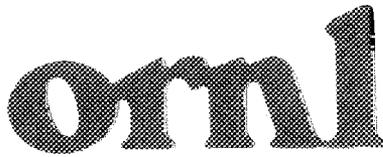


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User's Manual for SEPHIS MOD4,
Version 2.11

W. S. Groenier

MANAGED BY
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FOR THE UNITED STATES
DEPARTMENT OF ENERGY

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USER'S MANUAL FOR SEPHIS MOD4, VERSION 2.11

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Robotics and Process Systems Division

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ABSTRACT

SEPHIS MOD4, Version 2.11, is a significantly improved and enhanced version of the SEPHIS MOD4 calculational model for stagewise Purex and Thorex solvent extraction systems. Version 2.11, developed at the Oak Ridge National Laboratory, is especially suited for the casual user. All operations are carried out on a PC and extensive help features are included, enabling anyone familiar with liquid-liquid solvent extraction processes and PC operation to quickly become adept in applying the model to data analysis, flow sheet development, process monitoring, off-normal operational analysis, and studies of process response to changing inputs. This manual provides a brief description of the model and instructions for its use.

1. INTRODUCTION

SEPHIS MOD4, Version 2.11, is a PC-based calculational model for stagewise Purex and Thorex solvent extraction systems. Version 2.11 is the latest in a series of improvements to the original SEPHIS model developed in 1972,¹ which is termed SEPHIS MOD1. It was specific to the Purex process as applied to liquid-metal-cooled fast breeder reactor (LMFBR) fuels and considered only a single extractant concentration and temperature.

Improvements to the correlation of distribution coefficients were included in 1973.^{2,3} This model, SEPHIS MOD2, also allowed the use of various extractant concentrations and temperatures. In 1975, the distribution coefficient correlation was changed again, provision was made for the salting effect of inextractable nitrates, changes were made in order to perform calculations on a solute-free, rather than a molar, basis, and a means for handling a chemical reductant was included.⁴ This model, SEPHIS MOD3, was also adapted to the Thorex process in 1979.^{5,6}

SEPHIS MOD4 was developed in 1979 and adapted to both Purex and Thorex processes.⁷⁻⁹ Although following the same general concept of a mixer-settler bank as was used in previous SEPHIS models, MOD4 refined the concept slightly and, to a greater extent, changed the mathematical relationships that describe the concept. Major improvements were made in the handling of reactions by chemical reductants and in the integration procedures for accurately following process transient conditions.

The new Version 2.11 of SEPHIS MOD4 provides additional enhancements for the casual user. The most important is the adaptation to a PC. It offers unsurpassed flexibility for a range of solvent extraction applications, including data analysis, flow sheet development, process monitoring, off-normal operational analysis, and studies of process response to changing inputs.

1.1 OVERVIEW

This document is intended as a user's manual for SEPHIS MOD4, Version 2.11. In the sections to follow, sufficient information is provided to enable anyone familiar with liquid-liquid solvent extraction processes and with PC operation to become adept in the use of this model. An abbreviated description of the model is provided in Sect. 2. For a complete description of the model, including the programming logic, refer to the SEPHIS Technical Manual.¹⁰ The capabilities of Version 2.11 are discussed in Sect. 3, and the specific advantages over previous versions of the model are described in Sect. 4. Section 5 lists hardware requirements. In Sect. 6, detailed instructions are given for using the model. Sample problems are provided in Sect. 7. Appendixes show sample screen displays from the PC monitor, list common error messages, and offer a few hints that may be useful.

1.2 CONTENT OF THE DISTRIBUTION DISKETTE

The distribution diskette is a single 2S/2D, 5 1/4-in. floppy disk that contains the files listed in Table 1. This diskette may be obtained by writing to the Department of Energy National Energy Software Center, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439.

**Table 1. Files included in the
distribution diskette**

File	Size	Date
SECALC.EXE	136,093	7/16/90
SEPHIS.EXE	50,641	7/15/90
SEPREP.EXE	97,631	7/16/90
SEPRNT.EXE	74,343	7/16/90

2. DESCRIPTION OF THE MODEL

2.1 CONCEPTUAL AND MATHEMATICAL BASES

Version 2.11 employs the same conceptual and mathematical bases as the original SEPHIS MOD4. A stagewise representation of the liquid-liquid solvent extraction process is featured that would occur when using mixer-settler contactors in a countercurrent array. In a given stage, aqueous and organic streams from adjacent stages (and/or feed streams) are well mixed in the mixer section with any liquid inventory in the mixer where all mass transfer between the phases takes place. An equilibrium contact is assumed (i.e., a perfect mixer). The mixed-phase stream then flows to a settler that consists of three tanks (zones) in series. These three zones are of equal volume and serve as liquid holdup regions between mixers. No additional mass transfer between the phases occurs in the settler zones and the contents of each phase in each zone are assumed homogeneous. Aqueous and organic streams leaving the third settler zone proceed to adjacent stages or are withdrawn as products.

Feed streams can be admitted to any stage, and product streams can be withdrawn from any stage. A special routing provision is that the entire organic stream can be withdrawn from one stage and fed to any other stage.

Chemical reactions for plutonium (by the added reductant) are assumed to occur entirely within the aqueous phase. They may occur in the mixer, the aqueous portion of the settler zones, or both, depending on the time constant of the reaction and the relative quantities of reactants.

Provisions are made to specify stage volumes in one of three ways. Individual phase volumes for both mixers and settlers can be specified, total volumes for both mixers and settlers can be specified, or volumes can be assumed equal to the phase flow rate per unit time. The third method is adequate when only steady-state stage concentrations are desired. To accurately follow changing concentrations over a time period, stage volumes must be specified to closely approximate the contactor hardware being modeled.

The flow of solutes through the model is described by differential equations. Empirical correlations are used to distribute solutes between phases, to model chemical (reductant) reactions, to provide phase densities, and to account for water extracted into the organic phase. For simplification, certain assumptions and approximations are made; these are listed in Sect. 2.3. Integration of the differential equations is accomplished by using numerical techniques for a specified time increment. The user should specify a time increment for integrations that is no more than 25% of the mean stage solution residence time if accurate results for transient conditions are desired. If only steady-state results are desired, a time increment of 1 min is usually satisfactory. One of the numerical integration techniques will generally operate without failure at much larger time increments, as described in the remainder of this section.

Three numerical integration techniques are available for specification by the user for mixer calculations. (1) The Runge-Kutta technique is generally the most accurate (except when chemical

reduction of plutonium is occurring). It can be used to obtain transient or steady-state results. (2) The Trapezoidal technique will provide accurate steady-state results and consume somewhat less computer time than the Runge-Kutta technique for the same specified time increment for integrations. It is not recommended for transient results. (3) The Fast technique can be used for both transient and steady-state results, although the plutonium reduction profile differs somewhat from that generated by other techniques. Plutonium is reduced more slowly because of the set of concentrations used to calculate the reduction rate. When plutonium reduction is occurring, however, this is the only recommended technique for transient results. The Fast technique will consume more computer time than the Trapezoidal technique for the same specified time increment for integrations but in most cases is capable of handling relatively large time increments (10 min), thereby producing steady-state results at a rapid rate. Use the information in Table 2 as a guide when choosing an integration technique.

Table 2. Choice of numerical integration technique

Integration technique	Steady-state results		Transient results	
	No Pu reduction	Pu reduction	No Pu reduction	Pu reduction
Runge-Kutta	1	N	R	N
Trapezoidal	R	R	N	N
Fast	1	1,2	R	R

1 = Optional (generally consumes more computer time)

2 = Optional (plutonium profile may be in error)

N = Not recommended

R = Recommended

Only the Trapezoidal technique is used for settler calculations. Since no mass transfer between phases occurs in the settlers, this calculation merely has to propagate concentration changes through the settler zones.

Integrations continue for successive time increments until stopped by the user, stopped by a maximum time limitation, or stopped by the attainment of steady-state conditions as indicated by a user-specified tolerance.

When calculating the Purex process, plutonium reduction from Pu(IV) to Pu(III) can be modeled as (1) an instantaneous reduction, (2) reduction by uranium [U(IV)], or (3) reduction by hydroxylamine nitrate (HAN). The user specifies the quantity of reductant to be added in a feed stream (or initially added in inventory) and also specifies one of the three reaction mechanisms listed.

For a more complete description of the model (including programming logic) refer to the SEPHIS Technical Manual.¹⁰

2.2 PROGRAM FUNCTIONS

SEPHIS MOD4, Version 2.11, is a menu-driven set of computer programs. Program SEPHIS.EXE on the distribution diskette contains the menu program from which the user may select any of the three companion programs or exit to the computer system. On completion of any of the three companion programs, the menu reappears.

Program SECALC.EXE is the calculational routine that carries out all of the operations just described based on user input provided through the Problem Definition file. On completion, this routine prepares a Problem Results file. Hard-copy printouts of results are also managed by this routine. It must have available a previously prepared Problem Definition file to function.

Program SEPREP.EXE is used to prepare the Problem Definition file. It prompts the user to provide all of the input data for a particular problem to be solved.

The SEPRNT.EXE program enables the user to obtain hard-copy printouts of problems that were previously run without the necessity of rerunning them. This feature of the program is useful in instances where the original printout is destroyed or lost or when duplicate copies are desired.

2.3 APPROXIMATIONS AND ASSUMPTIONS

1. Solute concentrations in the contactor change rather slowly.

Approximations made to numerically integrate the differential equations become more exact if concentrations change slowly. By specifying a small time increment (significantly less than the mean stage residence time) over which integrations are performed, errors are minimized. This assumption does not apply when only steady-state results are desired.

2. Stage volumes and flow rates remain constant.

Because of nonideal solutions, which cause flow rates and volumes to vary with solute concentrations, SEPHIS MOD4 performs calculations on a solute-free, rather than a molar, basis. This convention greatly reduces the effect of nonideal solutions. Approximate relationships are used to convert molar to solute-free quantities.

3. The contactor operation conforms with the concept of the model.

Perfect mixing and all interphase mass transfers are assumed to occur in the mixers. The solutes are at an equilibrium distribution between the phases as defined by using approximate correlations of laboratory distribution data. In the settlers, phases separate completely, and interphase mass transfer is not allowed. Entrainment of one phase within the other is not considered. Each phase in every settler zone is homogeneous.

4. Chemical reactions occur entirely within the aqueous phase.

Pu (III), the reductant, and inextractable nitrate salts remain in the aqueous phase. The extent of reactions is governed by approximate chemical reaction kinetic data and expressions.

5. Solvent degradation products from radiolysis or chemical attack are not considered.

6. Nonideal heat effects are not considered.

Temperature profiles are calculated by using approximate heat capacities for the phases. Heats of mixing, heats of reaction (mass transfer), heat contributions from radiation, or heat transfer to the surrounding environment are not considered.

3. CAPABILITIES OF VERSION 2.11

3.1 APPLICATIONS

The SEPHIS MOD4, Version 2.11, calculational model will find many uses. Perhaps prominent among them is the development of a solvent extraction flow sheet to accomplish a specific purpose. A variety of input conditions can be quickly and inexpensively explored to result in a candidate flow sheet that is optimized for the purpose intended. Laboratory or pilot-plant verification of the chosen flow sheet conditions is, of course, a necessary step before constructing a plant owing to inaccuracies of the model brought about by the approximations and assumptions used. Operational data from such verification tests can then be compared to model results, and model parameters can be adjusted to provide a reasonable match.

Given an operational flow sheet, the model can be used for exploring off-normal operational scenarios and process response to changing input conditions. The solute concentration profile data generated by the model are useful for heavy metal inventory analyses.

The SEPHIS MOD4, Version 2.11, calculational model was developed for the Purex and Thorex solvent extraction systems. For Purex, the components considered are nitric acid, uranium, plutonium (IV), plutonium (III), a plutonium reductant, and inextractable nitrate salts. For Thorex, the components considered are nitric acid, uranium, thorium, and inextractable nitrate salts. Tri-*n*-butyl phosphate (TBP) is the organic-phase extracting agent for both systems.

The model assumes the use of up to 100 perfect mixer-settler stages, generally connected in a countercurrent array. As shown in Sect. 7, a range of problems can be set up for modeling. These include countercurrent arrays of stages for extraction, scrubbing, partitioning, and stripping operations. The flexibilities of the user-specified feed and product stream information permit modeling cross-current and batch processes as well. To model other types of equipment, such as pulsed columns, the user must have good information about the equivalent number of perfect stages represented by the column(s).

Applications are limited, to a certain degree, by the range of conditions for which distribution coefficient data are available. The empirical distribution coefficient models used in Version 2.11 were generated from a large population of laboratory distribution data^{5,11,12} covering the ranges shown in Table 3.

Table 3. Range of conditions for distribution coefficient data correlations

Process	HNO ₃ (M)	Uranium (g/L)	Plutonium (g/L)	Thorium (g/L)	TBP (%)	Temperature (°C)
Purex	0.0-5.0	0-200	0-100	—	10-30	10-40
Thorex	0.0-3.0	0-20	—	0-150	~30	15-70

3.2 CREATING PROBLEM DEFINITION FILES

Problem Definition files are created through the use of the SEPREP.EXE program, which can be run directly or invoked from the menu program SEPHIS.EXE. These files are created either on a diskette supplied by the user or on the user's hard disk. The contents of a Problem Definition file are as shown in Table 4. The SEPREP.EXE program prompts the user for all process and flow sheet information necessary to perform the calculations. On completion of problem definition, the user has the option of obtaining a hard-copy printout of the problem. Details for running this program are given in Sect. 6.

Table 4. Contents of a problem definition file

Data identification	
<u>General information</u>	
Date of problem preparation	
Time of problem preparation	
Problem title	
Number of stages	
Volume fraction of TBP	
Default temperature, °C	
Stage connection index	
Exit stage for organic (special routing)	
Entrance stage for organic (special routing)	
Pu reaction index	
Process index	
Time increment, min	
Time between printings, min	
Time to stop, min	
Tolerance (inventory change), %/min	
Index for extra products	
Index for mixer volume data	
Index for settler volume data	
Index for initial concentration profile data	
Integration technique index	
<u>Definition of each feed stream</u>	
(Purex process)	(Thorex process)
Stage number	Stage number
Index for type of stream	Index for type of stream
Feed rate, L/min	Feed rate, L/min
Acid concentration, <i>M</i>	Acid concentration, <i>M</i>
U concentration, g/L	U concentration, g/L
Pu(IV) concentration, g/L	Th concentration, g/L
Pu(III) concentration, g/L	Nitrate concentration, <i>M</i>
Reductant concentration, <i>M</i>	Feed temperature, °C
Nitrate concentration, <i>M</i>	Index for more streams
Feed temperature, °C	
Index for more streams	

Table 4. Contents of a problem definition file
(continued)

Data identification	
<u>Definition of extra products</u>	
Stage number	
Index for type of stream	
Product flow rate, L/min	
Index for more streams	
<u>Aqueous initial profile</u>	
(Purex process)	(Thorex process)
Acid concentration, <i>M</i>	Acid concentration, <i>M</i>
U concentration, g/L	U concentration, g/L
Pu(IV) concentration, g/L	Th concentration, g/L
Pu(III) concentration, g/L	Nitrate concentration, <i>M</i>
Reductant concentration, <i>M</i>	Temperature °C
Nitrate concentration, <i>M</i>	
Temperature, °C	
<u>Organic initial profile</u>	
(Purex process)	(Thorex process)
Acid concentration, <i>M</i>	Acid concentration, <i>M</i>
U concentration, g/L	U concentration, g/L
Pu(IV) concentration, g/L	Th concentration, g/L
<u>Mixer volume data</u>	
Stage number	
Aqueous volume, L	
Organic volume, L	
Index for more data	
<u>Settler volume data</u>	
Stage number	
Aqueous volume, L	
Organic volume, L	
Index for more data	

3.3 CALCULATING DEFINED PROBLEMS

The SECALC.EXE program performs all problem computations. It can be run directly or can be invoked from the menu program SEPHIS.EXE. The program uses a previously prepared Problem Definition file supplied on a diskette or on the hard disk and produces a Problem Results file on that disk medium. In the course of performing calculations, the program writes data to a scratch file on the diskette or hard disk that is then erased after the Problem Results file is created.

A screen display shows the status of operation. Initially, statements appear that indicate the status of problem setup (definition of feed streams, stage volumes, initial concentration profile, and others). The course of calculations is then monitored by showing time increments and stage numbers being calculated, as well as the largest inventory change (per minute) of a solute in a stage of the cascade. Finally, the screen display in the form of bar graphs shows the approach to steady-state conditions for all extracting solutes.

Calculations proceed for successive time increments until the maximum time allotment is met (as specified in the Problem Definition file) or until steady-state conditions are attained. In addition, by pressing any key on the PC keyboard, the user can abort the job at any time. If the job is stopped prematurely, or has reached the maximum time allowed, the user is given the option of continuing calculations for more time.

Hard-copy printouts of results are managed by this program and are provided at discrete times (as directed by the Problem Definition file) and whenever the job is stopped for any reason.

At the end of a computation job, the Problem Results file is created on the diskette or hard disk. The contents of this file are as shown in Table 5. Details for running this program are given in Sect. 6.

3.4 RETRIEVING RESULTS OF PAST PROBLEMS

The SEPRNT.EXE program can be run directly or can be invoked from the menu program SEPHIS.EXE. This program is used to obtain hard-copy printouts of past problems without the necessity of rerunning those problems. It must have available both the Problem Definition and the Problem Results files created previously on a diskette or on the hard disk. Details for running this program are given in Sect. 6.

Table 5. Contents of a problem results file

Data identification	
Problem title	
Date of calculations	
Time calculations begin	
Process run time, min	
<u>Concentration profile, each stage</u>	
(Purex process)	(Thorex process)
Stage number	Stage number
Aqueous acid concentration, <i>M</i>	Aqueous acid concentration, <i>M</i>
Aqueous U concentration, g/L	Aqueous U concentration, g/L
Aqueous Pu(IV) concentration, g/L	Aqueous Th concentration, g/L
Organic acid concentration, <i>M</i>	Organic acid concentration, <i>M</i>
Organic U concentration, g/L	Organic U concentration, g/L
Organic Pu(IV) concentration, g/L	Organic Th concentration, g/L
Aqueous Pu(III) concentration, g/L	Nitrate concentration, <i>M</i>
Aqueous reductant concentration, <i>M</i>	Aqueous flow rate, L/min
Aqueous nitrate concentration, <i>M</i>	Temperature, °C
Aqueous density, g/mL (Density data are at 25°C)	U extraction factor
Aqueous flow rate, L/min	Th extraction factor
Temperature, °C	Acid extraction factor
U extraction factor	Organic flow rate, L/min
Pu extraction factor	TBP saturation, %
Acid extraction factor	Maximum inventory change, %/min
Organic density, g/mL (Density data are at 25°C)	Time calculations stop
Organic flow rate, L/min	
TBP saturation, %	
Maximum inventory change, %/min	
Time calculations stop	
<u>Component material balances for the final time increments (up to 1000 min)</u>	
Process time, min	
Acid balance, %	
U balance, %	
Pu or Th balance, %	

4. ADVANTAGES OF VERSION 2.11

Compared to the original SEPHIS MOD4 model, Version 2.11 offers many improvements. The most important advantage is the ability to operate the programs on a PC with extensive user-oriented aids. The design of the various screen displays assists the user in providing input data in the correct form and in the proper sequence. After all requested information for a given display is completed, the user is given a chance to go back and correct that display before the data enter the computational routines.

An even more useful screen display appears while the calculations are being made. The continuous display of time increment and stage number, the automatically updated display of maximum inventory change per minute, and the bar-graph display of approach to steady-state conditions permit the user to monitor the transient approach to steady-state and stop calculations, if desired, at any time.

Another important advantage of the Version 2.11 programs is that they provide separate Problem Definition and Problem Results files for each job, which can be retained for other uses. These files are in an ASCII format and can be imported by other software, such as graphics programs or spreadsheets.

A new numerical integration technique (called Fast) has been developed since the publication of the original SEPHIS MOD4 model and is incorporated in Version 2.11. Although a little slower than the Trapezoidal technique for equivalent integration time increments, the Fast technique will function with large time increments and provide steady-state results at a rapid rate. This technique may produce a somewhat different plutonium reduction profile because of the way chemical effects are handled, but it is the only recommended method for obtaining transient results whenever plutonium reduction is occurring.

The correlation of Purex process distribution coefficient data has been further improved since the original SEPHIS MOD4 model and this correlation is incorporated in Version 2.11.

The mathematical description for the reduction of Pu(IV) by HAN has been improved in Version 2.11, eliminating the oscillations occasionally encountered in previous versions.

Calculations for estimates of aqueous- and organic-phase densities that appear in the printout of results have been corrected. The data are valid at a temperature of 25°C.

These programs retain all features and improvements used in the original SEPHIS MOD4 model and exhibit the same accuracy of calculations. Although written in the BASIC language, the programs have been compiled into .EXE files by using Microsoft's QuickBASIC, Version 4.0. Consequently, they operate quickly and efficiently on many PC systems.

5. HARDWARE REQUIREMENTS

Minimum PC hardware requirements are an IBM PC-XT or equivalent compatible (with 640-K RAM, two 360-K floppy disk drives or one 360-K floppy disk drive and an installed hard disk, and a math coprocessor chip) and a dot-matrix printer. Enhanced computational speed can be achieved with systems that operate at 8-MHz clock speed or higher. A 16-MHz (or faster) system with a 32-bit (80386) processor is ideal. On fast machines, a math coprocessor chip is not essential.

A color monitor is not required since color is not supported by the programs. To take full advantage of the hard-copy printout features, the dot-matrix printer should be configured to use the IBM character set.

6. USING THE MODEL

6.1 FIRST-TIME USAGE

As with any computer software, the user should prepare a backup copy of the distribution diskette for use and should store the original copy in a secure location. There are several options available for using these programs, as shown in Table 6. The choice will depend on the user's equipment and individual needs.

Table 6. Options for program usage

Location (drive) for:	
Program files	Data files
A\	B\
A\	C:\Subdir\
B\	A\
B\	C:\Subdir\
C:\Subdir\	A\
C:\Subdir\	B\
C:\Subdir\	C:\Subdir\

If the programs are to be run from an installed hard disk, the files on the distribution diskette should be directly copied to the hard disk. It is suggested that a special subdirectory be created on the hard disk for these programs (for example, C:\SEPHIS). To take full advantage of the hard-copy printout routines, the printer should be configured to use the IBM character set.

6.2 BEFORE STARTING

Before starting the SEPHIS MOD4, Version 2.11 programs, the user should have available an empty, formatted diskette or an appropriate subdirectory (C:\Subdir\) created on the installed hard disk. This can be the same subdirectory as that used for the programs, if desired. The programs will write Problem Definition and Problem Results files in that location. For diskettes, it is suggested that a separate diskette be used for each problem until it is determined that file sizes are sufficiently small to enable several problems to be stored on a diskette. In the course of performing calculations, the program will write data to a scratch file on the diskette or hard disk;

this file is erased at the end of the program after the Problem Results file is prepared. Since problems vary in length, the scratch file can become quite large. Only problems with a specified time to stop which are greatly in excess of 5000 min have resulted in a scratch file that exceeded the capacity of a 360-K diskette. It is generally safe to include up to six problems on a single diskette.

Before running the programs, the user should also have readily available all of the input data that will be requested. The necessary input information is described in Sect. 6.3.2.

6.3 HOW TO OPERATE

6.3.1 Program SEPHIS.EXE

Program SEPHIS.EXE is the menu program. The computer screen will display the menu and the user will be requested to select one of four options. Enter 1 to define a problem, 2 to run a problem, or 3 to print a problem. Note that to run a problem, the problem must first be defined by using option 1. Option 3 is used to obtain a new hard-copy printout of a previously run problem. The fourth option is to enter 0. This terminates the program and returns the computer to system status.

6.3.2 Program SEPREP.EXE

Normally, the program SEPHIS.EXE is run to obtain the beginning title screen and menu for the set of programs. The choice of option 1 from the menu invokes the program SEPREP.EXE. Alternatively, SEPREP.EXE can be started directly. The user will be asked if the Problem Definition file is to be created on a diskette, and if so, will be requested to insert the diskette.

A series of screen displays will prompt the user for process flow sheet and equipment information. When providing the requested information, the user should remember that stages are numbered following the flow of the heaviest phase (aqueous), or from the top down if one views the cascade as a pulsed column.

Initial Screen

The information on the first screen is requested in the following order:

1. Problem Title. Enter a title for the problem to be solved. **Do not use commas.** Limit the length to 60 characters.
2. Name of Process. Enter 0 for the Purex process; 1 for Thorex.
3. Number of Stages. Enter the number of stages as a whole number (up to 100).
4. TBP Content of the Solvent. Enter the TBP content as ##.# volume %.
5. Initial or Default Temperature. Enter the temperature as ##.# °C.

6. Unusual Stage Connections. Enter 0 if none, or 1 for special routing. Special routing is defined as the case where all of the organic phase leaving a particular stage is routed to some other stage. If a 1 is entered, two additional entries will be requested; the number of the stage from which organic is taken and the number of the stage to which it is returned.
7. Plutonium Reaction. Enter 0 for none, 1 for instantaneous reduction of Pu(IV), 2 for reduction of Pu(IV) by U(IV), or 3 for reduction of Pu(IV) by HAN. This request does not appear if the Thorex process is specified.
8. Time Increment. Specify a time increment for integrations (in minutes) that is <25% of the mean stage solution residence time if accurate results are desired for transient conditions; otherwise a good choice is 1.00 min. Enter the value as #.##. Hint: A multiple of the time increment should exactly equal the time between printing of results (specified in Item 9 that follows). For example, a time increment of 0.13 min will not permit results to be printed at 10 min, but a time increment of 0.125 min will allow a 10-min printing of results ($10/0.13 = 76.9$, not an even multiple).
9. Time Between Printing of Results. Enter the time interval (in minutes) at where results are to be printed. Remember that results will always be printed at the end of a job. This request allows more frequent printouts to be obtained. Enter the value as a whole number.
10. Time When Calculations Will Stop. Enter the maximum time (in minutes) that the job should run. It is generally wise to limit this value to 5000 min when data files are written to a diskette, to prevent exceeding diskette capacity for the scratch file. This time specification will terminate calculations if steady-state is not attained first or if the user does not abort the job prematurely. Enter the value as a whole number.
11. Tolerance for Steady State. An attainment of steady-state is assumed whenever the inventory change per minute of any solute in any stage is less than the user-defined tolerance. The tolerance should be set as low as possible without unduly adding to computation time. It is expressed as percentage inventory change per minute and is entered as #.####. Although values as low as 0.0001 are used frequently, values of 0.0010 provide essentially equivalent results.
12. Mixer Volume Index. Enter 1 if mixer volumes are to be defined for each phase, 2 if only total mixer volumes are defined, or 3 if volumes will be equal to phase flow multiplied by unit time.
13. Settler Volume Index. Enter 1 if settler volumes are to be defined for each phase, 2 if only total settler volumes are defined, or 3 if volumes will be equal to phase flow multiplied by unit time.
14. Initial Concentration Profile Index. Enter 0 if the initial concentration profile is 0, 1 if it is to be defined, or 2 if the profile is the result of a previous calculation.
15. Integration Technique Index. Enter 0 for the Runge-Kutta technique, 1 for the Trapezoidal technique, or 2 for the new, Fast technique. Refer to Table 2 when making choices.

16. Extra Product Stream Index. Enter 1 to indicate extra product streams, or 0 for none. Extra product streams are defined as those in addition to the normal product streams from the ends of a cascade of contactors.
17. Specification of Problem Definition File. A drive specification (path) and filename for the Problem Definition file must be entered. Examples are **B:\xxxxxxx** and **C:\Subdir\xxxxxxx** where up to eight characters (x) can represent a personalized filename. Only certain characters are allowed (using the standard DOS file naming convention). Do not add an extension to the filename since the program will automatically add .DAT to the filename to designate it as a data file.

This completes the information requested on the first screen. At this point, if any mistakes were made, the user is given the option of returning to Item 1, Problem Title.

Feed Stream Screens

The next set of screens will request information concerning feed streams. Information is provided in the following order:

1. Stage Number for Feed. Enter the stage number for a feed stream as a whole number.
 2. Type of Feed. Enter 1 for an aqueous stream, or 0 for an organic stream.
 3. Flow Rate. Enter the feed stream flow rate in L/min as ###.###.
 4. Nitric Acid Concentration. Enter the feed stream nitric acid concentration in molar units as ##.###.
 5. Uranium Concentration. Enter the feed stream uranium concentration in g/L as ###.###.
 6. (Purex). Plutonium (IV) Concentration. Enter the feed stream Plutonium (IV) concentration in g/L as ###.###
- or
- (Thorex). Thorium Concentration. Enter the feed stream Thorium concentration in g/L as ###.###.
7. (Purex, aqueous feed only). Plutonium (III) Concentration. Enter the aqueous feed stream Plutonium (III) concentration in g/L as ###.###.
 8. (Purex, aqueous feed only). Plutonium Reductant Concentration. Enter the plutonium reductant concentration in molar units as ##.###.
 9. (Aqueous feed only). Inextractable Nitrate Ion Concentration. Enter the inextractable nitrate ion concentration in molar units as ##.###.
 10. Feed Temperature. Enter the feed stream temperature in °C as ##.#. If the default temperature applies, enter 0.

This completes the information requested on this screen. At this point, if any mistakes were made, the user is given the option of returning to Item 1, Stage Number For Feed. The user is then asked if there is another feed stream. If so, the sequence is repeated for the next feed stream.

Extra Product Stream Screens

If extra product streams were indicated on the initial screen, the next set of screens will request information concerning these product streams. Information is provided in the following order:

1. Stage Number for Product. Enter the stage number for an extra product stream (a whole number).
2. Type of Product. Enter 1 for an aqueous stream, or 0 for an organic stream.
3. Flow Rate. Enter the product stream flow rate in L/min as ###.###.

This completes the information requested on the screen. If any mistakes were made, the user is given the option of returning to Item 1, Stage Number For Product. The user is then asked if there is another product stream. If so, the sequence is repeated for the next product stream.

Initial Concentration Profile Screens

If indications were made on the initial screen that the initial concentration profile is to be defined, the next set of screens will request information concerning that profile. The first screen(s) concern the aqueous-phase concentrations in each stage. The user will be asked to supply concentration data in the following order for each stage, beginning with Stage 1. The screen will show data for up to 17 stages. A new screen chart will appear, if required, for another 17 stages.

1. Nitric Acid Concentration. Enter the aqueous nitric acid concentration in molar units as ##.###.
2. Uranium Concentration. Enter the aqueous uranium concentration in g/L as ###.###.
3. (Purex). Plutonium (IV) Concentration. Enter the aqueous Plutonium (IV) concentration in g/L as ###.###
or
(Thorex). Thorium Concentration. Enter the aqueous Thorium concentration in g/L as ###.###.
4. (Purex). Plutonium (III) Concentration. Enter the aqueous Plutonium (III) concentration in g/L as ###.###.
5. (Purex). Plutonium Reductant Concentration. Enter the aqueous plutonium reductant concentration in molar units as ##.###.

6. Inextractable Nitrate Ion Concentration. Enter the aqueous nitrate ion concentration in molar units as ##.###.
7. Temperature. Enter the stage temperature in °C as ##.#. If the default temperature applies, enter 0.

This completes the information requested for the aqueous profile. The next screen(s) concern the organic-phase concentrations in each stage. The user will be asked to supply concentration data in the following order for each stage, beginning with Stage 1. The screen will show data for up to 17 stages. A new screen chart will appear, if required, for another 17 stages.

1. Nitric Acid Concentration. Enter the organic nitric acid concentration in molar units as ##.###.
2. Uranium Concentration. Enter the organic uranium concentration in g/L as ###.###.
3. (Purex). Plutonium (IV) Concentration. Enter the organic Plutonium (IV) concentration in g/L as ###.###

or

(Thorex). Thorium Concentration. Enter the organic Thorium concentration in g/L as ###.###.

This completes the information requested for the organic profile. If indications were made on the initial screen that the initial concentration profile is the result of a previous calculation, the user will be asked to enter a drive specification (path) and filename for the file that contains those data. If necessary, diskettes can be exchanged to access the data. If a diskette is removed, the user is given an opportunity to replace it after the profile data are read. There is a short waiting period, during which the concentration profile is read from the file.

Mixer Volume Definition Screen

If indications were made on the initial screen that mixer phase volumes or mixer total volumes will be defined, that information is requested on the next set of screens. Each screen chart will accommodate 34 sets of mixer volume data. After providing data for Stage 1, data entries need be made only for stages where the volume(s) change. The data must be entered in the order of increasing stage number. Information is requested in the order that follows:

1. Stage Number. Enter the stage number for which volumes will be given. Stage 1 must be entered first.
2. Aqueous Mixer Volume. Enter the aqueous-phase volume in L as ###.### if phase volumes are to be defined.
3. Organic Mixer Volume. Enter the organic-phase volume in L as ###.### if phase volumes are to be defined.
4. Total Mixer Volume. Enter the total mixer volume in L as ###.### if only total volumes are to be defined.

The user is then asked if volumes are to be defined for another stage. If so, the sequence is repeated for the next stage.

Settler Volume Definition Screen

If indications were made on the initial screen that settler phase volumes or settler total volumes will be defined, that information is requested on the next set of screens. Each screen chart will accommodate 34 sets of settler volume data. After providing data for Stage 1, data entries need be made only for stages where the volume(s) change. The data must be entered in the order of increasing stage number. Information is requested in the order that follows:

1. Stage Number. Enter the stage number for which volumes will be given. Stage 1 must be entered first.
2. Aqueous Settler Volume. Enter the aqueous-phase volume in L as ###.### if phase volumes are to be defined.
3. Organic Settler Volume. Enter the organic-phase volume in L as ###.### if phase volumes are to be defined.
4. Total Settler Volume. Enter the total settler volume in L as ###.### if only total volumes are to be defined.

The user is then asked if volumes are to be defined for another stage. If so, the sequence is repeated for the next stage.

Printout Requirements Screen

Finally, the user is asked if a hard-copy printout of the problem definition is desired. If so, a reminder to prepare the printer appears on the screen and the printout is prepared. Note that the printer should be configured to use the IBM character set.

The program terminates after preparing the Problem Definition file on the diskette or on the hard disk. The menu screen will reappear following termination of this program.

6.3.3 Program SECALC.EXE

Normally, the program SEPHIS.EXE is run to obtain the beginning title screen and menu for the set of programs. The choice of option 2 from the menu invokes the program SECALC.EXE. Alternatively, SECALC.EXE can be started directly. The user will be asked if the Problem Definition file is located on a diskette, and if so, will be requested to insert the diskette.

Two file specifications must now be entered. The first one requested is the drive specification (path) and filename for the Problem Definition file. It should take the form B:\xxxxxxx or C:\Subdir\xxxxxxx and conform to the filename established when the file was prepared. Do not include the extension .DAT since the program will automatically assume it is a data file. The second file specification will name the Problem Results file that will be prepared by SECALC.EXE. It should take the same general form as the Problem Definition filename. Examples of Problem Definition and Problem Results file specifications may be B:\PROB_DEF and B:\PROB_RES or C:\Subdir\PROB_DEF and C:\Subdir\PROB_RES.

A reminder to prepare the printer then appears on the screen and problem calculations proceed. The user will now see a status screen that permits the course of the calculations to be monitored. Calculations can be stopped prematurely merely by touching any key. Otherwise, calculations will continue until steady-state conditions are attained, or until the maximum time limitation specified by the Problem Definition file is reached.

Hard-copy printouts of results will be prepared at the time intervals specified by the Problem Definition file and at any termination of calculations.

When calculations are terminated prematurely (by pressing any key), the user is asked if calculations should continue for more time. If the answer is in the affirmative, calculations will continue as before, stopping only if a key is pressed, if the maximum time is reached, or on attainment of steady state. A negative answer terminates the program.

When calculations are stopped because the maximum time was reached, the user is also asked if calculations should continue for more time. If the answer is in the affirmative, the maximum time will be set at twice the original value. Calculations will continue as before, stopping only if a key is pressed, if the new maximum time is reached, or upon attainment of steady state. A negative answer terminates the program.

When calculations are stopped because steady-state conditions are attained (i.e., the user-defined tolerance is met), the program terminates.

At program termination the Problem Results file is prepared on the diskette or on the hard disk and the scratch file is erased. The menu screen will reappear following termination of this program.

6.3.4 Program SEPRNT.EXE

Normally, the program SEPHIS.EXE is run to obtain the beginning title screen and menu for the set of programs. The choice of option 3 from the menu invokes the program SEPRNT.EXE. Alternatively, SEPRNT.EXE can be started directly. The user will be asked if the Problem Definition and Problem Results files are located on a diskette, and if so, will be requested to insert the diskette.

Two file specifications must now be entered. The first one requested is that for the Problem Definition file. It should take the form `B:\xxxxxxx` or `C:\Subdir\xxxxxxx` and conform to the filename established when the file was prepared. The second file specification is that for the Problem Results file. It should take the same general form and conform to the filename established when the file was prepared. Do not include the extension `.DAT`, since the program will automatically assume these are data files.

A reminder to prepare the printer appears on the screen and the hard-copy printout is prepared. The program then terminates.

The menu screen will reappear following termination of this program.

7. SAMPLE PROBLEMS

The seven sample problems described in this section were first run by using earlier versions of the SEPHIS model, which required a mainframe computer. Although the computational times shown were very short (a few seconds), operation through the mainframe required the transportation of punched card input information and printed output information to and from the computing center. The total turnaround time for a job frequently took as much as 2 d. With today's use of PCs and modems to invoke mainframe computations, the turnaround time is admittedly much shorter, but transportation of printed output continues to be a limiting factor. Output files from mainframe calculations usually are available in a few hours, and printout information is received in 1 d or less. The computation times given for the same seven sample problems, run by using SEPHIS MOD4, Version 2.11, on a PC, range in the order of minutes. No add-on time for transporting data applies.

7.1 COEXTRACTION CONTACTOR

This first sample problem is for an 11-stage coextraction contactor employing a dilute (15.3% TBP) flow sheet for the extraction of uranium and plutonium, as shown in Fig. 1. Only the steady-state concentration profile is needed, so stage volume or initial profile information is unnecessary. The printout that follows Fig. 1 shows the final expected concentration profile.

The problem was previously calculated by using SEPHIS MOD1 and SEPHIS MOD3 on mainframe computers.^{1,4} Computation times were ~16 s for SEPHIS MOD1 on the Oak Ridge National Laboratory (ORNL) IBM System 360 and ~4 s for SEPHIS MOD3 on the ORNL IBM 360/91. These computer runs only carried the process through a 99.9% overall material balance. The computation time for SEPHIS MOD4, Version 2.11, on an IBM PC/XT without any upgrade features was ~6 min.

The use of an updated system (16-MHz with 32-bit processor) to carry the process to a tolerance of 0.0001% inventory change per minute resulted in a computation time of 1 min 51 sec. Note that the tolerance was not met within the maximum time specification of 200 min. The extra-time option was invoked to continue the process for an additional 56 min.

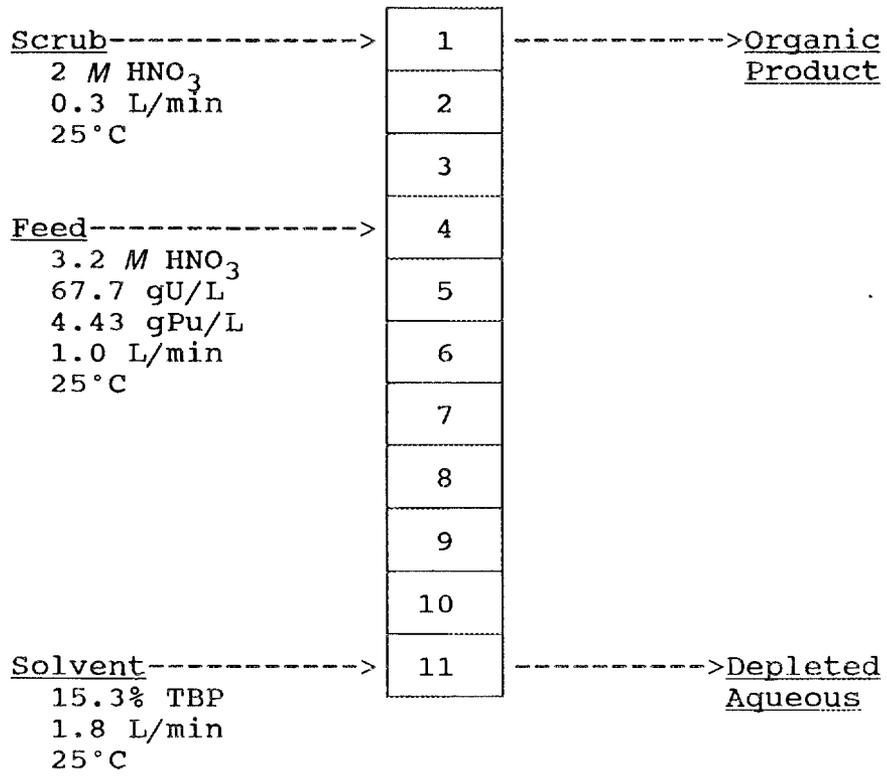


Fig. 1. Coextraction contactor.

PROBLEM DEFINITION DATA FOR SEPHIS MOD4, Ver. 2.11:

02-05-1990 11:23

Problem: Ex. 1 - ORNL-4746 - Coextraction

PUREX PROCESS

Total stages: 11

Volume % TBP in solvent: 15.3

Initial or default temperature (°C): 25.0

No unusual stage connections

No Plutonium reaction.

Minutes per time increment: 1.00

Minutes between printing of the concentration profile: 200

Calculations will stop after 200 minutes or when a tolerance of 0.0001 % per minute is reached.

Mixer volumes = (phase flow)(unit time).

Settler volumes = (phase flow)(unit time).

Initial concentration profile is zero.

Trapezoidal integration will be used.

No extra product streams.

The FILESPEC for this Problem Definition data file is: B:EX_01P.DAT

The FILESPEC for this Problem Results data file is: B:EX_01R.DAT

FEED AND PRODUCT STREAM DATA:

	STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	FLOW RATE (L/min)	TEMP (C)
AQUEOUS	1	2.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.00E-01	25.0
AQUEOUS	4	3.20E+00	6.77E+01	4.43E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	25.0
15.3 % TBP	11	0.00E+00	0.00E+00	0.00E+00				1.80E+00	25.0

STAGE VOLUME AND FLOW RATE DATA (Molal basis):

STAGE NO.	MIXER VOLUME BY PHASE		SETTLER VOLUME BY PHASE		MIXER FLOW RATE		INTERSTAGE FLOW RATE	
	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC
1	2.81E-01	1.79E+00	2.81E-01	1.79E+00	2.81E-01	1.79E+00	2.81E-01	1.79E+00
2	2.81E-01	1.79E+00	2.81E-01	1.79E+00	2.81E-01	1.79E+00	2.81E-01	1.79E+00
3	2.81E-01	1.79E+00	2.81E-01	1.79E+00	2.81E-01	1.79E+00	2.81E-01	1.79E+00
4	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00
5	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00
6	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00
7	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00
8	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00
9	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00
10	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00
11	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00	1.16E+00	1.79E+00

PROBLEM RESULTS FOR SEPHIS MOD4, Ver. 2.11:

06-08-1990 09:12

Problem: Ex. 1 - ORNL-4746 - Coextraction
(mixer concentrations shown)

TIME = 0.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	2.81E-01	25.0
2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	2.81E-01	25.0
3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	2.81E-01	25.0
4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.16E+00	25.0
5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.16E+00	25.0
6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.16E+00	25.0
7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.16E+00	25.0
8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.16E+00	25.0
9	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.16E+00	25.0
10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.16E+00	25.0
11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.16E+00	25.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.84E-01	1.80E+00	0.0	2.00E+02
2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.84E-01	1.80E+00	0.0	2.00E+02
3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.84E-01	1.80E+00	0.0	2.00E+02
4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.84E-01	1.80E+00	0.0	2.00E+02
5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.84E-01	1.80E+00	0.0	2.00E+02
6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.84E-01	1.80E+00	0.0	2.00E+02
7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.84E-01	1.80E+00	0.0	2.00E+02
8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.84E-01	1.80E+00	0.0	2.00E+02
9	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.84E-01	1.80E+00	0.0	2.00E+02
10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.84E-01	1.80E+00	0.0	2.00E+02
11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.84E-01	1.80E+00	0.0	2.00E+02

TIME = 200.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	1.94E+00	1.69E+01	3.73E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	3.02E-01	25.0
2	1.98E+00	2.15E+01	5.43E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	3.03E-01	25.0
3	2.23E+00	2.07E+01	5.37E+00	0.00E+00	0.00E+00	0.00E+00	1.11E+00	3.05E-01	25.0
4	3.25E+00	1.58E+01	3.31E+00	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.30E+00	25.0
5	3.36E+00	9.29E-01	5.03E-01	0.00E+00	0.00E+00	0.00E+00	1.11E+00	1.29E+00	25.0
6	3.37E+00	3.75E-02	5.25E-02	0.00E+00	0.00E+00	0.00E+00	1.11E+00	1.29E+00	25.0
7	3.37E+00	1.47E-03	5.34E-03	0.00E+00	0.00E+00	0.00E+00	1.11E+00	1.29E+00	25.0
8	3.37E+00	5.79E-05	5.42E-04	0.00E+00	0.00E+00	0.00E+00	1.11E+00	1.29E+00	25.0
9	3.36E+00	2.28E-06	5.52E-05	0.00E+00	0.00E+00	0.00E+00	1.11E+00	1.29E+00	25.0
10	3.30E+00	9.07E-08	5.72E-06	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.29E+00	25.0

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
11	2.86E+00	3.95E-09	6.69E-07	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.27E+00	25.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	9.01E-02	3.69E+01	2.42E+00	1.33E+01	3.94E+00	2.82E-01	8.39E-01	1.83E+00	75.3	3.02E-04
2	8.22E-02	3.97E+01	3.03E+00	1.12E+01	3.38E+00	2.51E-01	8.44E-01	1.84E+00	78.9	3.10E-04
3	9.06E-02	4.04E+01	3.31E+00	1.17E+01	3.70E+00	2.44E-01	8.45E-01	1.84E+00	81.9	3.19E-04
4	1.34E-01	4.02E+01	3.30E+00	3.62E+00	1.41E+00	5.83E-02	8.46E-01	1.84E+00	89.4	3.56E-04
5	3.16E-01	1.12E+01	2.34E+00	1.70E+01	6.59E+00	1.33E-01	8.11E-01	1.83E+00	76.8	4.70E-04
6	3.90E-01	6.58E-01	3.56E-01	2.48E+01	9.59E+00	1.64E-01	7.96E-01	1.83E+00	71.3	6.23E-04
7	3.96E-01	2.65E-02	3.71E-02	2.54E+01	9.83E+00	1.66E-01	7.95E-01	1.83E+00	70.9	7.00E-04
8	3.96E-01	1.04E-03	3.78E-03	2.55E+01	9.85E+00	1.66E-01	7.95E-01	1.83E+00	70.9	7.91E-04
9	3.95E-01	4.10E-05	3.83E-04	2.54E+01	9.81E+00	1.66E-01	7.95E-01	1.83E+00	70.7	8.84E-04
10	3.89E-01	1.61E-06	3.86E-05	2.51E+01	9.55E+00	1.67E-01	7.95E-01	1.83E+00	69.6	0.00E+00
11	3.40E-01	6.15E-08	3.58E-06	2.23E+01	7.68E+00	1.71E-01	7.94E-01	1.82E+00	60.8	0.00E+00

TIME = 256.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	1.94E+00	1.69E+01	3.73E+00	0.00E+00	0.00E+00	0.00E+00	1.09E+00	3.02E-01	25.0
2	1.98E+00	2.15E+01	5.43E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	3.03E-01	25.0
3	2.23E+00	2.07E+01	5.37E+00	0.00E+00	0.00E+00	0.00E+00	1.11E+00	3.05E-01	25.0
4	3.25E+00	1.58E+01	3.31E+00	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.30E+00	25.0
5	3.36E+00	9.29E-01	5.03E-01	0.00E+00	0.00E+00	0.00E+00	1.11E+00	1.29E+00	25.0
6	3.37E+00	3.75E-02	5.25E-02	0.00E+00	0.00E+00	0.00E+00	1.11E+00	1.29E+00	25.0
7	3.37E+00	1.48E-03	5.34E-03	0.00E+00	0.00E+00	0.00E+00	1.11E+00	1.29E+00	25.0
8	3.37E+00	5.79E-05	5.42E-04	0.00E+00	0.00E+00	0.00E+00	1.11E+00	1.29E+00	25.0
9	3.36E+00	2.28E-06	5.52E-05	0.00E+00	0.00E+00	0.00E+00	1.11E+00	1.29E+00	25.0
10	3.30E+00	9.08E-08	5.72E-06	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.29E+00	25.0
11	2.86E+00	3.95E-09	6.69E-07	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.27E+00	25.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	9.01E-02	3.69E+01	2.42E+00	1.33E+01	3.94E+00	2.82E-01	8.39E-01	1.83E+00	75.3	3.78E-05
2	8.22E-02	3.97E+01	3.03E+00	1.12E+01	3.38E+00	2.51E-01	8.44E-01	1.84E+00	78.9	3.61E-05
3	9.06E-02	4.04E+01	3.31E+00	1.17E+01	3.70E+00	2.44E-01	8.45E-01	1.84E+00	81.9	3.73E-05
4	1.34E-01	4.02E+01	3.30E+00	3.62E+00	1.41E+00	5.83E-02	8.46E-01	1.84E+00	89.4	3.40E-05
5	3.16E-01	1.12E+01	2.34E+00	1.70E+01	6.58E+00	1.33E-01	8.11E-01	1.83E+00	76.9	5.89E-05
6	3.90E-01	6.58E-01	3.56E-01	2.48E+01	9.59E+00	1.64E-01	7.96E-01	1.83E+00	71.3	6.92E-05
7	3.96E-01	2.65E-02	3.72E-02	2.54E+01	9.83E+00	1.66E-01	7.95E-01	1.83E+00	70.9	8.31E-05
8	3.96E-01	1.04E-03	3.78E-03	2.55E+01	9.85E+00	1.66E-01	7.95E-01	1.83E+00	70.9	9.03E-05
9	3.95E-01	4.10E-05	3.83E-04	2.54E+01	9.81E+00	1.66E-01	7.95E-01	1.83E+00	70.7	9.76E-05
10	3.89E-01	1.61E-06	3.86E-05	2.51E+01	9.55E+00	1.67E-01	7.95E-01	1.83E+00	69.6	0.00E+00
11	3.40E-01	6.15E-08	3.58E-06	2.23E+01	7.68E+00	1.71E-01	7.94E-01	1.82E+00	60.8	0.00E+00

7.2 PLUTONIUM EXTRACTION CONTACTOR

A simple ten-stage plutonium extraction contactor employing a dilute (15.0% TBP) flow sheet, shown in Fig. 2, is used in this example. Only the steady-state concentration profile is needed, so stage volume or initial profile information is unnecessary. The printout that follows Fig. 2 shows the final expected concentration profile.

The problem was previously calculated by using SEPHIS MOD1 and SEPHIS MOD3 on mainframe computers.^{1,4} Computation times were <3 s for SEPHIS MOD1 on the ORNL IBM System 360 and ~1 s for SEPHIS MOD3 on the ORNL IBM 360/91. These computer runs only carried the process through a 99.9% overall material balance. The computation time for SEPHIS MOD4, Version 2.11, on an IBM PC/XT without any upgrade features was ~2.5 min.

The use of an updated system (16-MHz with 32-bit processor) to carry the process to a tolerance of 0.0001% inventory change per minute resulted in a computation time of 1 min 2 s. Note that the tolerance was not met within the maximum time specification of 100 min. The extra-time option was invoked to continue the process for an additional 8 min.

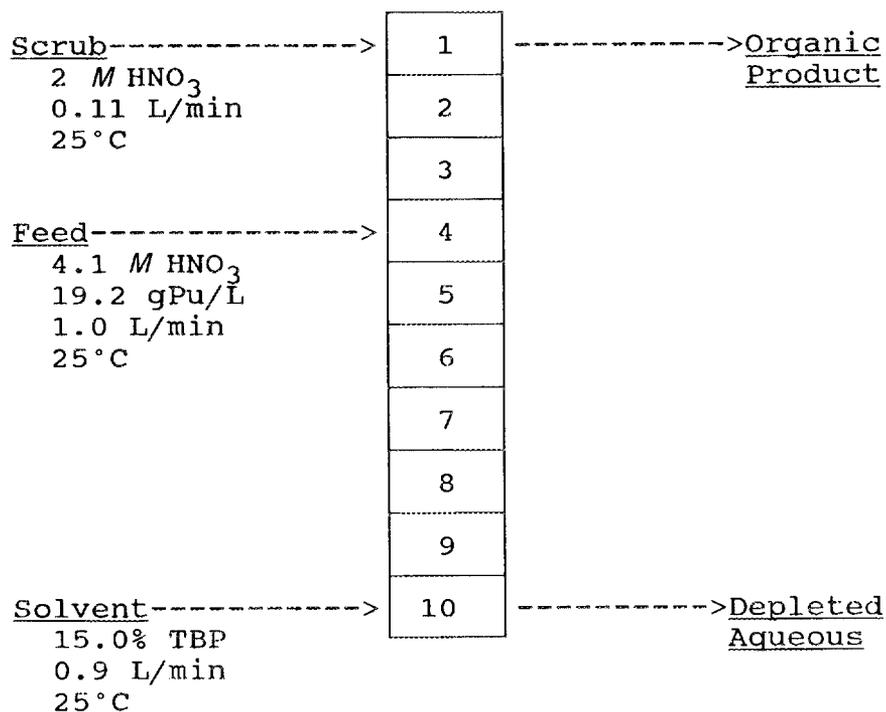


Fig. 2. Plutonium extraction contactor.

PROBLEM DEFINITION DATA FOR SEPHIS MOD4, Ver. 2.11:

02-05-1990 13:00

Problem: Ex. 2 - ORNL-4746 - Pu Extraction

PUREX PROCESS

Total stages: 10

Volume % TBP in solvent: 15.0

Initial or default temperature (°C): 25.0

No unusual stage connections

No Plutonium reaction.

Minutes per time increment: 1.00

Minutes between printing of the concentration profile: 100

Calculations will stop after 100 minutes or when a tolerance of 0.0001 % per minute is reached.

Mixer volumes = (phase flow)(unit time).

Settler volumes = (phase flow)(unit time).

Initial concentration profile is zero.

Trapezoidal integration will be used.

No extra product streams.

The FILESPEC for this Problem Definition data file is: B:EX_02P.DAT

The FILESPEC for this Problem Results data file is: B:EX_02R.DAT

FEED AND PRODUCT STREAM DATA:

	STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE IOM (M)	FLOW RATE (L/min)	TEMP (C)
AQUEOUS	1	2.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.10E-01	25.0
AQUEOUS	4	4.10E+00	0.00E+00	1.92E+01	0.00E+00	0.00E+00	0.00E+00	1.00E+00	25.0
15.0 % TBP	10	0.00E+00	0.00E+00	0.00E+00				9.00E-01	25.0

STAGE VOLUME AND FLOW RATE DATA (Molal basis):

STAGE NO.	MIXER VOLUME BY PHASE		SETTLER VOLUME BY PHASE		MIXER FLOW RATE		INTERSTAGE FLOW RATE	
	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC
1	1.03E-01	8.98E-01	1.03E-01	8.98E-01	1.03E-01	8.98E-01	1.03E-01	8.98E-01
2	1.03E-01	8.98E-01	1.03E-01	8.98E-01	1.03E-01	8.98E-01	1.03E-01	8.98E-01
3	1.03E-01	8.98E-01	1.03E-01	8.98E-01	1.03E-01	8.98E-01	1.03E-01	8.98E-01
4	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01
5	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01
6	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01
7	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01
8	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01
9	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01
10	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01	9.66E-01	8.98E-01

PROBLEM RESULTS FOR SEPHIS MOD4, Ver. 2.11:

06-08-1990 09:20

Problem: Ex. 2 - ORNL-4746 - Pu Extraction
(mixer concentrations shown)

TIME = 0.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.03E-01	25.0
2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.03E-01	25.0
3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.03E-01	25.0
4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	9.66E-01	25.0
5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	9.66E-01	25.0
6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	9.66E-01	25.0
7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	9.66E-01	25.0
8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	9.66E-01	25.0
9	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	9.66E-01	25.0
10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	9.66E-01	25.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.83E-01	9.00E-01	0.0	2.00E+02
2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.83E-01	9.00E-01	0.0	2.00E+02
3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.83E-01	9.00E-01	0.0	2.00E+02
4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.83E-01	9.00E-01	0.0	2.00E+02
5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.83E-01	9.00E-01	0.0	2.00E+02
6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.83E-01	9.00E-01	0.0	2.00E+02
7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.83E-01	9.00E-01	0.0	2.00E+02
8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.83E-01	9.00E-01	0.0	2.00E+02
9	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.83E-01	9.00E-01	0.0	2.00E+02
10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.83E-01	9.00E-01	0.0	2.00E+02

TIME = 100.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	2.16E+00	0.00E+00	1.16E+01	0.00E+00	0.00E+00	0.00E+00	1.08E+00	1.11E-01	25.0
2	2.48E+00	0.00E+00	1.05E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.12E-01	25.0
3	2.98E+00	0.00E+00	7.86E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.14E-01	25.0
4	4.09E+00	0.00E+00	5.20E+00	0.00E+00	0.00E+00	0.00E+00	1.14E+00	1.11E+00	25.0
5	4.13E+00	0.00E+00	8.45E-01	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.11E+00	25.0
6	4.13E+00	0.00E+00	1.17E-01	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.11E+00	25.0
7	4.13E+00	0.00E+00	1.59E-02	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.11E+00	25.0
8	4.13E+00	0.00E+00	2.14E-03	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.11E+00	25.0
9	4.12E+00	0.00E+00	2.85E-04	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.11E+00	25.0
10	3.80E+00	0.00E+00	3.71E-05	0.00E+00	0.00E+00	0.00E+00	1.12E+00	1.09E+00	25.0

ORGANIC PHASE:										
STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.69E-01	0.00E+00	2.09E+01	0.00E+00	1.49E+01	6.43E-01	8.21E-01	9.17E-01	62.8	2.70E-05
2	1.91E-01	0.00E+00	2.23E+01	0.00E+00	1.74E+01	6.30E-01	8.24E-01	9.18E-01	69.0	2.47E-05
3	2.32E-01	0.00E+00	2.22E+01	0.00E+00	2.27E+01	6.27E-01	8.25E-01	9.20E-01	76.2	1.68E-05
4	2.98E-01	0.00E+00	2.18E+01	0.00E+00	3.49E+00	6.06E-02	8.26E-01	9.22E-01	87.8	1.12E-05
5	4.07E-01	0.00E+00	6.28E+00	0.00E+00	6.16E+00	8.17E-02	8.05E-01	9.18E-01	83.9	3.19E-05
6	4.43E-01	0.00E+00	1.02E+00	0.00E+00	7.21E+00	8.88E-02	7.97E-01	9.17E-01	82.5	6.38E-05
7	4.49E-01	0.00E+00	1.42E-01	0.00E+00	7.39E+00	9.00E-02	7.96E-01	9.17E-01	82.3	8.65E-05
8	4.50E-01	0.00E+00	1.91E-02	0.00E+00	7.41E+00	9.01E-02	7.96E-01	9.16E-01	82.2	1.33E-04
9	4.49E-01	0.00E+00	2.54E-03	0.00E+00	7.38E+00	9.04E-02	7.96E-01	9.16E-01	82.0	2.01E-04
10	4.27E-01	0.00E+00	3.00E-04	0.00E+00	6.75E+00	9.38E-02	7.95E-01	9.16E-01	77.9	2.30E-04

TIME = 108.00 MINUTES

AQUEOUS PHASE:										
STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE IDN (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)	
1	2.16E+00	0.00E+00	1.16E+01	0.00E+00	0.00E+00	0.00E+00	1.08E+00	1.11E-01	25.0	
2	2.48E+00	0.00E+00	1.05E+01	0.00E+00	0.00E+00	0.00E+00	1.09E+00	1.12E-01	25.0	
3	2.98E+00	0.00E+00	7.86E+00	0.00E+00	0.00E+00	0.00E+00	1.10E+00	1.14E-01	25.0	
4	4.09E+00	0.00E+00	5.20E+00	0.00E+00	0.00E+00	0.00E+00	1.14E+00	1.11E+00	25.0	
5	4.13E+00	0.00E+00	8.45E-01	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.11E+00	25.0	
6	4.13E+00	0.00E+00	1.17E-01	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.11E+00	25.0	
7	4.13E+00	0.00E+00	1.59E-02	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.11E+00	25.0	
8	4.13E+00	0.00E+00	2.14E-03	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.11E+00	25.0	
9	4.12E+00	0.00E+00	2.85E-04	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.11E+00	25.0	
10	3.80E+00	0.00E+00	3.71E-05	0.00E+00	0.00E+00	0.00E+00	1.12E+00	1.09E+00	25.0	

ORGANIC PHASE:										
STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.69E-01	0.00E+00	2.09E+01	0.00E+00	1.49E+01	6.43E-01	8.21E-01	9.17E-01	62.8	9.14E-06
2	1.91E-01	0.00E+00	2.23E+01	0.00E+00	1.74E+01	6.30E-01	8.24E-01	9.18E-01	69.0	9.07E-06
3	2.32E-01	0.00E+00	2.22E+01	0.00E+00	2.27E+01	6.27E-01	8.25E-01	9.20E-01	76.2	2.42E-06
4	2.98E-01	0.00E+00	2.18E+01	0.00E+00	3.49E+00	6.06E-02	8.26E-01	9.22E-01	87.8	1.12E-05
5	4.07E-01	0.00E+00	6.28E+00	0.00E+00	6.16E+00	8.17E-02	8.05E-01	9.18E-01	83.9	7.57E-06
6	4.43E-01	0.00E+00	1.02E+00	0.00E+00	7.21E+00	8.88E-02	7.97E-01	9.17E-01	82.5	3.19E-05
7	4.49E-01	0.00E+00	1.42E-01	0.00E+00	7.39E+00	9.00E-02	7.96E-01	9.17E-01	82.3	3.84E-05
8	4.50E-01	0.00E+00	1.91E-02	0.00E+00	7.41E+00	9.01E-02	7.96E-01	9.16E-01	82.2	5.34E-05
9	4.49E-01	0.00E+00	2.54E-03	0.00E+00	7.38E+00	9.04E-02	7.96E-01	9.16E-01	82.0	7.54E-05
10	4.27E-01	0.00E+00	3.00E-04	0.00E+00	6.75E+00	9.38E-02	7.95E-01	9.16E-01	77.9	8.89E-05

7.3 URANIUM STRIPPING CONTACTOR

This calculation is for a simple, six-stage uranium stripping contactor employing a 30% TBP flow sheet, shown in Fig. 3. Only the steady-state concentration profile is desired, so stage volume or initial profile information is unnecessary. The printout that follows Fig. 3 shows the final expected concentration profile.

The problem was previously calculated by using SEPHIS MOD4 on a mainframe computer to a tolerance of 0.01% inventory change per minute.⁷ The computation time was 2.1 s on the ORNL IBM 360/91. The computation time for SEPHIS MOD4, Version 2.11, on an IBM PC/XT without any upgrade features was 6 min 49 s. The use of an upgraded system (16-MHz with 32-bit processor) resulted in a computation time of 1 min 14 s.

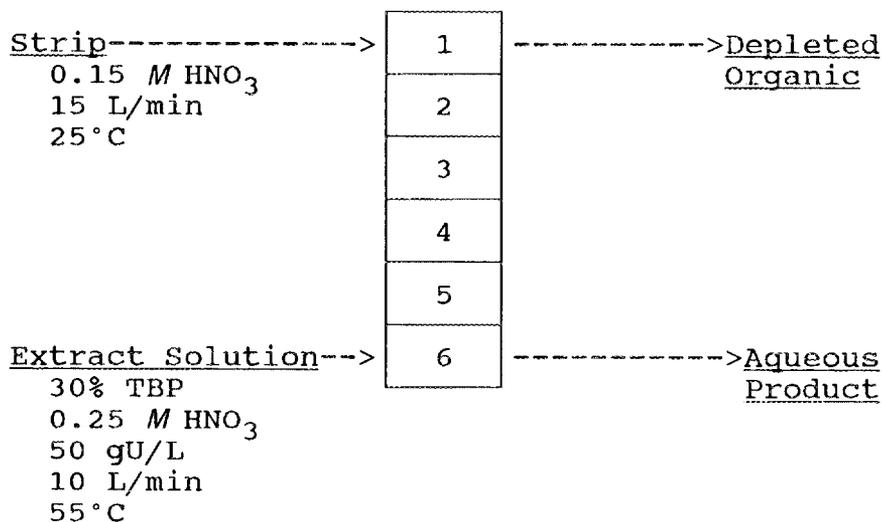


Fig. 3. Uranium stripping contactor.

PROBLEM DEFINITION DATA FOR SEPHIS MOD4, Ver. 2.11:

02-08-1990 08:29

Problem: Ex. 3 - ORNL-5471 - U Stripping

PUREX PROCESS

Total stages: 6

Volume X TBP in solvent: 30.0

Initial or default temperature (°C): 30.0

No unusual stage connections

No Plutonium reaction.

Minutes per time increment: 1.00

Minutes between printing of the concentration profile: 500

Calculations will stop after 500 minutes or when a tolerance of 0.0100 % per minute is reached.

Mixer volumes = (phase flow)(unit time).

Settler volumes = (phase flow)(unit time).

Initial concentration profile is zero.

Fast integration will be used.

No extra product streams.

The FILESPEC for this Problem Definition data file is: B:EX_03P.DAT

The FILESPEC for this Problem Results data file is: B:EX_03R.DAT

FEED AND PRODUCT STREAM DATA:

	STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	FLOW RATE (L/min)	TEMP (C)
AQUEOUS	1	1.50E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+01	25.0
30.0 % TBP	6	2.50E-01	5.00E+01	0.00E+00				1.00E+01	55.0

STAGE VOLUME AND FLOW RATE DATA (Molal basis):

STAGE NO.	MIXER VOLUME BY PHASE		SETTLER VOLUME BY PHASE		MIXER FLOW RATE		INTERSTAGE FLOW RATE	
	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC
1	1.49E+01	9.66E+00	1.49E+01	9.66E+00	1.49E+01	9.66E+00	1.49E+01	9.66E+00
2	1.49E+01	9.66E+00	1.49E+01	9.66E+00	1.49E+01	9.66E+00	1.49E+01	9.66E+00
3	1.49E+01	9.66E+00	1.49E+01	9.66E+00	1.49E+01	9.66E+00	1.49E+01	9.66E+00
4	1.49E+01	9.66E+00	1.49E+01	9.66E+00	1.49E+01	9.66E+00	1.49E+01	9.66E+00
5	1.49E+01	9.66E+00	1.49E+01	9.66E+00	1.49E+01	9.66E+00	1.49E+01	9.66E+00
6	1.49E+01	9.66E+00	1.49E+01	9.66E+00	1.49E+01	9.66E+00	1.49E+01	9.66E+00

PROBLEM RESULTS FOR SEPHIS MDD4, Ver. 2.11:

06-08-1996 09:24

Problem: Ex. 3 - ORNL-5471 - U Stripping
(mixer concentrations shown)

TIME = 0.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.49E+01	30.0
2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.49E+01	30.0
3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.49E+01	30.0
4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.49E+01	30.0
5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.49E+01	30.0
6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.97E-01	1.49E+01	30.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	9.74E+00	0.0	2.00E+02
2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	9.74E+00	0.0	2.00E+02
3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	9.74E+00	0.0	2.00E+02
4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	9.74E+00	0.0	2.00E+02
5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	9.74E+00	0.0	2.00E+02
6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.18E-01	9.74E+00	0.0	2.00E+02

TIME = 174.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	1.51E-01	2.73E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.01E+00	1.50E+01	25.0
2	1.51E-01	7.57E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.01E+00	1.50E+01	25.0
3	1.51E-01	1.38E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.02E+00	1.51E+01	25.1
4	1.52E-01	2.08E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.03E+00	1.51E+01	25.3
5	1.51E-01	2.82E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.04E+00	1.51E+01	26.5
6	3.05E-01	3.18E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.05E+00	1.52E+01	31.7

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.06E-02	1.60E+00	0.00E+00	3.81E-01	0.00E+00	4.57E-02	8.20E-01	9.75E+00	2.2	9.43E-03
2	1.20E-02	5.89E+00	0.00E+00	4.98E-01	0.00E+00	5.16E-02	8.26E-01	9.76E+00	5.5	7.26E-03
3	1.31E-02	1.32E+01	0.00E+00	6.22E-01	0.00E+00	5.81E-02	8.36E-01	9.79E+00	11.3	4.89E-03
4	1.35E-02	2.28E+01	0.00E+00	7.14E-01	0.00E+00	5.79E-02	8.48E-01	9.82E+00	18.7	3.01E-03
5	1.43E-02	3.34E+01	0.00E+00	7.71E-01	0.00E+00	5.79E-02	8.62E-01	9.86E+00	26.9	1.68E-03
6	2.88E-02	4.47E+01	0.00E+00	9.14E-01	0.00E+00	6.13E-02	8.77E-01	9.90E+00	36.9	8.22E-04

7.4 BATCH EXTRACTION/STRIPPING PROCESS

This sample calculation shows how a batch extraction process can be simulated. One volume of the aqueous phase is contacted with two separate portions of pure solvent. These are then combined and stripped by using five contacts with strip solution. Figure 4 shows how this can be represented as a series of cross-current contacts. An initial profile is specified for this problem. The printout that follows Fig. 4 shows the final expected concentration profile.

The problem was previously calculated by using SEPHIS MOD4 on a mainframe computer to a tolerance of 0.01% inventory change per minute.⁷ The computation time was 0.6 s on the ORNL IBM 360/91. The computation time for SEPHIS MOD4, Version 2.11, on an IBM PC/XT without any upgrade features was 1 min 51 s. The use of an upgraded system (16-MHz with 32-bit processor) resulted in a computation time of 46 s.

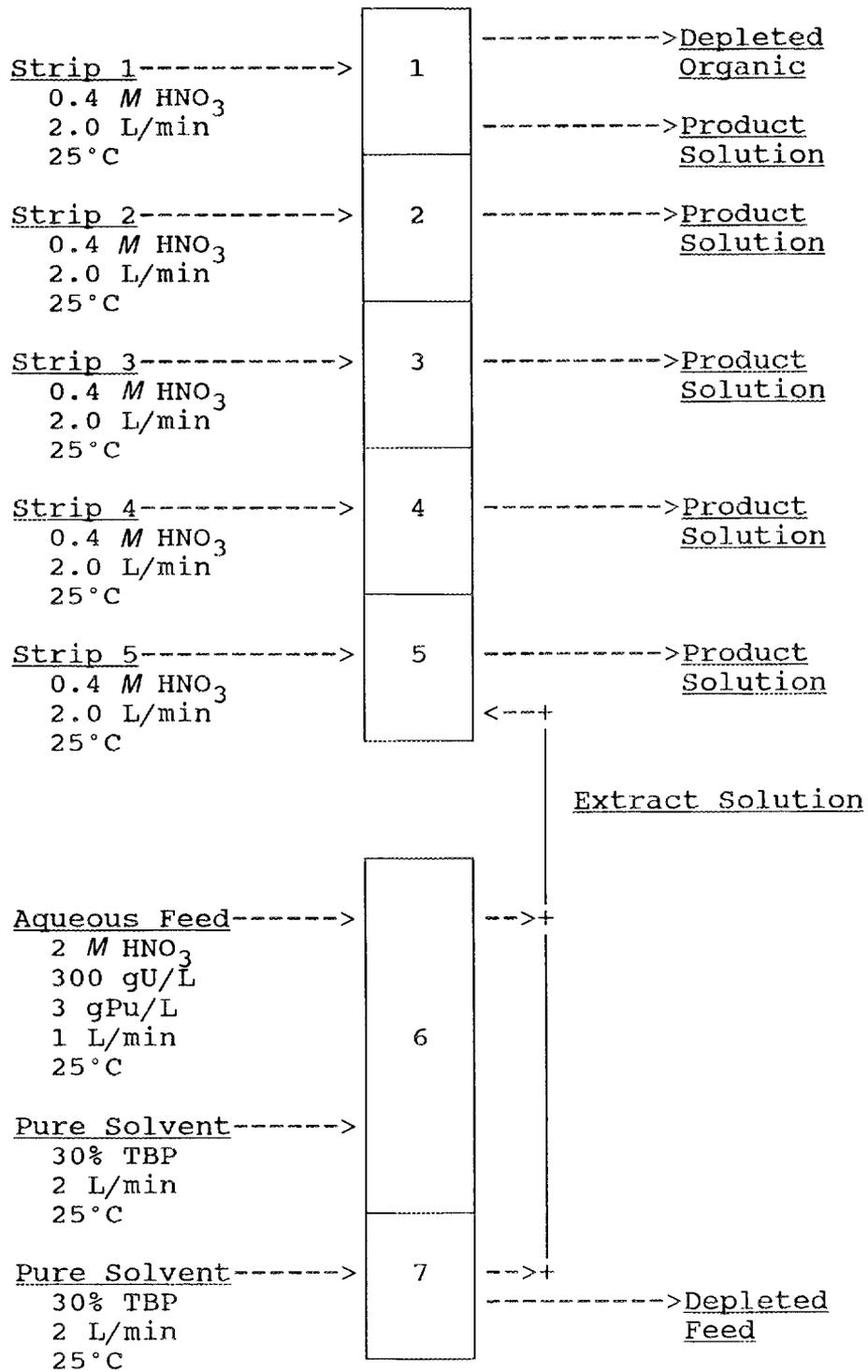


Fig. 4. Batch extraction/stripping process.

PROBLEM DEFINITION DATA FOR SEPHIS MOD4, Ver. 2.11:

02-08-1990 08:54

Problem: Ex. 4 - ORNL-5471 - Batch Extraction

PUREX PROCESS

Total stages: 7

Volume % TBP in solvent: 30.0

Initial or default temperature (°C): 25.0

Organic taken from stage 7 feeds stage 5.

No Plutonium reaction.

Minutes per time increment: 1.00

Minutes between printing of the concentration profile: 100

Calculations will stop after 100 minutes or when a tolerance of 0.0100 % per minute is reached.

Mixer volumes = (phase flow)(unit time).

Settler volumes = (phase flow)(unit time).

Initial concentration profile is defined.

Fast integration will be used.

Extra product stream(s).

The FILESPEC for this Problem Definition data file is: B:EX_04P.DAT

The FILESPEC for this Problem Results data file is: B:EX_04R.DAT

FEED AND PRODUCT STREAM DATA:

	STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	FLOW RATE (L/min)	TEMP (C)
AQUEOUS	1	4.00E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.00E+00	25.0
AQUEOUS	2	4.00E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.00E+00	25.0
AQUEOUS	3	4.00E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.00E+00	25.0
AQUEOUS	4	4.00E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.00E+00	25.0
AQUEOUS	5	4.00E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.00E+00	25.0
AQUEOUS	6	2.00E+00	3.00E+02	3.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	25.0
30.0 % TBP	6	0.00E+00	0.00E+00	0.00E+00				2.00E+00	25.0
30.0 % TBP	7	0.00E+00	0.00E+00	0.00E+00				2.00E+00	25.0
AQUEOUS	1	Product stream removed (actual flow rate to be computed)						3.00E+00	
AQUEOUS	2	Product stream removed (actual flow rate to be computed)						3.00E+00	
AQUEOUS	3	Product stream removed (actual flow rate to be computed)						3.00E+00	
AQUEOUS	4	Product stream removed (actual flow rate to be computed)						3.00E+00	
AQUEOUS	5	Product stream removed (actual flow rate to be computed)						3.00E+00	

INITIAL AQUEOUS PROFILE DATA:

	STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	TEMP (C)
	1	2.00E+00	3.00E+02	3.00E+00	0.00E+00	0.00E+00	0.00E+00	25.0
	2	2.00E+00	3.00E+02	3.00E+00	0.00E+00	0.00E+00	0.00E+00	25.0
	3	2.00E+00	3.00E+02	3.00E+00	0.00E+00	0.00E+00	0.00E+00	25.0
	4	2.00E+00	3.00E+02	3.00E+00	0.00E+00	0.00E+00	0.00E+00	25.0
	5	2.00E+00	3.00E+02	3.00E+00	0.00E+00	0.00E+00	0.00E+00	25.0
	6	2.00E+00	3.00E+02	3.00E+00	0.00E+00	0.00E+00	0.00E+00	25.0
	7	2.00E+00	3.00E+02	3.00E+00	0.00E+00	0.00E+00	0.00E+00	25.0

INITIAL ORGANIC PROFILE DATA:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)
1	0.00E+00	0.00E+00	0.00E+00
2	0.00E+00	0.00E+00	0.00E+00
3	0.00E+00	0.00E+00	0.00E+00
4	0.00E+00	0.00E+00	0.00E+00
5	0.00E+00	0.00E+00	0.00E+00
6	0.00E+00	0.00E+00	0.00E+00
7	0.00E+00	0.00E+00	0.00E+00

STAGE VOLUME AND FLOW RATE DATA (Molal basis):

STAGE NO.	MIXER VOLUME BY PHASE		SETTLER VOLUME BY PHASE		MIXER FLOW RATE		INTERSTAGE FLOW RATE	
	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC
1	1.98E+00	3.97E+00	1.98E+00	3.97E+00	1.98E+00	3.97E+00	0.00E+00	3.97E+00
2	1.98E+00	3.97E+00	1.98E+00	3.97E+00	1.98E+00	3.97E+00	0.00E+00	3.97E+00
3	1.98E+00	3.97E+00	1.98E+00	3.97E+00	1.98E+00	3.97E+00	0.00E+00	3.97E+00
4	1.98E+00	3.97E+00	1.98E+00	3.97E+00	1.98E+00	3.97E+00	0.00E+00	3.97E+00
5	1.98E+00	3.97E+00	1.98E+00	3.97E+00	1.98E+00	3.97E+00	0.00E+00	3.97E+00
6	8.45E-01	1.98E+00	8.45E-01	1.98E+00	8.45E-01	1.98E+00	8.45E-01	1.98E+00
7	8.45E-01	1.98E+00	8.45E-01	1.98E+00	8.45E-01	1.98E+00	8.45E-01	1.98E+00

PROBLEM RESULTS FOR SEPHTS MDD4, Ver. 2.11:

06-06-1990 09:27

Problem: Ex. 4 - ORNL-5471 - Batch Extraction
(mixer concentrations shown)

TIME = 0.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	2.02E+00	1.29E+02	2.03E+00	0.00E+00	0.00E+00	0.00E+00	1.24E+00	2.20E+00	25.0
1	PRODUCT STREAM								
2	2.02E+00	1.29E+02	2.03E+00	0.00E+00	0.00E+00	0.00E+00	1.24E+00	2.20E+00	25.0
2	PRODUCT STREAM								
3	2.02E+00	1.29E+02	2.03E+00	0.00E+00	0.00E+00	0.00E+00	1.24E+00	2.20E+00	25.0
3	PRODUCT STREAM								
4	2.02E+00	1.29E+02	2.03E+00	0.00E+00	0.00E+00	0.00E+00	1.24E+00	2.20E+00	25.0
4	PRODUCT STREAM								
5	2.02E+00	1.29E+02	2.03E+00	0.00E+00	0.00E+00	0.00E+00	1.24E+00	2.20E+00	25.0
5	PRODUCT STREAM								
6	2.01E+00	1.10E+02	1.86E+00	0.00E+00	0.00E+00	0.00E+00	1.21E+00	9.36E-01	25.0
7	2.01E+00	1.10E+02	1.86E+00	0.00E+00	0.00E+00	0.00E+00	1.21E+00	9.36E-01	25.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	5.44E-02	1.00E+02	6.14E-01	1.46E+00	5.72E-01	5.08E-02	9.52E-01	4.15E+00	82.4	2.00E+02
2	5.44E-02	1.00E+02	6.14E-01	1.46E+00	5.72E-01	5.08E-02	9.52E-01	4.15E+00	82.4	2.00E+02
3	5.44E-02	1.00E+02	6.14E-01	1.46E+00	5.72E-01	5.08E-02	9.52E-01	4.15E+00	82.4	2.00E+02
4	5.44E-02	1.00E+02	6.14E-01	1.46E+00	5.72E-01	5.08E-02	9.52E-01	4.15E+00	82.4	2.00E+02
5	5.44E-02	1.00E+02	6.14E-01	1.46E+00	5.72E-01	5.08E-02	9.52E-01	4.15E+00	82.4	2.00E+02
6	5.81E-02	9.51E+01	6.08E-01	1.91E+00	7.24E-01	6.40E-02	9.45E-01	2.07E+00	78.7	2.00E+02
7	5.81E-02	9.51E+01	6.08E-01	1.91E+00	7.24E-01	6.40E-02	9.45E-01	2.07E+00	78.7	2.00E+02

TIME = 31.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	3.95E-01	1.19E+01	4.41E-02	0.00E+00	0.00E+00	0.00E+00	1.03E+00	2.01E+00	25.0
1	PRODUCT STREAM								
2	3.95E-01	1.51E+01	8.84E-02	0.00E+00	0.00E+00	0.00E+00	1.03E+00	2.01E+00	25.0
2	PRODUCT STREAM								
3	3.98E-01	1.95E+01	1.80E-01	0.00E+00	0.00E+00	0.00E+00	1.04E+00	2.01E+00	25.0
3	PRODUCT STREAM								
4	4.25E-01	2.49E+01	3.64E-01	0.00E+00	0.00E+00	0.00E+00	1.05E+00	2.02E+00	25.0
4	PRODUCT STREAM								
5	5.98E-01	2.81E+01	6.47E-01	0.00E+00	0.00E+00	0.00E+00	1.06E+00	2.03E+00	25.0
5	PRODUCT STREAM								
6	1.99E+00	8.33E+01	1.62E+00	0.00E+00	0.00E+00	0.00E+00	1.18E+00	9.27E-01	25.0
7	1.53E+00	4.29E+00	2.62E-01	0.00E+00	0.00E+00	0.00E+00	1.05E+00	8.89E-01	25.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	4.57E-02	2.36E+01	2.28E-02	4.90E+00	1.04E+00	2.33E-01	8.50E-01	4.04E+00	22.3	6.89E-03
2	4.38E-02	2.94E+01	4.46E-02	3.91E+00	1.02E+00	2.24E-01	8.58E-01	4.05E+00	26.6	1.74E-03
3	4.19E-02	3.68E+01	8.82E-02	3.81E+00	9.91E-01	2.12E-01	8.67E-01	4.06E+00	32.1	5.06E-04
4	4.19E-02	4.63E+01	1.77E-01	3.75E+00	9.80E-01	1.99E-01	9.80E-01	4.07E+00	39.5	1.79E-04
5	5.59E-02	5.84E+01	3.55E-01	4.18E+00	1.11E+00	1.88E-01	8.96E-01	4.09E+00	50.2	7.95E-05
6	7.46E-02	1.07E+02	7.19E-01	2.89E+00	9.95E-01	8.42E-02	9.61E-01	2.08E+00	89.4	7.99E-06
7	2.38E-01	3.59E+01	6.22E-01	1.92E+01	5.47E+00	3.59E-01	8.72E-01	2.04E+00	49.8	7.82E-05

7.5 EXTRACTION/PARTIAL PARTITIONING - LOSS OF REDUCTANT

Two pulsed columns are modeled here as shown in Fig. 5. By using known data for the height of column equivalent to a theoretical stage (HETS), the SEPHIS MOD4 code can be set up to simulate this differential type of contactor. Volumes for the mixing and settling portions must be specified. In the interior of the column, the HETS determines the stage volume; the ratio of phases is assumed equal to the flow ratio, and the split between "mixers" and "settlers" is arbitrary. The volumes of solution in the phase disengagement sections at the ends of the column are merely added to the appropriate "settler."

The simulated situation is the complete loss of a small reductant stream fed to Stage 3 for 30 min. An initial profile is specified for this problem. The printout that follows Fig. 5 shows the expected concentration profile after 30 min.

The problem was previously calculated by using SEPHIS MOD4 on a mainframe computer.⁷ The computation time was ~13 s on the ORNL IBM 360/91. The computation time for SEPHIS MOD4, Version 2.11, on an IBM PC/XT without any upgrade features was 15 min 28 s. Use of an upgraded system (16-MHz with 32-bit processor) resulted in a computation time of 2 min 40 s.

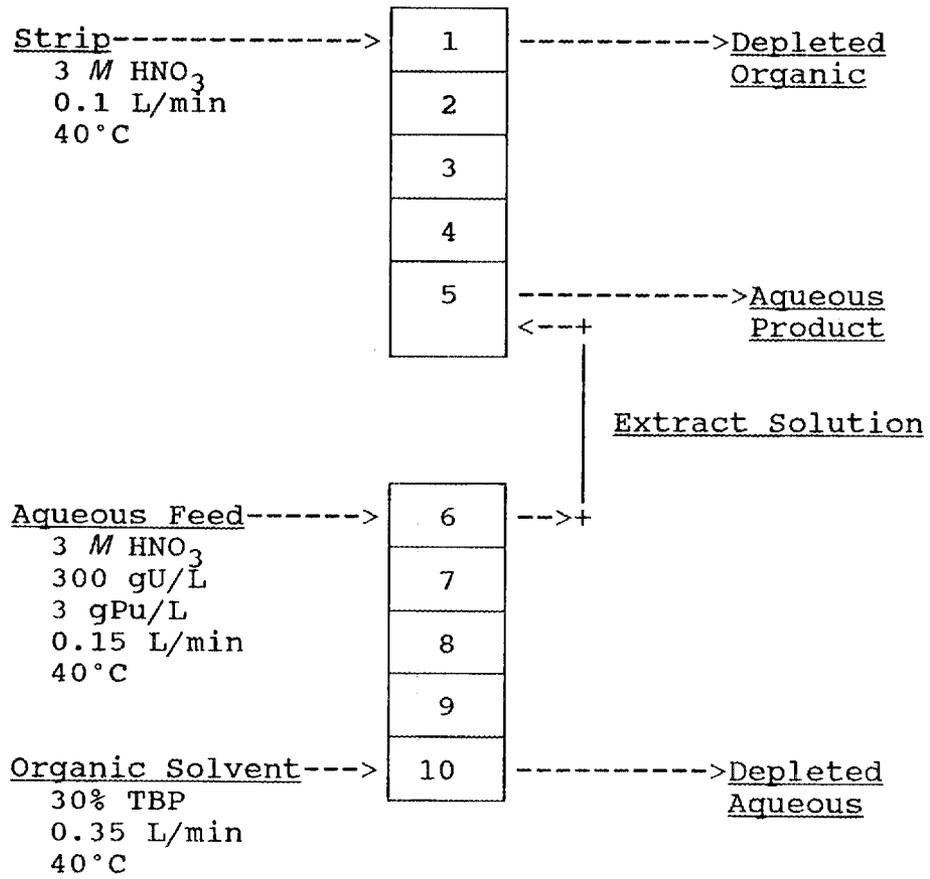


Fig. 5. Extraction/partial partitioning-loss of reductant.

PROBLEM DEFINITION DATA FOR SEPHIS MOD4, Ver. 2.11:

02-08-1990 10:08

Problem: Ex. 5 - ORNL-5471 - Pulsed Columns

PUREX PROCESS

Total stages: 10

Volume % TBP in solvent: 30.0

Initial or default temperature (°C): 40.0

No unusual stage connections

Instantaneous reduction of Pu(IV).

Minutes per time increment: 0.13

Minutes between printing of the concentration profile: 10

Calculations will stop after 30 minutes or when a tolerance of 0.0100 % per minute is reached.

Mixer volumes are defined for each phase.

Settler volumes are defined for each phase.

Initial concentration profile is defined.

Runge-Kutta integration will be used.

Extra product stream(s).

The FILESPEC for this Problem Definition data file is: B:EX_05P.DAT

The FILESPEC for this Problem Results data file is: B:EX_05R.DAT

FEED AND PRODUCT STREAM DATA:

	STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	FLOW RATE (L/min)	TEMP (C)
AQUEOUS	1	3.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E-01	40.0
AQUEOUS	6	3.00E+00	3.00E+02	3.00E+00	0.00E+00	0.00E+00	0.00E+00	1.50E-01	40.0
30.0 % TBP	10	0.00E+00	0.00E+00	0.00E+00				3.50E-01	40.0
AQUEOUS	5	Product stream removed (actual flow rate to be computed)						1.00E+01	

INITIAL AQUEOUS PROFILE DATA:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	TEMP (C)
1	2.84E+00	2.77E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	40.0
2	2.75E+00	4.28E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	40.0
3	2.64E+00	5.56E+01	0.00E+00	0.00E+00	1.72E-02	1.72E-02	40.0
4	2.55E+00	7.19E+01	0.00E+00	4.47E-02	1.70E-02	1.72E-02	40.0
5	2.41E+00	1.00E+02	1.75E-02	4.06E+00	0.00E+00	1.71E-02	40.0
6	3.00E+00	3.00E+02	2.87E+00	0.00E+00	0.00E+00	0.00E+00	40.0
7	3.00E+00	3.00E+02	2.74E+00	0.00E+00	0.00E+00	0.00E+00	40.0
8	3.05E+00	2.94E+02	2.55E+00	0.00E+00	0.00E+00	0.00E+00	40.0
9	3.48E+00	2.24E+02	1.91E+00	0.00E+00	0.00E+00	0.00E+00	40.0
10	3.14E+00	2.14E+01	2.67E-01	0.00E+00	0.00E+00	0.00E+00	40.0

INITIAL ORGANIC PROFILE DATA:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)
1	2.05E-01	8.75E+01	0.00E+00
2	1.63E-01	9.50E+01	0.00E+00
3	1.39E-01	9.91E+01	0.00E+00
4	1.19E-01	1.03E+02	0.00E+00
5	9.49E-02	1.07E+02	1.23E-02

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)
6	5.96E-02	1.15E+02	1.13E+00
7	5.97E-02	1.15E+02	1.08E+00
8	6.12E-02	1.15E+02	1.02E+00
9	8.00E-02	1.13E+02	9.47E-01
10	2.44E-01	8.31E+01	6.78E-01

STAGE VOLUME AND FLOW RATE DATA (Molal basis):

STAGE NO.	MIXER VOLUME BY PHASE		SETTLER VOLUME BY PHASE		MIXER FLOW RATE		INTERSTAGE FLOW RATE	
	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC
1	3.60E-02	1.20E-01	1.10E-01	5.80E-01	9.07E-02	3.47E-01	9.07E-02	3.47E-01
2	3.60E-02	1.20E-01	1.10E-01	3.80E-01	9.07E-02	3.47E-01	9.07E-02	3.47E-01
3	3.60E-02	1.20E-01	1.10E-01	3.80E-01	9.07E-02	3.47E-01	9.07E-02	3.47E-01
4	3.60E-02	1.20E-01	1.10E-01	3.80E-01	9.07E-02	3.47E-01	9.07E-02	3.47E-01
5	3.60E-02	1.20E-01	3.10E-01	3.80E-01	9.07E-02	3.47E-01	0.00E+00	3.47E-01
6	1.70E-01	4.00E-01	5.10E-01	1.70E+00	1.22E-01	3.47E-01	1.22E-01	3.47E-01
7	1.70E-01	4.00E-01	5.10E-01	1.18E+00	1.22E-01	3.47E-01	1.22E-01	3.47E-01
8	1.70E-01	4.00E-01	5.10E-01	1.18E+00	1.22E-01	3.47E-01	1.22E-01	3.47E-01
9	1.70E-01	4.00E-01	5.10E-01	1.18E+00	1.22E-01	3.47E-01	1.22E-01	3.47E-01
10	1.70E-01	4.00E-01	7.00E-01	1.18E+00	1.22E-01	3.47E-01	1.22E-01	3.47E-01

PROBLEM RESULTS FOR SEPHIS MOD4, Ver. 2.11:

06-08-1990 09:31

Problem: Ex. 5 - DRNL-5471 - Pulsed Columns
(mixer concentrations shown)

TIME = 0.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)	
1	2.86E+00	2.63E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	1.00E-01	40.0	
2	2.77E+00	4.13E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.14E+00	1.01E-01	40.0	
3	2.66E+00	5.45E+01	0.00E+00	0.00E+00	1.72E-02	1.72E-02	1.16E+00	1.01E-01	40.0	
4	2.57E+00	7.12E+01	0.00E+00	4.47E-02	1.70E-02	1.72E-02	1.18E+00	1.01E-01	40.0	
5	2.42E+00	9.92E+01	1.72E-02	4.08E+00	0.00E+00	1.71E-02	1.22E+00	1.01E-01	40.0	
5	PRODUCT STREAM								1.01E-01	
6	3.01E+00	3.00E+02	2.61E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0	
7	3.01E+00	2.99E+02	2.52E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0	
8	3.06E+00	2.94E+02	2.35E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0	
9	3.49E+00	2.23E+02	1.74E+00	0.00E+00	0.00E+00	0.00E+00	1.41E+00	1.48E-01	40.0	
10	3.16E+00	2.04E+01	2.50E-01	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.36E-01	40.0	

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.98E-01	8.78E+01	0.00E+00	1.21E+01	0.00E+00	2.51E-01	9.38E-01	3.64E-01	85.4	2.00E+02
2	1.57E-01	9.55E+01	0.00E+00	8.36E+00	0.00E+00	2.05E-01	9.47E-01	3.64E-01	87.5	2.00E+02
3	1.33E-01	9.95E+01	0.00E+00	6.61E+00	0.00E+00	1.80E-01	9.52E-01	3.64E-01	88.5	2.00E+02
4	1.13E-01	1.03E+02	0.00E+00	5.23E+00	0.00E+00	1.59E-01	9.56E-01	3.65E-01	89.3	2.00E+02
5	9.01E-02	1.09E+02	1.25E-02	3.91E+00	1.10E-02	1.34E-01	9.62E-01	3.65E-01	91.0	2.00E+02
6	5.63E-02	1.15E+02	1.23E-02	9.38E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.5	2.00E+02
7	5.63E-02	1.15E+02	1.19E+00	9.40E-01	1.15E+00	4.57E-02	9.72E-01	3.66E-01	94.5	2.00E+02
8	5.78E-02	1.15E+02	1.13E+00	9.57E-01	1.17E+00	4.61E-02	9.72E-01	3.66E-01	94.5	2.00E+02
9	7.57E-02	1.13E+02	1.03E+00	1.25E+00	1.45E+00	5.34E-02	9.69E-01	3.66E-01	94.4	2.00E+02
10	2.36E-01	8.36E+01	6.88E-01	1.09E+01	7.34E+00	2.00E-01	9.35E-01	3.64E-01	86.2	2.00E+02

TIME = 10.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)	
1	2.84E+00	2.65E+01	1.82E-01	0.00E+00	0.00E+00	0.00E+00	1.12E+00	1.00E-01	40.0	
2	2.76E+00	4.09E+01	3.97E-01	0.00E+00	0.00E+00	0.00E+00	1.14E+00	1.01E-01	40.0	
3	2.68E+00	5.34E+01	6.62E-01	2.90E-12	0.00E+00	1.22E-14	1.16E+00	1.01E-01	40.0	
4	2.59E+00	6.92E+01	9.99E-01	1.24E-07	0.00E+00	5.19E-10	1.18E+00	1.01E-01	40.0	
5	2.45E+00	9.94E+01	1.54E+00	5.45E-05	0.00E+00	2.28E-07	1.21E+00	1.02E-01	40.0	
5	PRODUCT STREAM								1.02E-01	
6	3.00E+00	3.00E+02	2.74E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0	
7	3.01E+00	3.00E+02	2.51E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0	
8	3.05E+00	2.94E+02	2.22E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0	
9	3.49E+00	2.23E+02	1.55E+00	0.00E+00	0.00E+00	0.00E+00	1.41E+00	1.48E-01	40.0	
10	3.15E+00	1.97E+01	2.85E-01	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.36E-01	40.0	

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.98E-01	8.83E+01	3.84E-01	1.21E+01	7.64E+00	2.52E-01	9.39E-01	3.64E-01	86.1	3.12E+01
2	1.57E-01	9.54E+01	5.92E-01	8.45E+00	5.39E+00	2.07E-01	9.48E-01	3.64E-01	88.0	1.71E+01
3	1.35E-01	9.92E+01	7.91E-01	6.72E+00	4.32E+00	1.82E-01	9.53E-01	3.65E-01	89.0	8.67E+00
4	1.15E-01	1.03E+02	9.62E-01	5.36E+00	3.48E+00	1.61E-01	9.57E-01	3.65E-01	89.9	3.79E+00
5	9.08E-02	1.07E+02	1.11E+00	3.87E+00	2.58E+00	1.33E-01	9.62E-01	3.65E-01	91.2	1.22E+00
6	5.61E-02	1.15E+02	1.29E+00	9.37E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	2.53E-02
7	5.62E-02	1.15E+02	1.18E+00	9.39E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	1.91E-01
8	5.77E-02	1.15E+02	1.07E+00	9.57E-01	1.17E+00	4.61E-02	9.72E-01	3.66E-01	94.6	4.33E-01
9	7.56E-02	1.13E+02	9.14E-01	1.25E+00	1.45E+00	5.34E-02	9.70E-01	3.66E-01	94.5	8.26E-01
10	2.41E-01	8.37E+01	5.83E-01	1.13E+01	7.59E+00	2.04E-01	9.35E-01	3.64E-01	86.6	9.48E-01

TIME = 20.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	2.84E+00	2.64E+01	3.87E-01	0.00E+00	0.00E+00	0.00E+00	1.12E+00	1.00E-01	40.0
2	2.76E+00	4.09E+01	6.28E-01	0.00E+00	0.00E+00	0.00E+00	1.14E+00	1.01E-01	40.0
3	2.68E+00	5.36E+01	8.48E-01	0.00E+00	0.00E+00	0.00E+00	1.16E+00	1.01E-01	40.0
4	2.59E+00	6.96E+01	1.12E+00	0.00E+00	0.00E+00	0.00E+00	1.18E+00	1.01E-01	40.0
5	2.45E+00	9.99E+01	1.61E+00	2.71E-15	0.00E+00	1.14E-17	1.21E+00	1.02E-01	40.0
5	PRODUCT STREAM								1.02E-01
6	3.00E+00	3.00E+02	2.72E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
7	3.00E+00	3.00E+02	2.45E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
8	3.05E+00	2.95E+02	2.13E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
9	3.49E+00	2.24E+02	1.45E+00	0.00E+00	0.00E+00	0.00E+00	1.41E+00	1.48E-01	40.0
10	3.15E+00	1.97E+01	1.89E-01	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.36E-01	40.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.97E-01	8.79E+01	8.15E-01	1.21E+01	7.64E+00	2.52E-01	9.40E-01	3.64E-01	86.1	1.16E+00
2	1.57E-01	9.51E+01	9.33E-01	8.43E+00	5.38E+00	2.06E-01	9.48E-01	3.64E-01	88.0	7.19E-01
3	1.34E-01	9.91E+01	1.01E+00	6.69E+00	4.30E+00	1.82E-01	9.53E-01	3.65E-01	89.1	3.71E-01
4	1.15E-01	1.03E+02	1.07E+00	5.32E+00	3.46E+00	1.60E-01	9.57E-01	3.65E-01	90.0	1.35E-01
5	9.05E-02	1.07E+02	1.15E+00	3.85E+00	2.57E+00	1.33E-01	9.62E-01	3.65E-01	91.2	9.92E-03
6	5.61E-02	1.15E+02	1.28E+00	9.37E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	1.12E-01
7	5.62E-02	1.15E+02	1.16E+00	9.38E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	2.57E-01
8	5.76E-02	1.15E+02	1.02E+00	9.55E-01	1.17E+00	4.60E-02	9.72E-01	3.66E-01	94.6	4.21E-01
9	7.55E-02	1.13E+02	8.55E-01	1.25E+00	1.45E+00	5.34E-02	9.70E-01	3.66E-01	94.5	5.67E-01
10	2.41E-01	8.37E+01	5.38E-01	1.13E+01	7.60E+00	2.04E-01	9.35E-01	3.64E-01	86.6	6.33E-01

TIME = 30.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	2.84E+00	2.65E+01	3.99E-01	0.00E+00	0.00E+00	0.00E+00	1.12E+00	1.00E-01	40.0

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
2	2.76E+00	4.10E+01	6.40E-01	0.00E+00	0.00E+00	0.00E+00	1.14E+00	1.01E-01	40.0
3	2.68E+00	5.37E+01	8.54E-01	0.00E+00	0.00E+00	0.00E+00	1.16E+00	1.01E-01	40.0
4	2.59E+00	6.97E+01	1.12E+00	0.00E+00	0.00E+00	0.00E+00	1.18E+00	1.01E-01	40.0
5	2.45E+00	1.00E+02	1.60E+00	0.00E+00	0.00E+00	0.00E+00	1.21E+00	1.02E-01	40.0
5	PRODUCT STREAM								
6	3.00E+00	3.00E+02	2.69E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
7	3.00E+00	3.00E+02	2.39E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
8	3.05E+00	2.95E+02	2.05E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
9	3.49E+00	2.24E+02	1.38E+00	0.00E+00	0.00E+00	0.00E+00	1.41E+00	1.48E-01	40.0
10	3.15E+00	1.98E+01	1.79E-01	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.36E-01	40.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.97E-01	8.79E+01	8.40E-01	1.21E+01	7.63E+00	2.52E-01	9.40E-01	3.64E-01	86.1	2.81E-02
2	1.57E-01	9.51E+01	9.49E-01	8.41E+00	5.37E+00	2.06E-01	9.48E-01	3.64E-01	88.0	5.86E-02
3	1.34E-01	9.91E+01	1.01E+00	6.68E+00	4.29E+00	1.81E-01	9.53E-01	3.65E-01	89.1	8.49E-02
4	1.14E-01	1.03E+02	1.07E+00	5.32E+00	3.45E+00	1.60E-01	9.57E-01	3.65E-01	90.0	1.05E-01
5	9.05E-02	1.07E+02	1.14E+00	3.84E+00	2.57E+00	1.33E-01	9.62E-01	3.65E-01	91.2	1.19E-01
6	5.61E-02	1.15E+02	1.27E+00	9.37E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	1.26E-01
7	5.62E-02	1.16E+02	1.13E+00	9.38E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	2.52E-01
8	5.75E-02	1.16E+02	9.82E-01	9.55E-01	1.17E+00	4.60E-02	9.72E-01	3.66E-01	94.6	3.69E-01
9	7.54E-02	1.13E+02	8.13E-01	1.25E+00	1.45E+00	5.33E-02	9.70E-01	3.66E-01	94.5	4.51E-01
10	2.41E-01	8.38E+01	5.08E-01	1.13E+01	7.58E+00	2.04E-01	9.35E-01	3.64E-01	86.6	4.78E-01

7.6 EXTRACTION/PARTIAL PARTITIONING - REDUCTANT REGAINED

The problem described in Sect. 7.5 is continued in this section, but with the reductant stream restored (Fig. 6). The concentration profile existing after 30 min with no reductant is the starting profile for this new sample calculation. An additional 30 min of operating time is permitted.

The problem was previously calculated by using SEPHIS MOD4 on a mainframe computer.⁷ The computation time was ~13 s on the ORNL IBM 360/91 (a total of 27 s for this example and the previous example). The computation time for SEPHIS MOD4, Version 2.11, on an IBM PC/XT without any upgrade features was 16 min 54 s. The use of an upgraded system (16-MHz with 32-bit processor) resulted in a computation time of 4 min 55 s.

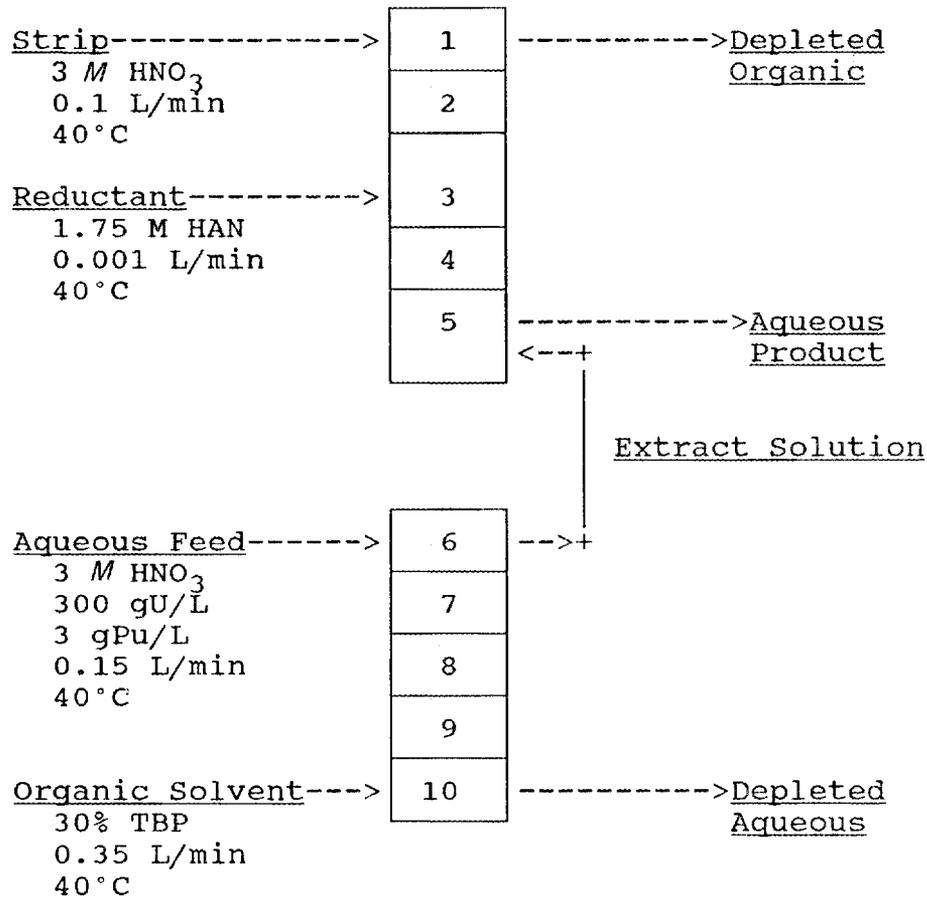


Fig. 6. Extraction/partial partitioning—reductant regained.

PROBLEM DEFINITION DATA FOR SEPHIS MOD4, Ver. 2.11:

02-08-1990 13:55

Problem: Ex. 6 - ORNL-5471 - Pulsed Columns II

PUREX PROCESS

Total stages: 10

Volume % TBP in solvent: 30.0

Initial or default temperature (°C): 40.0

No unusual stage connections

Instantaneous reduction of Pu(IV).

Minutes per time increment: 0.13

Minutes between printing of the concentration profile: 10

Calculations will stop after 30 minutes or when a tolerance of 0.0100 % per minute is reached.

Mixer volumes are defined for each phase.

Settler volumes are defined for each phase.

Initial concentration profile is from a previous problem.

Fast integration will be used.

Extra product stream(s).

The FILESPEC for this Problem Definition data file is: B:EX_06P.DAT

The FILESPEC for this Problem Results data file is: B:EX_06R.DAT

FEED AND PRODUCT STREAM DATA:

	STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	FLOW RATE (L/min)	TEMP (C)
AQUEOUS	1	3.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E-01	40.0
AQUEOUS	3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.75E+00	1.75E+00	1.00E-03	40.0
AQUEOUS	6	3.00E+00	3.00E+02	3.00E+00	0.00E+00	0.00E+00	0.00E+00	1.50E-01	40.0
30.0 % TBP	10	0.00E+00	0.00E+00	0.00E+00				3.50E+01	40.0
AQUEOUS	5	Product stream removed (actual flow rate to be computed)						1.00E+01	

INITIAL AQUEOUS PROFILE DATA:

	STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU(III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	TEMP (C)
	1	2.84E+00	2.65E+01	3.99E-01	0.00E+00	0.00E+00	0.00E+00	40.0
	2	2.76E+00	4.10E+01	6.40E-01	0.00E+00	0.00E+00	0.00E+00	40.0
	3	2.68E+00	5.37E+01	8.54E-01	0.00E+00	0.00E+00	0.00E+00	40.0
	4	2.59E+00	6.97E+01	1.12E+00	0.00E+00	0.00E+00	0.00E+00	40.0
	5	2.45E+00	1.00E+02	1.60E+00	0.00E+00	0.00E+00	0.00E+00	40.0
	6	3.00E+00	3.00E+02	2.69E+00	0.00E+00	0.00E+00	0.00E+00	40.0
	7	3.00E+00	3.00E+02	2.39E+00	0.00E+00	0.00E+00	0.00E+00	40.0
	8	3.05E+00	2.95E+02	2.05E+00	0.00E+00	0.00E+00	0.00E+00	40.0
	9	3.49E+00	2.24E+02	1.38E+00	0.00E+00	0.00E+00	0.00E+00	40.0
	10	3.15E+00	1.98E+01	1.79E-01	0.00E+00	0.00E+00	0.00E+00	40.0

INITIAL ORGANIC PROFILE DATA:

	STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)
	1	1.97E-01	8.79E+01	8.40E-01
	2	1.57E-01	9.51E+01	9.49E-01
	3	1.34E-01	9.91E+01	1.01E+00
	4	1.14E-01	1.03E+02	1.07E+00

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)
5	9.05E-02	1.07E+02	1.14E+00
6	5.61E-02	1.15E+02	1.27E+00
7	5.62E-02	1.16E+02	1.13E+00
8	5.75E-02	1.16E+02	9.82E-01
9	7.54E-02	1.13E+02	8.13E-01
10	2.41E-01	8.38E+01	5.08E-01

STAGE VOLUME AND FLOW RATE DATA (Molal basis):

STAGE NO.	MIXER VOLUME BY PHASE		SETTLER VOLUME BY PHASE		MIXER FLOW RATE		INTERSTAGE FLOW RATE	
	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC
1	3.60E-02	1.20E-01	1.10E-01	5.80E-01	9.07E-02	3.47E-01	9.07E-02	3.47E-01
2	3.60E-02	1.20E-01	1.10E-01	3.80E-01	9.07E-02	3.47E-01	9.07E-02	3.47E-01
3	3.60E-02	1.20E-01	1.10E-01	3.80E-01	9.17E-02	3.47E-01	9.17E-02	3.47E-01
4	3.60E-02	1.20E-01	1.10E-01	3.80E-01	9.17E-02	3.47E-01	9.17E-02	3.47E-01
5	3.60E-02	1.20E-01	3.10E-01	3.80E-01	9.17E-02	3.47E-01	0.00E+00	3.47E-01
6	1.70E-01	4.00E-01	5.10E-01	1.70E+00	1.22E-01	3.47E-01	1.22E-01	3.47E-01
7	1.70E-01	4.00E-01	5.10E-01	1.18E+00	1.22E-01	3.47E-01	1.22E-01	3.47E-01
8	1.70E-01	4.00E-01	5.10E-01	1.18E+00	1.22E-01	3.47E-01	1.22E-01	3.47E-01
9	1.70E-01	4.00E-01	5.10E-01	1.18E+00	1.22E-01	3.47E-01	1.22E-01	3.47E-01
10	1.70E-01	4.00E-01	7.00E-01	1.18E+00	1.22E-01	3.47E-01	1.22E-01	3.47E-01

PROBLEM RESULTS FOR SEPHIS MOD4, Ver. 2.11:

06-08-1990 09:36

Problem: Ex. 6 - ORNL-5471 - Pulsed Columns II
 (mixer concentrations shown)

TIME = 0.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	2.84E+00	2.65E+01	3.99E-01	0.00E+00	0.00E+00	0.00E+00	1.12E+00	1.00E-01	40.0
2	2.76E+00	4.10E+01	6.40E-01	0.00E+00	0.00E+00	0.00E+00	1.14E+00	1.01E-01	40.0
3	2.68E+00	5.37E+01	8.54E-01	0.00E+00	0.00E+00	0.00E+00	1.16E+00	1.02E-01	40.0
4	2.59E+00	6.97E+01	1.12E+00	0.00E+00	0.00E+00	0.00E+00	1.18E+00	1.02E-01	40.0
5	2.45E+00	1.00E+02	1.60E+00	0.00E+00	0.00E+00	0.00E+00	1.21E+00	1.03E-01	40.0
5	PRODUCT STREAM								1.03E-01
6	3.00E+00	3.00E+02	2.69E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
7	3.00E+00	3.00E+02	2.39E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
8	3.05E+00	2.95E+02	2.05E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
9	3.49E+00	2.24E+02	1.38E+00	0.00E+00	0.00E+00	0.00E+00	1.41E+00	1.48E-01	40.0
10	3.15E+00	1.98E+01	1.79E-01	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.36E-01	40.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.97E-01	8.79E+01	8.40E-01	1.21E+01	7.63E+00	2.52E-01	9.40E-01	3.64E-01	86.1	2.00E+02
2	1.57E-01	9.51E+01	9.49E-01	8.41E+00	5.37E+00	2.06E-01	9.48E-01	3.64E-01	88.0	2.00E+02
3	1.34E-01	9.91E+01	1.01E+00	6.61E+00	4.25E+00	1.79E-01	9.53E-01	3.65E-01	89.1	2.00E+02
4	1.14E-01	1.03E+02	1.07E+00	5.26E+00	3.42E+00	1.58E-01	9.57E-01	3.65E-01	90.0	2.00E+02
5	9.05E-02	1.07E+02	1.14E+00	3.80E+00	2.55E+00	1.31E-01	9.62E-01	3.65E-01	91.2	2.00E+02
6	5.61E-02	1.15E+02	1.27E+00	9.37E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	2.00E+02
7	5.62E-02	1.16E+02	1.13E+00	9.38E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	2.00E+02
8	5.75E-02	1.16E+02	9.82E-01	9.55E-01	1.17E+00	4.60E-02	9.72E-01	3.66E-01	94.6	2.00E+02
9	7.54E-02	1.13E+02	8.13E-01	1.25E+00	1.45E+00	5.33E-02	9.70E-01	3.66E-01	94.5	2.00E+02
10	2.40E-01	8.38E+01	5.08E-01	1.13E+01	7.58E+00	2.04E-01	9.35E-01	3.64E-01	86.6	2.00E+02

TIME = 10.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	2.85E+00	2.65E+01	1.56E-03	0.00E+00	0.00E+00	0.00E+00	1.12E+00	1.00E-01	40.0
2	2.76E+00	4.07E+01	7.97E-04	0.00E+00	0.00E+00	0.00E+00	1.14E+00	1.01E-01	40.0
3	2.66E+00	5.21E+01	0.00E+00	1.83E+00	9.55E-03	1.72E-02	1.16E+00	1.02E-01	40.0
4	2.56E+00	6.69E+01	4.00E-01	4.09E+00	7.74E-05	1.72E-02	1.18E+00	1.02E-01	40.0
5	2.42E+00	9.74E+01	1.37E+00	4.08E+00	0.00E+00	1.71E-02	1.22E+00	1.03E-01	40.0
5	PRODUCT STREAM								1.03E-01
6	3.00E+00	3.00E+02	2.65E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
7	3.00E+00	3.00E+02	2.33E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
8	3.05E+00	2.95E+02	1.97E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
9	3.48E+00	2.25E+02	1.32E+00	0.00E+00	0.00E+00	0.00E+00	1.41E+00	1.48E-01	40.0
10	3.15E+00	1.99E+01	1.71E-01	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.36E-01	40.0

ORGANIC PHASE:										
STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.98E-01	8.86E+01	3.30E-03	1.21E+01	7.67E+00	2.52E-01	9.39E-01	3.64E-01	86.1	7.52E+01
2	1.58E-01	9.58E+01	1.20E-03	8.53E+00	5.44E+00	2.08E-01	9.48E-01	3.64E-01	88.0	7.51E+01
3	1.36E-01	9.97E+01	0.00E+00	6.86E+00	0.00E+00	1.83E-01	9.52E-01	3.64E-01	88.9	1.49E+01
4	1.16E-01	1.03E+02	4.00E-01	5.52E+00	3.19E-01	1.62E-01	9.56E-01	3.65E-01	89.9	1.85E+01
5	9.07E-02	1.07E+02	1.01E+00	3.91E+00	6.59E-01	1.33E-01	9.62E-01	3.65E-01	91.2	1.65E+00
6	5.61E-02	1.15E+02	1.25E+00	9.37E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	1.09E-01
7	5.62E-02	1.16E+02	1.10E+00	9.38E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	2.16E-01
8	5.75E-02	1.16E+02	9.44E-01	9.54E-01	1.17E+00	4.60E-02	9.72E-01	3.66E-01	94.6	3.08E-01
9	7.53E-02	1.13E+02	7.74E-01	1.25E+00	1.45E+00	5.33E-02	9.70E-01	3.66E-01	94.5	3.67E-01
10	2.40E-01	8.40E+01	4.82E-01	1.13E+01	7.54E+00	2.03E-01	9.35E-01	3.64E-01	86.7	3.92E-01

TIME = 20.00 MINUTES

AQUEOUS PHASE:										
STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)	
1	2.84E+00	2.65E+01	1.18E-06	0.00E+00	0.00E+00	0.00E+00	1.12E+00	1.00E-01	40.0	
2	2.76E+00	4.08E+01	6.04E-07	0.00E+00	0.00E+00	0.00E+00	1.14E+00	1.01E-01	40.0	
3	2.66E+00	5.27E+01	0.00E+00	2.82E-04	1.72E-02	1.72E-02	1.16E+00	1.02E-01	40.0	
4	2.57E+00	6.69E+01	0.00E+00	2.94E+00	4.87E-03	1.72E-02	1.18E+00	1.02E-01	40.0	
5	2.42E+00	9.64E+01	9.96E-01	4.07E+00	6.84E-05	1.71E-02	1.22E+00	1.02E-01	40.0	
5	PRODUCT STREAM								1.02E-01	
6	3.00E+00	3.00E+02	2.63E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0	
7	3.00E+00	3.00E+02	2.28E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0	
8	3.05E+00	2.95E+02	1.92E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0	
9	3.48E+00	2.25E+02	1.27E+00	0.00E+00	0.00E+00	0.00E+00	1.42E+00	1.48E-01	40.0	
10	3.15E+00	2.00E+01	1.65E-01	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.36E-01	40.0	

ORGANIC PHASE:										
STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.98E-01	8.86E+01	2.50E-06	1.21E+01	7.67E+00	2.53E-01	9.39E-01	3.64E-01	86.1	3.37E-03
2	1.58E-01	9.59E+01	9.05E-07	8.52E+00	5.43E+00	2.08E-01	9.48E-01	3.64E-01	88.0	2.03E-03
3	1.35E-01	9.98E+01	0.00E+00	6.79E+00	0.00E+00	1.83E-01	9.52E-01	3.64E-01	88.9	2.55E+02
4	1.17E-01	1.03E+02	0.00E+00	5.52E+00	0.00E+00	1.63E-01	9.56E-01	3.65E-01	89.8	1.85E+01
5	9.14E-02	1.07E+02	7.39E-01	3.96E+00	5.20E-01	1.34E-01	9.62E-01	3.65E-01	91.2	1.01E+01
6	5.61E-02	1.15E+02	1.24E+00	9.37E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	9.25E-02
7	5.62E-02	1.16E+02	1.08E+00	9.38E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	1.83E-01
8	5.75E-02	1.16E+02	9.18E-01	9.54E-01	1.17E+00	4.60E-02	9.72E-01	3.66E-01	94.6	2.60E-01
9	7.53E-02	1.13E+02	7.48E-01	1.24E+00	1.45E+00	5.32E-02	9.70E-01	3.66E-01	94.5	3.10E-01
10	2.39E-01	8.41E+01	4.65E-01	1.12E+01	7.52E+00	2.03E-01	9.35E-01	3.64E-01	86.7	3.30E-01

TIME = 30.00 MINUTES

AQUEOUS PHASE:									
STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
1	2.84E+00	2.65E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+00	1.00E-01	40.0

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	PU (III) (g/L)	REDUCTANT (M)	NITRATE ION (M)	DENSITY (g/mL)	FLOW RATE (L/min)	TEMP (C)
2	2.76E+00	4.09E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.14E+00	1.01E-01	40.0
3	2.66E+00	5.30E+01	0.00E+00	0.00E+00	1.72E-02	1.72E-02	1.16E+00	1.02E-01	40.0
4	2.57E+00	6.89E+01	0.00E+00	1.59E+00	1.05E-02	1.72E-02	1.18E+00	1.02E-01	40.0
5	2.43E+00	9.63E+01	5.53E-01	4.08E+00	2.54E-05	1.71E-02	1.22E+00	1.02E-01	40.0
5	PRODUCT STREAM								1.02E-01
6	3.00E+00	3.00E+02	2.61E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
7	3.00E+00	3.00E+02	2.24E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
8	3.05E+00	2.95E+02	1.87E+00	0.00E+00	0.00E+00	0.00E+00	1.50E+00	1.50E-01	40.0
9	3.48E+00	2.25E+02	1.24E+00	0.00E+00	0.00E+00	0.00E+00	1.42E+00	1.48E-01	40.0
10	3.15E+00	2.01E+01	1.61E-01	0.00E+00	0.00E+00	0.00E+00	1.13E+00	1.36E-01	40.0

ORGANIC PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	PU (IV) (g/L)	U EXTRACT FACTOR	PU EXTRACT FACTOR	H+ EXTRACT FACTOR	DENSITY (g/mL)	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	1.98E-01	8.87E+01	0.00E+00	1.21E+01	0.00E+00	2.52E-01	9.39E-01	3.64E-01	86.1	6.71E-03
2	1.58E-01	9.59E+01	0.00E+00	8.50E+00	0.00E+00	2.07E-01	9.48E-01	3.64E-01	88.0	1.13E-02
3	1.35E-01	9.99E+01	0.00E+00	6.75E+00	0.00E+00	1.82E-01	9.52E-01	3.64E-01	88.9	1.84E-02
4	1.16E-01	1.03E+02	0.00E+00	5.44E+00	0.00E+00	1.61E-01	9.56E-01	3.65E-01	89.8	5.08E+00
5	9.17E-02	1.08E+02	4.12E-01	3.98E+00	3.17E-01	1.35E-01	9.62E-01	3.65E-01	91.2	9.57E+00
6	5.61E-02	1.15E+02	1.23E+00	9.37E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	7.71E-02
7	5.62E-02	1.16E+02	1.06E+00	9.38E-01	1.15E+00	4.56E-02	9.72E-01	3.66E-01	94.6	1.54E-01
8	5.75E-02	1.16E+02	8.96E-01	9.54E-01	1.17E+00	4.60E-02	9.72E-01	3.66E-01	94.6	2.19E-01
9	7.52E-02	1.14E+02	7.27E-01	1.24E+00	1.45E+00	5.32E-02	9.70E-01	3.66E-01	94.5	2.61E-01
10	2.39E-01	8.41E+01	4.51E-01	1.12E+01	7.50E+00	2.02E-01	9.35E-01	3.64E-01	86.7	2.78E-01

7.7 THORIUM EXTRACTION

This sample problem is for an 11-stage acid Thorex extraction flow sheet using 30% TBP for the extraction of uranium and thorium shown in Fig. 7. Only the steady-state concentration profile is needed, so stage volume or initial profile information is unnecessary. The printout that follows Fig. 7 shows the final expected concentration profile.

The problem was previously calculated by using SEPHIS MOD3 on a mainframe computer.⁶ The computation time was ~6 s on the ORNL IBM 360/91 for an overall material balance of 99.9%. The computation time for SEPHIS MOD4, Version 2.11, on an IBM PC/XT without any upgrade features was 34 min 13 s to carry the process to a tolerance of 0.01% inventory change per minute.

The use of an upgraded system (16-MHz with 32-bit processor) resulted in a computation time of 8 min 48 s to carry the process to a tolerance of 0.0001% inventory change per minute. Note that the tolerance was not met within the maximum time specification of 200 min or the extra-time option of 400 min. The extra-time option had to be invoked a second time (providing a maximum time of 800 min) to attain the tolerance.

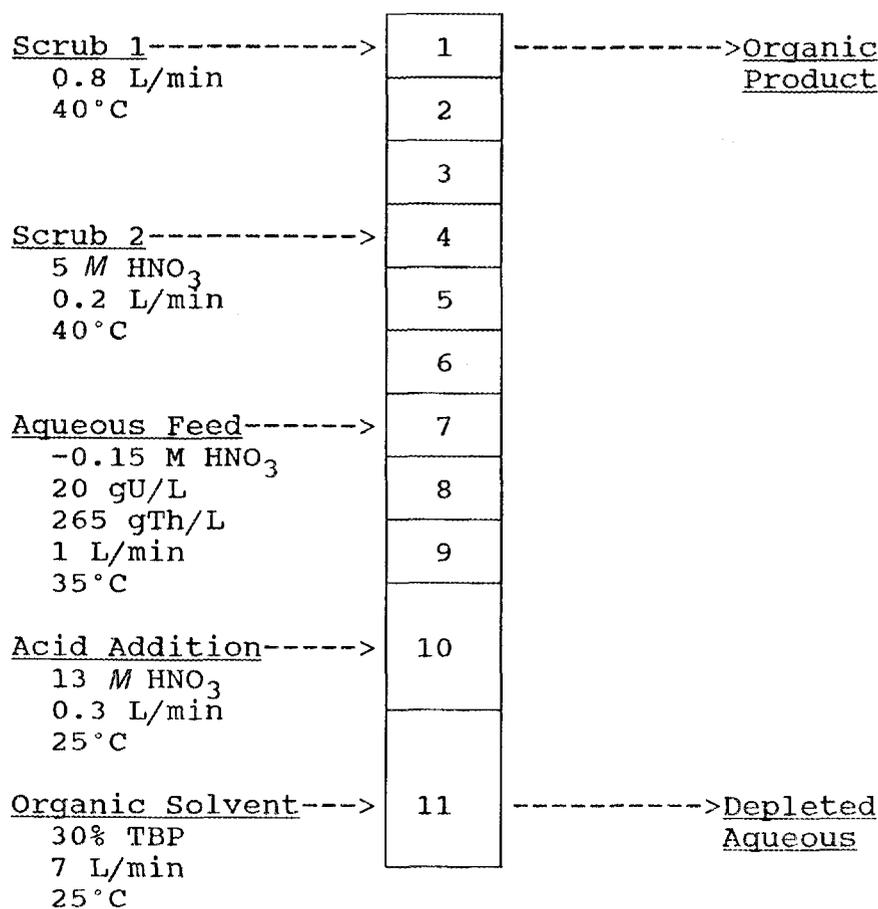


Fig. 7. Thorium extraction.

PROBLEM DEFINITION DATA FOR SEPHIS MOD4, Ver. 2.11:

02-05-1990 13:15

Problem: Ex. 7 - ORNL/CSD/TM-70 - U+Th Extraction

THOREX PROCESS

Total stages: 11

Volume % TBP in solvent: 30.0

Initial or default temperature (°C): 40.0

No unusual stage connections

Minutes per time increment: 1.00

Minutes between printing of the concentration profile: 200

Calculations will stop after 200 minutes or when a tolerance of 0.0001 % per minute is reached.

Mixer volumes = (phase flow)(unit time).

Settler volumes = (phase flow)(unit time).

Initial concentration profile is zero.

Trapezoidal integration will be used.

No extra product streams.

The FILESPEC for this Problem Definition data file is: B:EX_07P.DAT

The FILESPEC for this Problem Results data file is: B:EX_07R.DAT

FEED AND PRODUCT STREAM DATA:

	STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	THORIUM (g/L)	NITRATE ION (M)	FLOW RATE (L/min)	TEMP (C)
AQUEOUS	1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.00E-01	40.0
AQUEOUS	4	5.00E+00	0.00E+00	0.00E+00	0.00E+00	2.00E-01	40.0
AQUEOUS	7	-1.50E-01	2.00E+01	2.65E+02	0.00E+00	1.00E+00	35.0
AQUEOUS	10	1.30E+01	0.00E+00	0.00E+00	0.00E+00	3.00E-01	25.0
30.0 % TBP	11	0.00E+00	0.00E+00	0.00E+00		7.00E+00	25.0

STAGE VOLUME AND FLOW RATE DATA (Molal basis):

STAGE NO.	MIXER VOLUME BY PHASE		SETTLER VOLUME BY PHASE		MIXER FLOW RATE		INTERSTAGE FLOW RATE	
	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC	AQUEOUS	ORGANIC
1	8.00E-01	7.00E+00	8.00E-01	7.00E+00	8.00E-01	7.00E+00	8.00E-01	7.00E+00
2	8.00E-01	7.00E+00	8.00E-01	7.00E+00	8.00E-01	7.00E+00	8.00E-01	7.00E+00
3	8.00E-01	7.00E+00	8.00E-01	7.00E+00	8.00E-01	7.00E+00	8.00E-01	7.00E+00
4	1.00E+00	7.00E+00	1.00E+00	7.00E+00	1.00E+00	7.00E+00	1.00E+00	7.00E+00
5	1.00E+00	7.00E+00	1.00E+00	7.00E+00	1.00E+00	7.00E+00	1.00E+00	7.00E+00
6	1.00E+00	7.00E+00	1.00E+00	7.00E+00	1.00E+00	7.00E+00	1.00E+00	7.00E+00
7	2.00E+00	7.00E+00	2.00E+00	7.00E+00	2.00E+00	7.00E+00	2.00E+00	7.00E+00
8	2.00E+00	7.00E+00	2.00E+00	7.00E+00	2.00E+00	7.00E+00	2.00E+00	7.00E+00
9	2.00E+00	7.00E+00	2.00E+00	7.00E+00	2.00E+00	7.00E+00	2.00E+00	7.00E+00
10	2.30E+00	7.00E+00	2.30E+00	7.00E+00	2.30E+00	7.00E+00	2.30E+00	7.00E+00
11	2.30E+00	7.00E+00	2.30E+00	7.00E+00	2.30E+00	7.00E+00	2.30E+00	7.00E+00

PROBLEM RESULTS FOR SEPHIS MOD4, Ver. 2.11:

06-08-1990 09:43

Problem: Ex. 7 - DRNL/CSD/TM-70 - U+Th Extraction
(mixer concentrations shown)

TIME = 0.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	THORIUM (g/L)	NITRATE ION (M)	FLOW RATE (L/min)	TEMP (C)
1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.00E-01	40.0
2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.00E-01	40.0
3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.00E-01	40.0
4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	40.0
5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	40.0
6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E+00	40.0
7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.00E+00	40.0
8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.00E+00	40.0
9	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.00E+00	40.0
10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.30E+00	40.0
11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.30E+00	40.0

ORGANIC PHASE (The indication of 3 phases is within a 10% tolerance):

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	THORIUM (g/L)	U EXTRACT FACTOR	TH EXTRACT FACTOR	H+ EXTRACT FACTOR	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.00E+00	0.0	2.00E+02
2	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.00E+00	0.0	2.00E+02
3	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.00E+00	0.0	2.00E+02
4	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.00E+00	0.0	2.00E+02
5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.00E+00	0.0	2.00E+02
6	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.00E+00	0.0	2.00E+02
7	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.00E+00	0.0	2.00E+02
8	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.00E+00	0.0	2.00E+02
9	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.00E+00	0.0	2.00E+02
10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.00E+00	0.0	2.00E+02
11	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.00E+00	0.0	2.00E+02

TIME = 200.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	THORIUM (g/L)	NITRATE ION (M)	FLOW RATE (L/min)	TEMP (C)
1	4.22E-01	6.30E-01	9.89E+01	0.00E+00	8.00E-01	34.6
2	8.79E-01	4.55E-01	1.13E+02	0.00E+00	8.00E-01	32.9
3	1.38E+00	4.03E-01	1.10E+02	0.00E+00	8.00E-01	32.3
4	1.97E+00	3.70E-01	1.03E+02	0.00E+00	1.00E+00	32.1
5	1.81E+00	3.49E-01	1.11E+02	0.00E+00	1.00E+00	31.4
6	1.58E+00	3.46E-01	1.16E+02	0.00E+00	1.00E+00	31.1
7	1.25E+00	3.54E-01	1.20E+02	0.00E+00	2.00E+00	30.9
8	1.97E+00	1.75E-02	5.06E+01	0.00E+00	2.00E+00	29.2
9	2.61E+00	3.56E-04	9.45E+00	0.00E+00	2.00E+00	27.8
10	3.30E+00	3.32E-06	1.06E+00	0.00E+00	2.30E+00	26.6

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	THORIUM (g/L)	NITRATE ION (M)	FLOW RATE (L/min)	TEMP (C)
11	1.91E+00	5.05E-08	1.72E-01	0.00E+00	2.30E+00	25.8

ORGANIC PHASE (The indication of 3 phases is within a 10% tolerance):

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	THORIUM (g/L)	U EXTRACT FACTOR	TH EXTRACT FACTOR	H+ EXTRACT FACTOR	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	5.08E-02	2.86E+00	3.79E+01	3.97E+01	3.36E+00	1.05E+00	7.00E+00	51.6	1.80E-02
2	9.91E-02	2.93E+00	4.92E+01	5.64E+01	3.81E+00	9.86E-01	7.00E+00	69.4	1.50E-02
3	1.51E-01	2.91E+00	5.08E+01	6.32E+01	4.06E+00	9.56E-01	7.00E+00	76.1	1.26E-02
4	2.09E-01	2.90E+00	5.04E+01	5.49E+01	3.43E+00	7.43E-01	7.00E+00	80.9	9.81E-03
5	1.90E-01	2.91E+00	5.26E+01	5.84E+01	3.32E+00	7.35E-01	7.00E+00	81.6	1.15E-02
6	1.67E-01	2.91E+00	5.37E+01	5.88E+01	3.25E+00	7.38E-01	7.00E+00	80.8	1.39E-02
7	1.34E-01	2.91E+00	5.44E+01	2.87E+01	1.58E+00	3.75E-01	7.00E+00	78.7	1.98E-02
8	2.88E-01	1.01E-01	3.44E+01	2.02E+01	2.38E+00	5.12E-01	7.00E+00	67.0	2.22E-02
9	4.92E-01	5.01E-03	1.44E+01	4.93E+01	5.34E+00	6.59E-01	7.00E+00	62.0	3.62E-02
10	6.77E-01	1.02E-04	2.65E+00	9.33E+01	7.61E+00	6.24E-01	7.00E+00	65.0	5.13E-02
11	4.59E-01	1.07E-06	2.92E-01	6.47E+01	5.18E+00	7.33E-01	7.00E+00	42.3	5.44E-02

TIME = 400.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	THORIUM (g/L)	NITRATE ION (M)	FLOW RATE (L/min)	TEMP (C)
1	4.25E-01	6.31E-01	9.85E+01	0.00E+00	8.00E-01	34.6
2	8.85E-01	4.57E-01	1.13E+02	0.00E+00	8.00E-01	32.9
3	1.39E+00	4.95E-01	1.09E+02	0.00E+00	8.00E-01	32.3
4	1.98E+00	3.72E-01	1.02E+02	0.00E+00	1.00E+00	32.1
5	1.82E+00	3.52E-01	1.10E+02	0.00E+00	1.00E+00	31.4
6	1.59E+00	3.49E-01	1.15E+02	0.00E+00	1.00E+00	31.1
7	1.26E+00	3.57E-01	1.20E+02	0.00E+00	2.00E+00	30.9
8	1.98E+00	1.76E-02	4.98E+01	0.00E+00	2.00E+00	29.2
9	2.62E+00	3.52E-04	9.19E+00	0.00E+00	2.00E+00	27.8
10	3.31E+00	3.25E-06	1.02E+00	0.00E+00	2.30E+00	26.6
11	1.91E+00	4.94E-08	1.66E-01	0.00E+00	2.30E+00	25.8

ORGANIC PHASE (The indication of 3 phases is within a 10% tolerance):

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	THORIUM (g/L)	U EXTRACT FACTOR	TH EXTRACT FACTOR	H+ EXTRACT FACTOR	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)
1	5.12E-02	2.86E+00	3.78E+01	3.96E+01	3.36E+00	1.05E+00	7.00E+00	51.5	3.25E-04
2	9.97E-02	2.93E+00	4.91E+01	5.61E+01	3.81E+00	9.87E-01	7.00E+00	69.3	2.80E-04
3	1.52E-01	2.91E+00	5.07E+01	6.29E+01	4.07E+00	9.57E-01	7.00E+00	75.9	2.38E-04
4	2.10E-01	2.90E+00	5.03E+01	5.46E+01	3.44E+00	7.44E-01	7.00E+00	80.8	1.93E-04

ORGANIC PHASE (The indication of 3 phases is within a 10% tolerance):							FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)	
STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	THORIUM (g/L)	U EXTRACT FACTOR	TH EXTRACT FACTOR	H+ EXTRACT FACTOR				
5	1.91E-01	2.91E+00	5.24E+01	5.79E+01	3.34E+00	7.36E-01	7.00E+00	81.5	2.15E-04	
#####	3 Phases Possible in the above stage									
6	1.68E-01	2.91E+00	5.35E+01	5.83E+01	3.26E+00	7.39E-01	7.00E+00	80.7	2.59E-04	
#####	3 Phases Possible in the above stage									
7	1.35E-01	2.91E+00	5.42E+01	2.85E+01	1.59E+00	3.75E-01	7.00E+00	78.6	3.69E-04	
#####	3 Phases Possible in the above stage									
8	2.91E-01	1.02E-01	3.41E+01	2.03E+01	2.40E+00	5.14E-01	7.00E+00	66.9	4.13E-04	
9	4.95E-01	5.02E-03	1.42E+01	4.99E+01	5.40E+00	6.61E-01	7.00E+00	62.0	6.79E-04	
10	6.79E-01	1.01E-04	2.57E+00	9.41E+01	7.64E+00	6.24E-01	7.00E+00	65.0	9.54E-04	
11	4.60E-01	1.05E-06	2.82E-01	6.49E+01	5.19E+00	7.33E-01	7.00E+00	42.3	1.01E-03	

TIME = 516.00 MINUTES

AQUEOUS PHASE:

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	THORIUM (g/L)	NITRATE IDN (M)	FLOW RATE (L/min)	TEMP (C)
1	4.25E-01	6.31E-01	9.85E+01	0.00E+00	8.00E-01	34.6
2	8.85E-01	4.57E-01	1.13E+02	0.00E+00	8.00E-01	32.9
3	1.39E+00	4.05E-01	1.09E+02	0.00E+00	8.00E-01	32.3
4	1.98E+00	3.73E-01	1.02E+02	0.00E+00	1.00E+00	32.1
5	1.82E+00	3.52E-01	1.10E+02	0.00E+00	1.00E+00	31.4
6	1.59E+00	3.49E-01	1.15E+02	0.00E+00	1.00E+00	31.1
7	1.26E+00	3.57E-01	1.20E+02	0.00E+00	2.00E+00	30.9
8	1.98E+00	1.76E-02	4.98E+01	0.00E+00	2.00E+00	29.2
9	2.62E+00	3.52E-04	9.18E+00	0.00E+00	2.00E+00	27.8
10	3.31E+00	3.25E-06	1.02E+00	0.00E+00	2.30E+00	26.6
11	1.91E+00	4.93E-08	1.65E-01	0.00E+00	2.30E+00	25.8

ORGANIC PHASE (The indication of 3 phases is within a 10% tolerance):

STAGE NO.	NITRIC ACID (M)	URANIUM (g/L)	THORIUM (g/L)	U EXTRACT FACTOR	TH EXTRACT FACTOR	H+ EXTRACT FACTOR	FLOW RATE (L/min)	TBPSAT (%)	INVENTORY CHANGE (%)	
1	5.12E-02	2.86E+00	3.78E+01	3.96E+01	3.36E+00	1.05E+00	7.00E+00	51.5	4.29E-05	
2	9.98E-02	2.93E+00	4.91E+01	5.61E+01	3.81E+00	9.87E-01	7.00E+00	69.3	2.16E-05	
3	1.52E-01	2.91E+00	5.07E+01	6.29E+01	4.07E+00	9.57E-01	7.00E+00	75.9	1.83E-05	
#####	3 Phases Possible in the above stage									
4	2.10E-01	2.90E+00	5.03E+01	5.46E+01	3.44E+00	7.44E-01	7.00E+00	80.8	1.60E-05	
#####	3 Phases Possible in the above stage									
5	1.91E-01	2.91E+00	5.24E+01	5.79E+01	3.34E+00	7.36E-01	7.00E+00	81.5	2.61E-05	
#####	3 Phases Possible in the above stage									
6	1.68E-01	2.91E+00	5.35E+01	5.83E+01	3.26E+00	7.39E-01	7.00E+00	80.7	2.86E-05	
#####	3 Phases Possible in the above stage									
7	1.35E-01	2.91E+00	5.42E+01	2.85E+01	1.59E+00	3.75E-01	7.00E+00	78.6	3.65E-05	
#####	3 Phases Possible in the above stage									
8	2.91E-01	1.02E-01	3.41E+01	2.03E+01	2.40E+00	5.14E-01	7.00E+00	66.9	4.39E-05	
9	4.96E-01	5.02E-03	1.42E+01	4.99E+01	5.40E+00	6.61E-01	7.00E+00	62.0	6.11E-05	
10	6.79E-01	1.01E-04	2.57E+00	9.42E+01	7.64E+00	6.24E-01	7.00E+00	65.0	9.40E-05	
11	4.60E-01	1.05E-06	2.82E-01	6.49E+01	5.19E+00	7.33E-01	7.00E+00	42.3	9.20E-05	

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APPENDIX A
SAMPLE SCREEN DISPLAYS

PC - S E P H I S - MOD4
Version 2.11 (1990)

A Solvent Extraction Process Having Interacting Solutes

For Uranium, Plutonium, Thorium, and Nitric Acid
Mass Transfer in Purex- or Thorex-type Flowsheets

W.S. Groenier
Fuel Recycle Division
Oak Ridge National Laboratory

*** MENU ***

1. Define a problem.
2. Run a problem.
3. Print a problem.

Enter the number (1 to 3) of your choice (0 to quit).

FEED STREAMS:

Feed to Stage No.: 6

Feed is Aqueous.

Feed flow rate (L/min.) is: 0.150

Nitric Acid (M): 3.000

Uranium (g/L): 300.000

Plutonium (IV) (g/L): 3.000

Plutonium (III) (g/L): 0.000

Plutonium Reductant (M): 0.000

Inextractable Nitrate Ion (M): 0.000

Temperature (°C): 40.0

Is the above information correct (Y/N)?

PRODUCT STREAMS:
(in addition to usual end streams)

Product from Stage No.: 5

Product is Aqueous.

Product flow rate (L/min.): 10.000

Is the above information correct (Y/N)?

INITIAL CONCENTRATION PROFILE: (Aqueous)							
Stage No.	HNO3 (M)	U (g/L)	Pu(IV) (g/L)	Pu(III) (g/L)	REDUCTANT (M)	NITRATE (M)	TEMP (C)
1	2.84E+00	2.77E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	40.00
2	2.75E+00	4.28E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	40.00
3	2.64E+00	5.56E+01	0.00E+00	0.00E+00	1.72E-02	1.72E-02	40.00
4	2.55E+00	7.19E+01	0.00E+00	4.47E-02	1.70E-02	1.72E-02	40.00
5	2.41E+00	1.00E+02	1.75E-02	4.08E+00	0.00E+00	1.71E-02	40.00
6	3.00E+00	3.00E+02	2.87E+00	0.00E+00	0.00E+00	0.00E+00	40.00
7	3.00E+00	3.00E+02	2.74E+00	0.00E+00	0.00E+00	0.00E+00	40.00
8	3.05E+00	2.94E+02	2.55E+00	0.00E+00	0.00E+00	0.00E+00	40.00
9	3.48E+00	2.24E+02	1.91E+00	0.00E+00	0.00E+00	0.00E+00	40.00
10	3.14E+00	2.14E+01	2.67E-01	0.00E+00	0.00E+00	0.00E+00	40.00

Are the entries for the last stage correct (Y/N)?

INITIAL CONCENTRATION PROFILE: (Organic)			
Stage No.	HNO3 (M)	U (g/L)	Pu(IV) (g/L)
1	2.05E-01	8.75E+01	0.00E+00
2	1.63E-01	9.50E+01	0.00E+00
3	1.39E-01	9.91E+01	0.00E+00
4	1.19E-01	1.03E+02	0.00E+00
5	9.48E-02	1.07E+02	1.23E-02
6	5.96E-02	1.15E+02	1.13E+00
7	5.97E-02	1.15E+02	1.08E+00
8	6.12E-02	1.15E+02	1.02E+00
9	8.00E-02	1.13E+02	9.47E-01
10	2.44E-01	8.31E+01	6.78E-01

Are the entries for the last stage correct (Y/N)?

MIXER VOLUMES:

(Provide data only for first stage and stages where volume changes)

Mixer Volume (L)				Mixer Volume (L)			
Stage No.	Aqueous	Organic	Total	Stage No.	Aqueous	Organic	Total
1	3.60E-02	1.20E-01					
6	1.70E-01	4.00E-01					

More Mixer Volume Data (Y/N)? N

SETTLER VOLUMES:

(Provide data only for first stage and stages where volume changes)

Settler Volume (L)				Settler Volume (L)			
Stage No.	Aqueous	Organic	Total	Stage No.	Aqueous	Organic	Total
1	1.10E-01	5.80E-01					
2	1.10E-01	3.80E-01					
5	3.10E-01	3.80E-01					
6	5.10E-01	1.70E+00					
7	5.10E-01	1.18E+00					
10	7.00E-01	1.18E+00					

More Settler Volume Data (Y/N)? N

Steady-state condition is met ---
 Press any key to continue

TIME (min.)	STAGE NO.
256.00	1

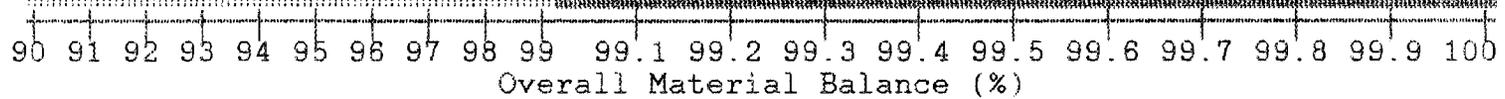
Problem is defined.
 Feed and product streams are identified.
 Initial concentration profile is established.
 Cascade flows are established.
 Stage volumes and flows are defined.
 Using trapezoidal integration.
 No plutonium reaction.
 Print time = 200 min.
 Maximum time = 400 min.

INVENTORY CHANGE (%/min.):		
Max.:	0.0001	>Stage: 9
Tol.:	0.0001	>Comp.: 3
OVERALL MATERIAL BALANCE (%):		
Nitric Acid:	100.00	
Uranium:	100.00	
Plutonium:	100.00	

NITRIC ACID:

URANIUM:

PLUTONIUM:



Maximum time reached ----
Press any key to continue

Problem is defined.
Feed and product streams are identified.
Initial concentration profile is established.
Cascade flows are established.
Stage volumes and flows are defined.
Using Runge-Kutta integration.
Pu(IV) reduced instantaneously.
Print time = 30 min.
Maximum time \square 30 min.

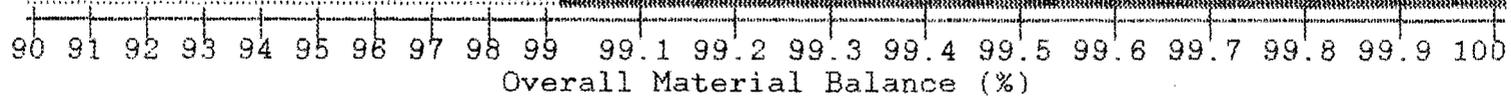
TIME (min.)	STAGE NO.
30.00	1

INVENTORY CHANGE (%/min.):	
Max.:	0.4780 >Stage: 10
Tol.:	0.0100 >Comp.: 3
OVERALL MATERIAL BALANCE (%):	
Nitric Acid:	100.04
Uranium:	99.69
Plutonium:	109.64

NITRIC ACID:

URANIUM:

PLUTONIUM:



APPENDIX B COMMON ERROR MESSAGES

Error trapping routines are included in the programs for the most common errors. They include:

Bad File Name	The file specification provided is not in a recognizable format. Enter correct file specification.
Disk Full	The user-supplied diskette is full. The problem will have to be rerun using a new diskette.
Disk Not Ready	The user-supplied diskette is not in place. Insert diskette and press any key.
File Not Found	The file specification provided is incorrect or the wrong diskette was placed in the drive. Check the diskette and press any key. Provide correct file specification when requested.
Printer Not Ready	The printer is not turned on. Turn printer on.

APPENDIX C HINTS

1. Do not use commas in problem names.
2. Since the Problem Definition and Problem Results files are in ASCII format, they can be edited with the on-screen editor for minor changes.
3. Also, the Problem Results file can be imported to graphics software to produce graphs of concentration profiles, the approach to steady-state, the effect of system changes, etc.
4. A multiple of the value of the specified time increment should exactly equal the specified time between printing of results. Otherwise, printouts of results will not be obtained at the desired times.
5. When conducting a study of the effect of varying flow sheet parameters, it is easy to complete one computation, prepare a new Problem Definition file for the changed parameter(s), and resume calculations by using as an initial concentration profile the final profile from the previous computation without changing diskettes. Be aware, however, that with more than six such computations, one may run out of diskette space. The use of an installed hard disk to store data files effectively eliminates this problem. When such a sequential study involves the chemical reduction of Pu(IV), an additional caution is noted below.
6. At the start of a new problem, mixer and settler zone concentrations in each stage are set equal to each other. If the new problem begins with a concentration profile from a previous problem, and that previous problem involved the chemical reduction of Pu(IV) and/or was not run to a steady state, note that the settler concentrations from the previous problem are not retained for use in the new problem. Only mixer concentrations are retained. Settler concentrations can differ from mixer concentrations during unsteady-state operation and when chemical reduction continues to occur in the settler zones. Consequently, a perturbation will occur when such problems are linked. It will prevail for only a few time increments and is of concern only when closely studying transient conditions.
7. The use of the Runge-Kutta integration technique for problems where plutonium reduction is occurring may produce incomplete material balances. It is recommended that the Fast technique be used for such problems. The Trapezoidal technique is also recommended if only a steady-state solution is desired.

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