STAGE AT TIME T AND T+DTHETA.
C
BANK(J,1,9,2)=E*BANK(J,1,9,1)+VS(J)+D/VKA(J)-E*(VS(J)+V/VKA(J))
. +(E-1)*(D-V)/(DTHETA*VKA(J)**2)
IF(BANK(J,1,9,1).GE.VS(J)) GO TO 20
C
C
C THIS EQUATION IS FOR FILLING THE STAGE SINCE NO AQUEOUS IS FLOWING
C OUT AT TIME T OR T+DTHETA.
C
BANK(J,1,9,2)=BANK(J,1,9,1)+(V+D)*DTHETA/2.0
IF(BANK(J,1,9,2).LE.VS(J)) GO TO 20
C
C
C THIS EQUATION IS FOR THE 'NO FLOW' TO 'FLOW' TRANSITION. IT ASSUMES
C THAT THE FLOW OUT OF THE STAGE VARIES LINEARLY OVER THE TIME INCREMENT,
C AND THAT TOTAL VOLUME IS CONSERVED.
C
BANK(J,1,9,2)=(BANK(J,1,9,1)+(V+D*VKA(J)*VS(J))*DTHETA/2.0)
. /(1.0+DTHETA*VKA(J)/2.0)
20 CONTINUE
IF(BANK(J,1,9,2).LE.1.E-4) BANK(J,1,9,2)=0.0
BANK(J,1,8,2)=AMAX1(0.0,VKA(J)*(BANK(J,1,9,2)-VS(J)))
IF(BANK(J,1,8,2).LE.1.E-6) BANK(J,1,8,2)=0.0
IF(BANK(J,1,9,2).LE.0.95*VT(J)) GO TO 30
BANK(J,1,9,2)=0.95*VT(J)
BANK(J,1,8,2)=V+D-BANK(J,1,8,1)-2.0*(0.95*VT(J)-BANK(J,1,9,1))
. /DTHETA
30 CONTINUE
C
C
C CALCULATING ORGANIC FLOWS AND VOLUMES.
C V = ORGANIC FLOW INTO THE STAGE AT TIME T.
C D = ORGANIC FLOW INTO THE STAGE AT TIME T+DTHETA.
C E = EXPONENTIAL FUNCTION.
C
DO 60 JJ=1,NTOST
J=NTOST-JJ+1
V=FEED(J,2,8,1)
D=FEED(J,2,8,2)

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```

IF(J.EQ.NTOST) GO TO 40
V=V+AMAX1(0.0,BANK(J+1,2,8,1)-PROD(J+1,2))
D=D+AMAX1(0.0,BANK(J+1,2,8,2)-PROD(J+1,2))
40 CONTINUE
E=EXP(-DTHETA*VKO(J))
IF(BANK(J,1,9,1).LT.VT(J)-BANK(J,2,9,1)) GO TO 45
C
C
C THIS EQUATION IS FOR THE REGULAR OPERATION OF THE STAGE. ORGANIC IS
C FLOWING OUT OF THE STAGE AT TIME T AND T+DTHETA.
C
BANK(J,2,9,2)=E*BANK(J,2,9,1)+VT(J)-BANK(J,1,9,2)+D/VKO(J)
-E*(VT(J)-BANK(J,1,9,1)+V/VKO(J))+ (E-1.0)*(D-V-VKO(J)*
(BANK(J,1,9,2)-BANK(J,1,9,1)))/(DTHETA*VKO(J)**2)
IF(BANK(J,1,9,2)+BANK(J,2,9,1)-VT(J)+DTHETA*(V+D)/2.0.GE.0.0)
GO TO 50
C
C
C THIS EQUATION IS FOR THE 'FLOW' TO 'NO FLOW' TRANSITION. IT ASSUMES
C THAT THE FLOWS VARY LINEARLY OVER THE TIME INCREMENT, AND THAT
C TOTAL VOLUME IS CONSERVED.
C
BANK(J,2,9,2)=BANK(J,2,9,1)+DTHETA*(D+V-BANK(J,2,9,1))/2.0
GO TO 50
45 CONTINUE
C
C
C THIS EQUATION IS FOR FILLING THE STAGE WITH ORGANIC SINCE NONE IS
C FLOWING OUT.
C
BANK(J,2,9,2)=BANK(J,2,9,1)+DTHETA*(D+V)/2.0
IF(BANK(J,1,9,2)+BANK(J,2,9,2).LE.VT(J)) GO TO 50
C
C
C THIS EQUATION IS FOR THE 'NO FLOW' TO 'FLOW' TRANSITION SINCE THE
C ORGANIC IS NOT FLOWING OUT OF THE STAGE AT TIME T, BUT IS FLOWING
C OUT AT T+DTHETA. THE EQUATION ASSUMES THAT THE FLOWS VARY LINEARLY
C OVER THE TIME INCREMENT, AND THAT VOLUME IS CONSERVED.
C
BANK(J,2,9,2)=(BANK(J,2,9,1)+DTHETA*(D+V-VKO(J))*(BANK(J,1,9,2)
-VT(J))/2.0)/(1.0+DTHETA*VKO(J)/2.0)
50 CONTINUE
IF(BANK(J,2,9,2).LE.1.E-4) BANK(J,2,9,2)=0.0
BANK(J,2,8,2)=AMAX1(0.,VKO(J)*(BANK(J,2,9,2)+BANK(J,1,9,2)-VT(J)))
IF(BANK(J,2,8,2).LE.1.E-6) BANK(J,2,8,2)=0.0
60 CONTINUE
C
C
C THE 'DO 250' LOOP IS FOR CALCULATING CONCENTRATIONS. THE CONCENTRATIONS
C FOR A STAGE REQUIRE THE REACHING OF EQUILIBRIUM IN THE 'MIXER,' AND
C THE SUBSEQUENT MIXING OF THE 'MIXER' PRODUCTS WITH THE CONTENTS OF
C THE 'SETTLERS.'
C ANUMER = AMOUNT OF SOLUTE ENTERING IN AQUEOUS STREAMS.
C BNUMER = AMOUNT OF SOLUTE ENTERING IN ORGANIC STREAMS.
C ADENOM = AQUEOUS FLOW INTO THE STAGE.
C BDEWOM = ORGANIC FLOW INTO THE STAGE.
C TIN = TEMPERATURE IN THE 'MIXER.'
C XTRY = TRIAL AQUEOUS CONCENTRATION LEAVING THE 'MIXER.'
C YTRY = TRIAL ORGANIC CONCENTRATION LEAVING THE 'MIXER.'
C NCOFF IS USED TO SCAN THE STAGES MULTIPLE TIMES FOR EACH TIME
C INCREMENT. IT WAS FOUND THAT SMALL BUT SIGNIFICANT INTEGRATION
C ERRORS OCCURRED WHEN THE STAGES WERE SCANNED ONLY ONCE.
C
DO 250 NCOFF=1,2
NDIREC=-NDIREC
DO 250 NSCAN=1,NTOST
J=NSCAN
IF(NDIREC.LT.0) J=NTOST-J+1
JP=J-1
JS=J+1
C
C
C THIS SECTION IS JUST ACCUMULATING THE SOLUTE FLOWS INTO THE STAGE.
C
ADENOM=FEED(J,1,8,2)+FEED(J,1,8,1)
BDEWOM=FEED(J,2,8,2)+FEED(J,2,8,1)
DO 100 L=1,7
XTRY(L)=BANK(J,1,L,2)
ANUMER(L)=FEED(J,1,9,2)*FEED(J,1,L,2)+FEED(J,1,8,1)*FEED(J,1,L,1)
BNUMER(L)=FEED(J,2,8,2)*FEED(J,2,L,2)+FEED(J,2,8,1)*FEED(J,2,L,1)
100 CONTINUE

```

```

IF(J.EQ.1) GO TO 110
TERONE=AMAX1(0.0,BANK(JP,1,8,1)-PROD(JP,1))
TERTWO=AMAX1(0.0,BANK(JP,1,8,2)-PROD(JP,1))
ADENOM=ADENOM+TERONE+TERTWO
DO 105 L=1,7
ANUMER(L)=ANUMER(L)+TERONE*BANK(JP,1,L,1)+TERTWO*BANK(JP,1,L,2)
105 CONTINUE
110 CONTINUE
IF(J.EQ.NTOST) GO TO 120
TERONE=AMAX1(0.0,BANK(JS,2,8,1)-PROD(JS,2))
TERTWO=AMAX1(0.0,BANK(JS,2,8,2)-PROD(JS,2))
BDENOM=BDENOM+TERCNE+TERTWO
DO 115 L=1,7
BNUMER(L)=BNUMER(L)+TERONE*BANK(JS,2,L,1)+TERTWO*BANK(JS,2,L,2)
115 CONTINUE
120 CONTINUE
C
C
C CALCULATING TIN, THE MIXER TEMPERATURE, WHICH IS USED AS THE
C TEMPERATURE FOR CALCULATING DISTRIBUTION COEFFICIENTS IN UCOR.
C
TIN=TEMPI
IF(ADENOM+SPH*BDENOM.GE.1.E-10) TIN=(ANUMER(7)+SPH*BNUMER(7))
  / (ADENOM+SPH*BDENOM)
MCK=0
C
C
C HERE THE PROGRAM TESTS THE FLOW RATIO INTO THE STAGE TO DETERMINE
C IF THE STREAMS ENTERING THE STAGE CAN BE MIXED. EXTREME FLOW RATIOS
C CANNOT BE MIXED WITHOUT POTENTIAL PROBLEMS APPEARING. THIS PRIMARILY
C IS A GUARD AGAINST UNREALISTIC VALUES BEING CALCULATED DURING STARTUP.
C
IF(ADENOM.LT.25.0*BDENOM.AND.PDENOM.LT.25.0*ADENOM) GO TO 160
C
C THE PHASES ARE NOT TO BE MIXED DUE TO A LACK OF ONE OR BOTH PHASES,
C OR AN IMPROPER FLOW RATIO. THE CONCENTRATIONS LEAVING THE 'MIXER'
C ARE SET TO AN AVERAGE OF THE INPUT STREAMS.
C
DO 135 L=1,NSOLU
XTRY(L)=0.0
YTRY(L)=0.0
135 CONTINUE
IF(ADENOM.LE.0.0) GO TO 145
DO 140 L=1,NSOLU
XTRY(L)=ANUMER(L)/ADENOM
140 CONTINUE
145 CONTINUE
IF(BDENOM.LE.0.0) GO TO 155
DO 150 L=1,NSOLU
YTRY(L)=BNUMER(L)/BDENOM
150 CONTINUE
155 CONTINUE
GO TO 172
C
C
160 CONTINUE
C
C BOTH AQUEOUS AND ORGANIC PHASES ENTER THE 'MIXER' SO THE SOLUTES MUST
C BE RE-DISTRIBUTED BETWEEN THE PHASES. UCORPU CALCULATES THE APPROPRIATE
C DISTRIBUTION COEFFICIENTS (DTRY). THE ITERATION IS USED TO ENSURE
C THAT A MATCHING SET OF XTRY AND DTRY ARE FOUND. A GOOD MATCH IS
C DESIRED DUE TO THE INTERRELATION BETWEEN THEM.
C
IF(IPROC.EQ.0) CALL UCORPU
IF(IPROC.EQ.1) CALL UCORTH
ICK=0
DO 170 L=1,NSOLU
XSAV=XTRY(L)
XTRY(L)=(ANUMER(L)+BNUMER(L))/(ADENOM+DTRY(L)*BDENOM)
YTRY(L)=XTRY(L)*DTRY(L)
IF(XTRY(L).GT.1.E-6.AND.ABS(XTRY(L)-XSAV).GT.CONTOL*XTRY(L)) ICK=1
170 CONTINUE
MCK=MCK+ICK
IF(ICK.EQ.1.AND.MCK.LE.20) GO TO 160
172 CONTINUE

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C
C
C THE PRODUCTS OF THE 'MIXER' HAVE BEEN DETERMINED, AND ARE NOW COMBINED
C WITH THE CONTENTS OF THE 'SETTLER.' THE EQUATIONS FOR THE 'SETTLER'
C ARE SIMPLY PERFECT MIXING EQUATIONS FOR AN AQUEOUS AND AN ORGANIC
C TANK.
C DAVOL = THE CHANGE IN AQUEOUS VOLUME DURING THE TIME INTERVAL.
C DOVOL = THE CHANGE IN ORGANIC VOLUME DURING THE TIME INTERVAL.
C DAFLO = THE CHANGE IN AQUEOUS FLOWS INTO THE STAGE.
C DOFLO = THE CHANGE IN ORGANIC FLOWS INTO THE STAGE.
C TAFLO = THE AQUEOUS FLOW INTO THE STAGE AT TIME T.
C TOFLO = THE ORGANIC FLOW INTO THE STAGE AT TIME T.
C
C
C   DAVOL=BANK(J,1,9,2)-BANK(J,1,9,1)
C   DOVOL=BANK(J,2,9,2)-BANK(J,2,9,1)
C   DAFLO=FEED(J,1,8,2)
C   DOFLO=FEED(J,2,8,2)
C   TAFLO=FEED(J,1,8,1)
C   TOFLO=FEED(J,2,8,1)
C   IF(J.EQ.1) GO TO 175
C   DAFLO=DAFLO+AMAX1(0.0,BANK(JP,1,8,2)-PROD(JP,1))
C   TAFLO=TAFLO+AMAX1(0.0,BANK(JP,1,8,1)-PROD(JP,1))
175 CONTINUE
C   IF(J.EQ.NTOST) GO TO 180
C   DOFLO=DOFLO+AMAX1(0.0,BANK(JS,2,8,2)-PROD(JS,2))
C   TOFLO=TOFLO+AMAX1(0.0,BANK(JS,2,8,1)-PROD(JS,2))
180 CONTINUE
C
C
C IN THE CALCULATION FOR THE 'SETTLER,' THE IMPORTANT QUANTITY IS THE
C VALUE FOR THE EXPONENTIAL WHICH DETERMINES HOW TO WEIGHT THE CONTENTS
C OF THE 'SETTLER' AS OPPOSED TO THE INCOMING STREAM. IF THE PREVIOUS
C CONTENTS OF THE 'SETTLER' ARE A SMALL FRACTION OF WHAT IS IN THE
C INCOMING STREAM, THE EXPONENTIAL IS ZERO (THE CONCENTRATION OF THE
C INCOMING STREAM WILL BE THE 'SETTLER' CONCENTRATION FOR TIME T+DTHETA).
C ANOTHER EXPONENTIAL IS USED IF THE VOLUME REMAINS CONSTANT (DAVOL=0),
C AND ANOTHER IF THE VOLUME AT TIME T AND THE VOLUME CHANGE ARE BOTH
C SIGNIFICANT.
C
C
C THE ZERO VALUE OF 'E' IS FOR WHEN THERE IS NO AQUEOUS PRESENT, AND FOR
C WHEN THE AQUEOUS AT TIME T+DTHETA IS ALMOST ENTIRELY DUE TO THE STREAM
C ENTERING THE 'SETTLER.'
C
C   E=0.0
C   DAFLO=DAPLO-TAFLO
C   DOFLO=DOFLO-TOFLO
C   GENWT=0.0
C   FIN=TAFLO+0.5*DAFLO
C   IF(BANK(J,1,9,2).EQ.0.0) GO TO 200
C   IF(BANK(J,1,9,1).LE.0.001*BANK(J,1,9,2)) GO TO 200
C   IF(ABS(DAVOL).LE.0.001*BANK(J,1,9,2)) GO TO 190
C
C
C THIS VALUE OF 'E' IS THE GENERAL CASE. DAVOL AND THE AQUEOUS VOLUME
C AT TIME T ARE SIGNIFICANT.
C
C   E=(TAFLO-BANK(J,1,9,1)*DAPLO/DAVOL)*ALOG(BANK(J,1,9,2)
C     /BANK(J,1,9,1))
C   E=EXP(-DTHETA*(E+DAFLO)/DAVOL)
C   GENWT=ALOG(BANK(J,1,9,2)/BANK(J,1,9,1))*DTHETA/DAVOL
C   IF(FIN.LE.1.0E-6) GO TO 200
C   GENWT=((BANK(J,1,9,2)/BANK(J,1,9,1))** (FIN*DTHETA/DAVOL)-1.0)/FIN
C   GO TO 200
190 CONTINUE
C
C
C THIS VALUE OF 'E' IS FOR CONSTANT VOLUME (DAVOL=0).
C
C   E=EXP(-DTHETA*ADENOM/(2.0*BANK(J,1,9,2)))
C   GENWT=DTHETA/BANK(J,1,9,2)
C   IF(FIN.GT.1.0E-6) GENWT=(EXP(FIN*DTHETA/BANK(J,1,9,2))-1.0)/FIN
200 CONTINUE
C
C
C CALCULATING FOR THE AQUEOUS PHASE.
C
C   DO 205 L=1,NSOLU
C   IF(BANK(J,1,9,2).EQ.0.0) XTRY(L)=0.0
C   BANK(J,1,L,2)=XTRY(L)-(XTRY(L)-BANK(J,1,L,1))*E
C   IF(BANK(J,1,L,2).LE.1.0E-10) BANK(J,1,L,2)=0.0
205 CONTINUE
C   GENWTA=E*GENWT

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C
C
C SIMILAR CALCULATIONS FOR THE ORGANIC PHASE.
C
E=0.0
GENWT=0.0
FIN=TOPLO+0.5*DOFLO
IF (BANK (J,2,9,2) .EQ.0.0) GO TO 220
IF (BANK (J,2,9,1) .LE.0.001*BANK (J,2,9,2)) GO TO 220
IF (ABS (DOVOL) .LE.0.001*BANK (J,2,9,2)) GO TO 210
E=(TOPLO-BANK (J,2,9,1)*DOFLO/DOVOL)*ALOG (BANK (J,2,9,2)
/BANK (J,2,9,1))
E=EXP (-DTHETA*(DOFLO+E)/DOVOL)
GENWT=ALOG (BANK (J,2,9,2)/BANK (J,2,9,1))*DTHETA/DOVOL
IF (FIN .LE.1.0E-6) GO TO 220
GENWT=(BANK (J,2,9,2)/BANK (J,2,9,1))** (FIN*DTHETA/DOVOL)-1.0)/FIN
GO TO 220
210 CONTINUE
E=EXP (-DTHETA*BDENM/(BANK (J,2,9,2)+BANK (J,2,9,1)))
GENWT=DTHETA/BANK (J,2,9,2)
IF (FIN .GT.1.0E-6) GENWT=(EXP (FIN*DTHETA/BANK (J,2,9,2))-1.0)/FIN
220 CONTINUE
DO 230 L=1, NSOLU
IF (BANK (J,2,9,2) .EQ.0.0) YTRY (L)=0.0
BANK (J,2,L,2)=YTRY (L)-(YTRY (L)-BANK (J,2,L,1))*E
IF (BANK (J,2,L,2) .LE.1.0E-10) BANK (J,2,L,2)=0.0
230 CONTINUE
GENWTO=E*GENWT
C
C
C SIMILAR CALCULATION FOR THE TEMPERATURE.
C
E=0.0
IF (BANK (J,1,9,2) .EQ.0.0 .AND. BANK (J,2,9,2) .EQ.0.0) GO TO 240
IF (BANK (J,1,9,1)+SPH*BANK (J,2,9,1) .LE.0.001*(DAVOL+SPH*DOVOL))
GO TO 240
IF (ABS (DAVOL+SPH*DOVOL) .LE.0.001*(BANK (J,1,9,2)+SPH*BANK (J,2,9,2)))
GO TO 235
E=(BANK (J,1,9,1)+SPH*BANK (J,2,9,1))*(DAFLO+SPH*DOFLO)
E=(TAFLO+SPH*TOFLC-E)/(DAVOL+SPH*DOVOL)
E=E*ALOG ((BANK (J,1,9,2)+SPH*BANK (J,2,9,2))/(BANK (J,1,9,1)+
SPH*BANK (J,2,9,1)))
E=EXP (-DTHETA*(DAFLO+SPH*DOFLO+E)/(DAVOL+SPH*DOVOL))
GO TO 240
235 CONTINUE
E=EXP (-DTHETA*(ADENOM+SPH*BDENM)/(BANK (J,1,9,2)+BANK (J,1,9,1)
+SPH*(BANK (J,2,9,2)+BANK (J,2,9,1))))
240 CONTINUE
T=TIN-(TIN-BANK (J,1,7,1))*E
BANK (J,1,7,2)=T
BANK (J,2,7,2)=T
C
C
C RXNDEN CALCULATES REACTION PRODUCTS AND SOLUTION DENSITIES FOR THE PROGRAM.
C THE REACTION PRODUCTS ARE FACTORED INTO THE CONCENTRATIONS AS GENERATION
C TERMS USING GENWTA AND GENWTO AS THE INTEGRATED WEIGHTING FACTORS
C
CALL RXNDEN (J, GENWTA, GENWTO)
C
DO 250 K=1,2
IF (BANK (J,K,9,1) .GT.0.0) GO TO 250
BANK (J,K,10,1)=BANK (J,K,10,2)
DO 250 L=1,7
BANK (J,K,L,1)=BANK (J,K,L,2)
250 CONTINUE
C
C
C THE 'DO 300' LOOP IS FOR EVALUATING THE CONTROLLERS
C
DO 300 J=1, NTOST
IF (ICNTFL (J) .EQ.0) GO TO 300
DO 300 K=1,2
IF (ICNTFL (J) .NE.K .AND. ICNTPL (J) .NE.3) GO TO 300
DO 295 L=1,8
IF (FEED (J,K,L,3) .EQ.0.0) GO TO 295
PDSAVE=FEED (J,K,L,2)

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C
C
C EVALUATING THE CONTRCLLERS.
C JM = MONITORED STAGE.
C KM = MONITORED PHASE (MAY BE EITHER FOR THE FEED OR THE BANK).
C LM = MONITORED VARIABLE.
C
C JM=ABS (FEED (J,K,L,3))
C KM=1
C IF (FEED (J,K,L,4) .EQ.2.0 .OR. FEED (J,K,L,4) .EQ.4.0) KM=2
C LM=FEED (J,K,L,5)
C IF (FEED (J,K,L,3) .LT.0.0) GO TO 275
C
C
C 3-MODE CONTROLLING.
C EONE = ERROR AT TIME T.
C ETWO = ERROR AT TIME T+DTHETA.
C
C IF (FEED (J,K,L,4) .GT.2.5) GO TO 255
C
C
C CONTROLLED BY A BANK VARIABLE.
C
C EONE=BANK (JM,KM,LM,1) -FEED (J,K,L,6)
C ETWO=BANK (JM,KM,LM,2) -FEED (J,K,L,6)
C GO TO 260
C 255 CONTINUE
C
C
C CONTROLLED BY A FEED STREAM VARIABLE.
C
C EONE=FEED (JM,KM,LM,1) -FEED (J,K,L,5)
C ETWO=FEED (JM,KM,LM,2) -FEED (J,K,L,6)
C 260 CONTINUE
C
C
C KEEPING THE INTEGRATED ERROR.
C
C FEED (J,K,L,14) =FEED (J,K,L,14) +DTHETA*(ETWO+EONE)/2.0
C
C
C COMPUTING THE NEW VALUE FOR THE CONTROLLER OUTPUT.
C
C FEED (J,K,L,2) =FEED (J,K,L,10) +FEED (J,K,L,7) * (ETWO
C . +FEED (J,K,L,14) /FEED (J,K,L,8) +FEED (J,K,L,9) * (ETWO-EONE)
C . /DTHETA)
C
C
C IMPOSING MINIMUM AND MAXIMUM VALUES TO LIMIT THE CONTROLLER.
C
C FEED (J,K,L,2) =AMIN1 (FEED (J,K,L,2) ,FEED (J,K,L,12))
C FEED (J,K,L,2) =AMAX1 (FEED (J,K,L,2) ,FEED (J,K,L,13))
C GO TO 290
C 275 CONTINUE
C
C
C ON/OFF CONTROLLING.
C
C IF (FEED (J,K,L,4) .GT.2.5) GO TO 280
C
C
C CONTROLLED BY A BANK VARIABLE.
C
C
C THESE 'IF' STATEMENTS DETERMINE IF THE UPPER OR LOWER SET POINTS FOR
C THE CONTROLLER HAVE BEEN EXCEEDED.
C
C IF (BANK (JM,KM,LM,2) .GT. FEED (J,K,L,6)) GO TO 285
C IF (BANK (JM,KM,LM,2) .LT. FEED (J,K,L,7)) GO TO 288
C GO TO 283
C 280 CONTINUE
C
C
C CONTROLLED BY A FEED STREAM VARIABLE.
C
C IF (FEED (JM,KM,LM,2) .GT. FEED (J,K,L,6)) GO TO 285
C IF (FEED (JM,KM,LM,2) .LT. FEED (J,K,L,7)) GO TO 288
C 283 CONTINUE

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C
C
C NEITHER LIMIT WAS EXCEEDED SO THE PROGRAM MUST DETERMINE WHAT THE
C PREVIOUS SETTING WAS (ON OR OFF).
C
      IF (ABS (FDSAVE-FEED (J,K,L,12)) .GT. ABS (FDSAVE-FEED (J,K,L,13)))
      .   GO TO 288
295 CONTINUE
C
C
C SWITCHING TO THE 'ON' VALUE.
C
      FEED (J,K,L,2) = FEED (J,K,L,12)
      GO TO 290
288 CONTINUE
C
C
C SWITCHING TO THE 'OFF' VALUE.
C
      FEED (J,K,L,2) = FEED (J,K,L,13)
290 CONTINUE
      FEED (J,K,L,1) = FDSAVE
C
C
C IMPOSING THE ERROR ON THE OUTGOING VALUE WITH THE CONDITION THAT NO
C NEGATIVE VALUES ARE ALLOWED (WITH THE EXCEPTION OF TEMPERATURE).
C
      FEED (J,K,L,2) = FEED (J,K,L,2) * (1.0 + FEED (J,K,L,11) * (RANF (0.) - .5) / 50.)
      IF (L.NP.7) FEED (J,K,L,2) = AMAX1 (0.0, FEED (J,K,L,2))
      IF (ABS (FEED (J,K,L,2)) .LE. 1.0E-9) FEED (J,K,L,2) = 0.0
295 CONTINUE
      IF (FEED (J,K,8,1) .GT. 0.0) GO TO 300
      DO 300 L=1,7
      FEED (J,K,L,1) = FEED (J,K,L,2)
300 CONTINUE
      DO 350 J=1, NTOST
      DO 350 K=1,2
      CONVRG (J,K) = 0.0
C
C
C CHECKING THE CONVERGENCE OF THE FEED STREAMS.
C
      IF (ICNTRL (J) .NE. K .AND. ICNTRL (J) .NE. 3) GO TO 310
      DO 305 L=1,3
      IF (FEED (J,K,L,2) .GT. 1.0E-6) CONVRG (J,K) = AMAX1 (CONVRG (J,K) ,
      .   100. * ABS (FEED (J,K,L,2) - FEED (J,K,L,1)) / (DTHETA * FEED (J,K,L,2)))
305 CONTINUE
310 CONTINUE
C
C
C CHECKING THE CONVERGENCE OF THE BANK.
C
      IF (BANK (J,K,9,2) .LE. 1.0E-8) GO TO 320
      DO 315 L=1,9
      IF (BANK (J,K,L,2) .GT. 1.0E-6) CONVRG (J,K) = AMAX1 (CONVRG (J,K) ,
      .   100. * ABS (BANK (J,K,L,2) - BANK (J,K,L,1)) / (DTHETA * BANK (J,K,L,2)))
315 CONTINUE
320 CONTINUE
C
C
C INCREMENTING TIME IN THE BANK.
C
      DO 325 L=1,10
      BANK (J,K,L,1) = BANK (J,K,L,2)
325 CONTINUE
350 CONTINUE
      RETURN
      END

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SUBROUTINE UCORPU

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C
C
C SUBROUTINE UCORPU CALCULATES DISTRIBUTION COEFFICIENTS FOR THE PUBEX
C PROCESS. THE AQUEOUS CONCENTRATIONS ARE FIRST CONVERTED TO MOLAR
C UNITS. THE MOLAR QUANTITIES ARE CONVERTED TO MOLAL UNITS. THE
C MOLAL QUANTITIES ARE PUT INTO THE CORRELATIONS TO GET A MOLAL
C DISTRIBUTION COEFFICIENT AND ORGANIC CONCENTRATION. THE ORGANIC
C MOLAL CONCENTRATION IS CONVERTED TO MOLAR UNITS. THE FINAL
C DISTRIBUTION COEFFICIENT IS THEN THE RATIO OF THE ORGANIC MOLAR
C CONCENTRATION TO THE AQUEOUS MOLAR CONCENTRATION.
C
COMMON/DISTPB/ XTRY (7), DTPY (6), TEMP
COMMON/SWITCH/ NTOST, NSOLU, CTBP, SPH, NEWIN, N*WOUT, IVOL, IPPO, TEMPI,
. DTHETA, ISOL (10), CONVEG (100, 2), IPXM, IPROCE, ICTRL (100)
DIMENSION XMOLAR (6), XMOAL (6), YMOLAL (6)
DO 5 I=1, 6
XMOLAR (I) = AMAX 1 (0.0, XTRY (I))
5 CONTINUE
XMOLAR (2) = XMOLAR (2) / 238.
XMOLAR (3) = XMOLAR (3) / 239.
XMOLAR (4) = XMOLAR (4) / 239.
CONVA = 1.0 / AMAX 1 (0.1, 1.0 - 0.0309 * XMOLAR (1) - 0.0724 * XMOLAR (2)
. - 0.13 * XMOLAR (3) - 0.031 * XMOLAR (6))
DO 10 I=1, 6
XMOAL (I) = XMOLAR (I) * CONVA
10 CONTINUE
TNM = XMOAL (1) + 2. * XMOAL (2) + 2. * XMOAL (3) + 4. * XMOAL (4) + XMOAL (6)
IF (TNM .LT. 1.0E-10) TNM = 1.0E-10
DRT = 1000. / (TEMP + 273.16) - 3.3529
UK = (3.7 * TNM ** 1.57 + 1.4 * TNM ** 3.9 +).011 * TNM ** 7.3)
. * (4.0 * CTBP ** (-0.17) - 3.0)
PUK = UK * (0.20 + 0.55 * CTBP ** 1.25 + 0.0074 * TNM ** 2)
HK1 = (0.135 * TH ** 0.82 + 0.0052 * TNM ** 3.44) * (1.0 - 0.54 * EXP (-15.0 * CTBP))
HK1 = HK1 * EXP (0.34 * DRT)
UK = UK * EXP (2.5 * DRT)
PUK = PUK * EXP (-0.2 * DRT)
HK2 = HK1
A = 2. * (UK * XMOAL (2) + PUK * XMOAL (2) + HK2 * XMOAL (1))
B = 1.0 + HK1 * XMOAL (1)
C = -3.65145 * CTBP
TF = -C / B
IF (A .GE. 1.E-6) TF = (-B + SQRT (B ** 2 - 4. * A * C)) / (2. * A)
DIRY (1) = HK1 * TF + HK2 * TF ** 2
DTPY (2) = UK * TF ** 2
C
C
C THIS IS THE CORRECTION SUGGESTED BY P.T.JUBIN
C
DIRY (3) = PUK * TF ** 2
. / (1.0 - 0.43223 + 0.013118 * TEMP + 0.74358 * XMOAL (2)
. - 0.175829 * XMOAL (1) * XMOAL (2))
DIRY (4) = 0.0
DIRY (5) = 0.0
DIRY (6) = 0.0
DO 20 I=1, 6
YMOLAL (I) = XMOAL (I) * DIRY (I)
20 CONTINUE
WO = (4.2 - 0.015 * TEMPI) * (CTBP ** 1.69) * (3.65145 * CTBP - 2.0 * YMOLAL (2)
. - 2.0 * YMOLAL (3) - 0.6 * YMOLAL (1)) / (3.65145 * CTBP)
CONVO = 1.0 + 0.097 * YMOLAL (2) + 0.139 * YMOLAL (3) + 0.043 * YMOLAL (1) + 0.174 * WO
DO 30 I=1, 6
DIRY (I) = DIRY (I) * CONVO / CONVO
IF (XMOLAR (I) .NE. 0.0) DTPY (I) = YMOLAL (I) / (XMOLAR (I) * CONVO)
30 CONTINUE
RETURN
END

```

```

SUBROUTINE UCORTH
C
C UCOR RETURNS A VALUE OF THE DISTRIBUTION COEFFICIENTS- DTRY(I)
C Z - TOTAL IONIC STRENGTH
C TEMP - TEMPERATURE IN DEGREES CENTIGRADE
C XTRY - AQUEOUS PHASE COMPOSITION
C KU, KTH, KH - MASS ACTION EQUILIBRIUM CONSTANTS=A+B*C*Z+D*Z*Z
C FOR KU(I) - A,B,C,D ARE COEF(1,I), COEF(2,I), COEF(3,I), AND COEF(4,I)
C FOR KTH(I) - A,B,C,D ARE COEF(5,I), COEF(6,I), COEF(7,I), AND COEF(8,I)
C FOR KH(I) - A,B,C,D ARE COEF(9,I), COEF(10,I), COEF(11,I), AND COEF(12,I)
C
C     FOR I=1 U ACCURACY
C     I=2 TH ACCURACY
C     I=3 H ACCURACY
C
COMMON/DISTRB/ XTRY(7),DTRY(6),TEMP
COMMON/SWITCH/ NTCST,NSOLU,CTEP,SPH,NEWIN,NEWOUT,IVOL,IPRO,TEMPI,
  . DTRFTA,ISOL(10),CONVRG(100,2),IRXN,IPROCE,ICNTRL(100)
DIMENSION XMOLAR(6),YMOLAL(6),YMOLAL(6)
REAL*4 COEF(12,3),KU(3),KH(3),A(4),TBP(3)
DATA COEF/5.16764,12.7385,-6.10939,0.825665,
  . 0.895314,-0.258242,0.0628435,0.00145494,
  . 0.480975,-0.222463,0.0320684,-0.000857849,
  . 4.98513,13.7875,-7.02178,.883582,
  . 1.52821,-.527579,.0324897,.00416738,
  . .538601,-.207956,.0204384,-.00118140,
  . 2.55963,-7.66961,2.03295,1.58978,
  . 1.31060,-0.475194,0.0370571,0.00577316,
  . 0.398195,-0.158715,0.0312264,-0.00164366/
DO 5 I=1,6
  XMOLAR(I)=XTRY(I)
5 CONTINUE
  XMOLAR(2)=XMOLAR(2)/238.
  XMOLAR(3)=XMOLAR(3)/232.
DO 10 I=1,6
  YMOLAL(I)=XMOLAR(I)
10 CONTINUE
  Z=AMIN1(XMOLAL(1)+3.0*XMOLAL(2)+10.0*XMOLAL(3),10.0)
  TNM=XMOLAL(1)+2.0*XMOLAL(2)+4.0*XMOLAL(3)
C
C CALCULATE MASS ACTION EQUILIBRIUM CONSTANTS
C
DO 30 I=1,3
  KU(I)=COEF(1,I)+CCEF(2,I)*Z+COEF(3,I)*Z**2+COEF(4,I)*Z**3
  KU(I)=AMAX1(0.0,KU(I))
  KTH(I)=COEF(5,I)+COEF(6,I)*Z+COEF(7,I)*Z**2+COEF(8,I)*Z**3
  KH(I)=COEF(9,I)+CCEF(10,I)*Z+COEF(11,I)*Z**2+COEF(12,I)*Z**3
C
C SOLVE CUBIC EQUATION FOR TBP
C
  A(1)=-3.65145*CTBP
  A(2)=1.0+KH(I)*XMOLAL(1)*TNM
  A(3)=2.0*KU(I)*XMOLAL(2)*TNM**2
  A(4)=3.0*KTH(I)*XMOLAL(3)*TNM**4
  Y=AMIN1(-A(1),-A(1)/A(2))
  IF(Y.LT.0.) Y=-A(1)
  DO 20 J=1,20
  C=A(2)+2.0*A(3)*Y+3.0*A(4)*Y**2
  D=A(1)+A(2)*Y+A(3)*Y**2+A(4)*Y**3
  DELTY=D/C
  Y=Y-DELTY
  IF(ABS(DELTY).LT.1.E-5.AND.ABS(D).LT.1.E-5) GO TO 25
20 CONTINUE
25 CONTINUE
  TBP(I)=Y
30 CONTINUE
  DTRY(1)=KH(3)*TNM*TBP(3)
  DTRY(2)=KU(1)*TNM**2*TBP(1)**2
  DTRY(3)=KTH(2)*TNM**4*TBP(2)**3
  DTRY(4)=0.
  DTRY(5)=0.
  DTRY(6)=0.
C
C TEMPERATURE ADJUSTMENT
C
  DRT=1./(273.+TEMP)-1./298.
  DTRY(1)=DTRY(1)*EXP(-818.902*DRT)
  DTRY(2)=DTRY(2)*EXP(2500.*DRT)
  DTRY(3)=DTRY(3)*EXP((891.664+879.689*XMOLAL(2)
  . -1474.38*XMOLAL(3)**2)*DRT)
  RETURN
END

```



```

CC=R*B
DO 78 I=1,10
A=1.0/(1.0-EXTENT)
IF (FOR.GT.0.01) GO TO 72

```

```

C
C THIS INTEGRATED FORM ASSUMES A LARGE EXCESS OF THE REDUCTANT
C

```

```

AMTINT=AA*A*EXTENT-2.0*BB*ALOG(A)+CC*EXTENT
GO TO 76
72 CONTINUE
IF (ABS(1.0-FOR).LT.0.05) GO TO 74

```

```

C
C THIS INTEGRATED RATE EQUATION IS THE GENERAL CASE
C

```

```

FOR=DUMFUN(FOR)
B=1.0-FOR*EXTENT
C=1.0/(1.0-FOR)
AMTINT=(FOR-A*EXTENT-FOR/B+2.0*C*FOR*ALOG(A*B))*AA*C*C
AMTINT=AMTINT-2.0*BB*C*(FOR*EXTENT/B-C*ALOG(A*B))-CC*EXTENT/B
AMTINT=-AMTINT
GO TO 76

```

```

C
C THIS INTEGRATED FORM ASSUMES A STOICHIOMETRIC AMOUNT OF REDUCTANT
C

```

```

74 CONTINUE
AMTINT=AA*(A*A-1.0)/3.0-BB*(A-1.0)+CC*(A-1.0)
76 CONTINUE
IF (AMTINT.GT.RK) EXTENT=EXTENT-EXTINC
IF (AMTINT.LT.FK) EXTENT=EXTENT+EXTINC
EXTINC=EXTINC/2.0
78 CONTINUE
RXNAMT=EXTENT*SOLAMT(3)
GO TO 100
80 CONTINUE

```

```

C
C IPXN = 2 REACTION BETWEEN PU (IV) AND O (IV)
C
C RK = RATE CONSTANT
C
C RCU = RATIO OF PU (IV) TO REDUCTANT
C
C EXTMAX = MAXIMUM EXTENT BASED ON PU (IV) AND A TEN SECOND HALF TIME
C

```

```

IF (RX(3).LT.1.0E-10.OR.RX(5).LT.1.0E-10) GO TO 90
EXTMAX=AMIN1(1.0,1.0-0.5*(DTHETA/10.),2.0*SOLAMT(5)/SOLAMT(3))
RK=170.0/60.0
RK=RK*DTHETA*RX(5)
RCU=SOLAMT(3)/(2.0*SOLAMT(5))
RHO=RX(1)*RX(1)
REXP=1.0E40
IF (RK*(1.0-RCU).LT.100.0*RHO) REXP=EXP(RK*(1.0-RCU)/RHO)
EXTENT=RK/(RK+RHO)
IF (ABS(1.0-RCU).GT.0.05) EXTENT=(1.0-REXP)/(RCU-REXP)
EXTENT=AMIN1(EXTENT,EXTMAX)
RXNAMT=SOLAMT(3)*EXTENT
GO TO 100
90 CONTINUE

```

```

C
C IPXN = 1 INSTANTANEOUS REDUCTION OF PU (IV)
C
C THIS MECHANISM IS USED BY ALL REDUCTION REACTIONS WHEN THE
C
C CONCENTRATIONS FALL BELOW A THRESHOLD LEVEL
C
C INSTANTANEOUS REDUCTION WORKS MORE TO JUST ELIMINATE THE PU(IV)
C
C AND REDUCTANT CONCENTRATIONS THAN TO CALCULATE A GENERATION TERM.
C

```

```

IF (GENWTO.GT.1.F-6) RX(3)=RX(2)+BANK(J,2,2)*GENWTA/(GENWTO*239.)
RXNAMT=AMIN1(-RX(3)/STOIC(3,IPXN),-RX(5)/STOIC(5,IRXN))
RXNAMT=RXNAMT*DTHETA/GENWTA
100 CONTINUE
DO 105 L=1,6
GENAMT(1,L)=RXNAMT*STOIC(L,IRXN)/DTHETA
GENAMT(2,L)=0.0
105 CONTINUE
GENAMT(1,2)=GENAMT(1,2)*239.
GENAMT(1,3)=GENAMT(1,3)*239.
GENAMT(1,4)=GENAMT(1,4)*239.

```


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