

To the Graduate Council:

I am submitting herewith a thesis written by Alan M. Krichinsky entitled "NUMATH: A Nuclear Material Holdup Estimator for Unit Operations and Chemical Processes." I recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Chemical Engineering.

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NUMATH: A NUCLEAR MATERIAL HOLDUP ESTIMATOR FOR
UNIT OPERATIONS AND CHEMICAL PROCESSES

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ABSTRACT

A computer program, NUMATH (Nuclear Material Holdup Estimator), has been developed to permit inventory estimation in vessels involved in unit operations and chemical processes. This program has been implemented in an operating nuclear fuel processing plant.

NUMATH's purpose is to provide steady-state composition estimates for material residing in process vessels until representative samples can be obtained and chemical analyses can be performed. Since these compositions are used for inventory estimation, the results are determined for and cataloged in container-oriented files. The estimated compositions represent material collected in applicable vessels--including consideration for material previously acknowledged in these vessels.

The program utilizes process measurements and simple material balance models to estimate material holdups and distribution within unit operations. During simulated run testing, NUMATH-estimated inventories typically produced material balances within 7% of the associated measured material balances for uranium and within 16% of the associated, measured material balances for thorium during steady-state process operation.

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LIST OF SYMBOLS

A	elemental conversion constant
B	elemental conversion factor
C	elemental concentration (in grams per liter or gram per gram)
D	elemental distribution factor
F	isotopic weight fraction (in gram of isotope per gram of element)
M	molarity
MSpG	molarity-to-specific gravity conversion factor
P	performance function
Q	bulk quantity contribution (in grams or liters for collecting vessels; in grams per hour or liter per hour for flow-through vessels)
SpG	measured specific gravity
W	molecular weight
X	source material vector
Y	resultant material vector
$\sum_s X^s$	sum of all X^s 's for all s

Subscripts

i	isotope
j	element
k	summation variable for m
m	number of elements (or components) significantly affecting the specific gravity correction

Superscripts

- n number of source materials (or source vessels)
- v estimated material in subject (central) vessel
- s source material and summation variable for n

1. INTRODUCTION

Purpose of NUMATH

In recent years, there has been widespread concern about the possible loss or diversion of nuclear materials at various points in the nuclear fuel cycle.¹ To minimize the possibility of material diversion and theft, the nuclear industry utilizes physical protection systems (guards, fences, intrusion alarms, etc.). To enhance the detection of possible material diversion or theft, the industry relies on material accountability.

Nuclear material accountability may be defined as the capability of a facility to account for nuclear material. This includes performing inventory measurements and maintaining inventory records.²

A material balance drawn around a unit operation, a chemical process,^a or an entire plant for a given period of time is simply stated as:

$$\text{inputs} - \text{outputs} = \text{ending inventory} - \text{beginning inventory.} \quad (1)$$

If measurements are taken to verify the balance, this relationship becomes only approximately correct due to the measurement errors affecting each term of the balance.

^aUnit operation pertains to the application of equipment for physical treatment (e.g., separation, purification, mixing, etc.) of material to provide a desired product; chemical process pertains to the application of equipment for chemical treatment (i.e., chemical reaction) of material to provide a desired product.³ In this study, no formal distinction is made between unit operations and chemical processes; furthermore, every occurrence of each term implies both types of treatment.

In chemical processing of nuclear material, a "closed" material balance⁴ for an inventory period is used and may be expressed as:

$$\begin{aligned} &\text{beginning inventory} + \text{inputs} - \text{outputs} - \text{ending inventory} \\ &= \text{physical inventory difference.} \quad (2) \end{aligned}$$

This material balance, by definition, includes all components and considers measurement error. The term introduced in the closed material balance, physical inventory difference (PID), has special significance in the nuclear industry since the material accounted for is of strategic importance. If this number becomes significant (as defined by propagated measurement errors), then certain procedures are initiated to find the source of this difference.

For transfers which are in progress, the inventories include unmeasured holdups (in-process inventories for which the quantities have not been determined by both bulk quantity measurement and quantitative composition analysis) with indeterminate uncertainty. When unit operations are involved in a transfer, that transfer might typically last days with commensurate "in-process" material contributing to the inventories. If the contribution of unmeasured holdups can be acceptably estimated from information about the system, then the uncertainties may be defined and more confidence may be placed on the PID. It is to these inventory estimations that NUMATH (Nuclear Material Holdup Estimator) is directed.

Present accountability systems maintain inventories on a batch-by-batch basis, with the more advanced systems being implemented by computer. Batch accounting typically requires material homogenization, multiple sampling, and chemical analysis to account for any nuclear

material within vessels of a process system. Such procedures require a minimum of 1.5 hours and average 4 to 8 hours. If the materials can be accounted for by established nondestructive analysis (NDA) techniques,^a the lag time for batch accounting may be reduced to as little as 0.1 hour.⁵⁻⁷ However, at present, remote processing of such materials usually precludes the use of NDA techniques or results in measurements of questionable utility.

Nondestructive analysis has been applied, nevertheless, to determine inventories of residual fissile material^b in equipment enclosed by glove boxes.⁸⁻¹⁰ It is significant to note that these measurements were *not* used for accountability purposes; they were obtained to assist in formulating material recovery and cleanup strategy in anticipation of site and equipment renovation or deactivation. Additionally, the amounts of material involved in such measurements were very small relative to the plant throughput. These measurements occupied one or more survey teams for periods of time ranging from one day to greater than one month (depending on the measurement technique employed and the number and complexity of the glove boxes surveyed), during which time all material movements were curtailed. Under these conditions, measurement accuracies ranging from $\pm 16\%$ to $\pm 50\%$ were achieved. Considering the costs (in plant downtime and manpower) and constraints (of no material movement) required to achieve this degree of accuracy, it is

^aNondestructive analysis is the characterization of material without altering its chemical or physical condition.

^bFissile material is any material (i.e., ^{233}U , ^{235}U , and Pu) which will split its nucleus (fission) to form two or more smaller nuclei.

considered a vast improvement merely to match this accuracy (i.e., $\pm 16\%$) while estimating the inventory on a timely basis without interfering with plant operations. It should be noted that such techniques have only been applied to measuring inventories of fissile material (i.e., plutonium and certain isotopes of uranium). NDA has not been applied to directly measure less valuable, fertile material^a which is also monitored for nuclear material accountability; however, an accuracy of $\pm 25\%$ is believed to be reasonably achievable for estimating inventories of fertile materials by NUMATH.

Thorough measurement of physical inventories requires cessation of plant operations, draining and flushing of process equipment into measured tanks, homogenization of tank contents, sampling, and chemical analysis--a procedure which could interrupt plant operations for several days. An alternative to shutting down the plant is to infer the quantity of in-process materials while the plant is operating. This inference (inventory estimation) can be of practical importance if acceptably accurate estimates of in-process nuclear materials can be provided while imposing less disruption to plant operations than would be necessitated by physical inventories at the required frequency.¹¹

NUMATH is designed to provide inventory estimation by utilizing previous inventory measurements, operating data, and, where available, on-line process measurements. For the present time, NUMATH's purpose is to provide a reasonable, temporary estimate of material inventory until accurate inventory determination can be obtained from chemical analysis.

^aFertile material is any material (i.e., Th and ²³⁸U) which, upon capturing neutrons, will be transmuted into fissile material.

Ultimately, it is believed that NUMATH will utilize on-line analyzers in addition to more advanced calculational techniques to provide accurate inventory determinations and estimates.

NUMATH Implementation Facility

The plant in which NUMATH has been implemented is the ^{233}U Radiochemical Processing Pilot Plant (RPPP) in operation at Oak Ridge National Laboratory. In addition to liquid and solids blending, unit operations employed in the plant include solids dissolution, solvent extraction, ion exchange, evaporation, and solidification. It should be noted that all of these processes (with the exception of solidification) are performed remotely--behind 5-foot-thick concrete walls--due to a significant radiation hazard. Although all of the processes mentioned above have had files (to be discussed in Section 5) prepared for NUMATH estimation, only two of them (solvent extraction and ion exchange) will be addressed in this study.

Solutions containing ^{233}U are subjected to solvent extraction and ion exchange purification to achieve desired product purity and to remove radioactive products of decay. The single-cycle solvent extraction system (Figure 1) recovers uranium from bulk thorium (and decay product) contaminants. An aqueous uranium-thorium feed solution enters the extraction-scrub column (V-4/V-5) where uranium (and trace thorium) is extracted to the organic phase. The bulk contaminants exit the bottom of the column as aqueous waste. The organic phase exits the top of the extraction-scrub column and is introduced into the bottom of the strip column (V-6/V-7) where the uranium (and trace thorium) in the

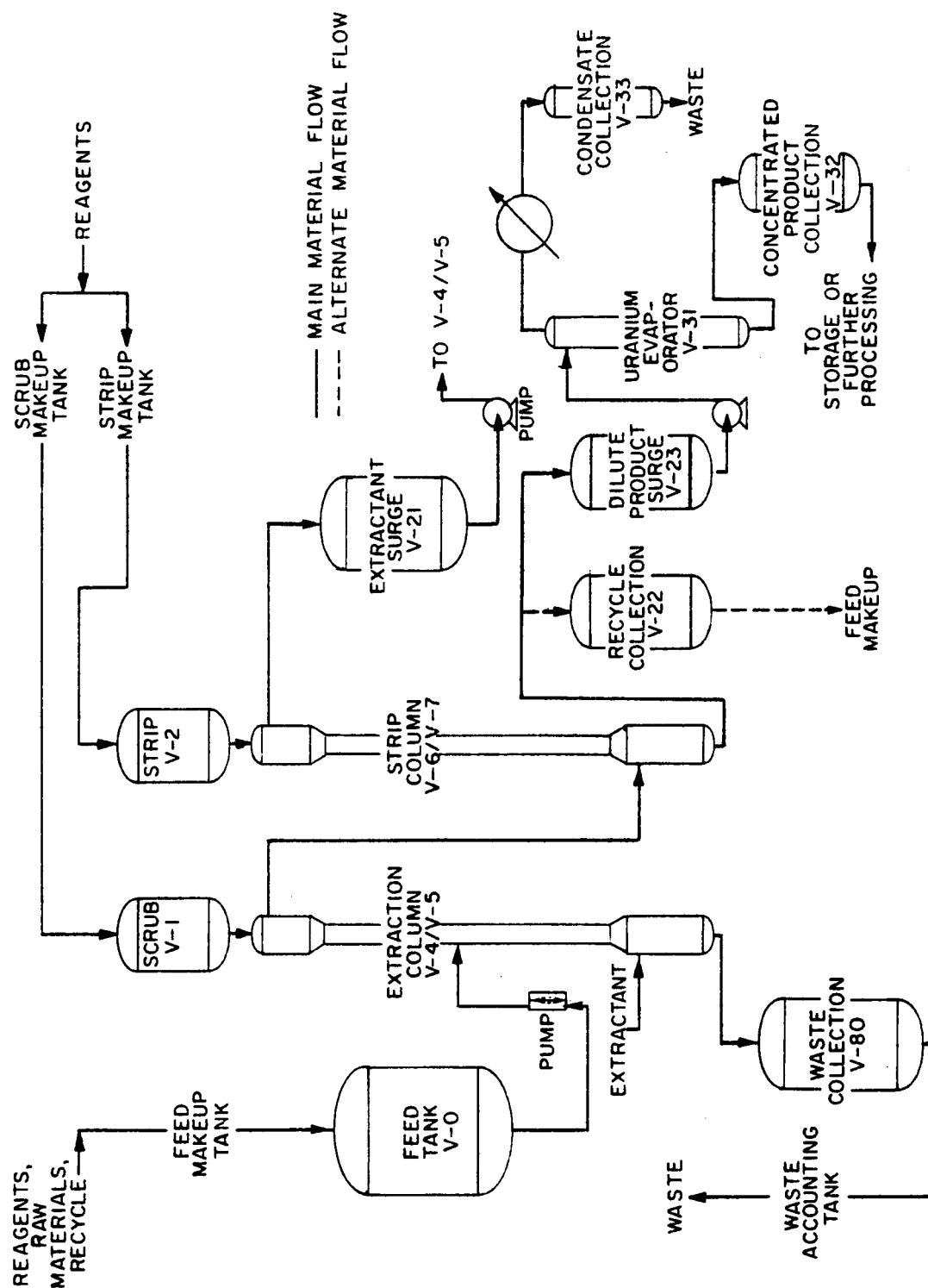


Figure 1. Flowsheet of a single-cycle solvent extraction system.

extractant (organic phase) transfers to the strip solution (aqueous phase). After evaporation of excess water, the aqueous phase is collected as concentrated product solution.

The ion exchange system (Figure 2) removes residual thorium (and some decay products) from aqueous uranium feed solutions. This system is operated in batch mode to (1) pretreat the stationary ion exchange resin with acid, (2) convert resin from acid to uranyl (UO_2^{+2}) form, (3) displace uranyl ions with thorium ions, and (4) regenerate the resin to acid form. Feed solutions flow through the system during steps 2 and 3. Useful product is collected only during step 3; all other effluents are collected as recycle or waste.

Material balances are regularly determined around these processes while they are in operation. The amounts of material actively involved in such processes are small relative to the entire plant inventory. It is significant to note, however, that while material may be categorized as "in process" (and not precisely measured) when it is actively involved in a unit operation, *all* material entering or leaving the plant boundary is accurately characterized.

Remote plant instrumentation directly useful in nuclear material accountability utilizes bubbler probes, pneumatic differential pressure transmitters, and strip chart recorders to indicate liquid level and specific gravity and includes thermocouples and recorders to indicate temperature on steam-jacketed vessels. For vessels in which solutions bearing nuclear material normally reside, a recent instrument upgrading (to improve measurement accuracy) augmented the existing volume determination system with electronic differential pressure transmitters

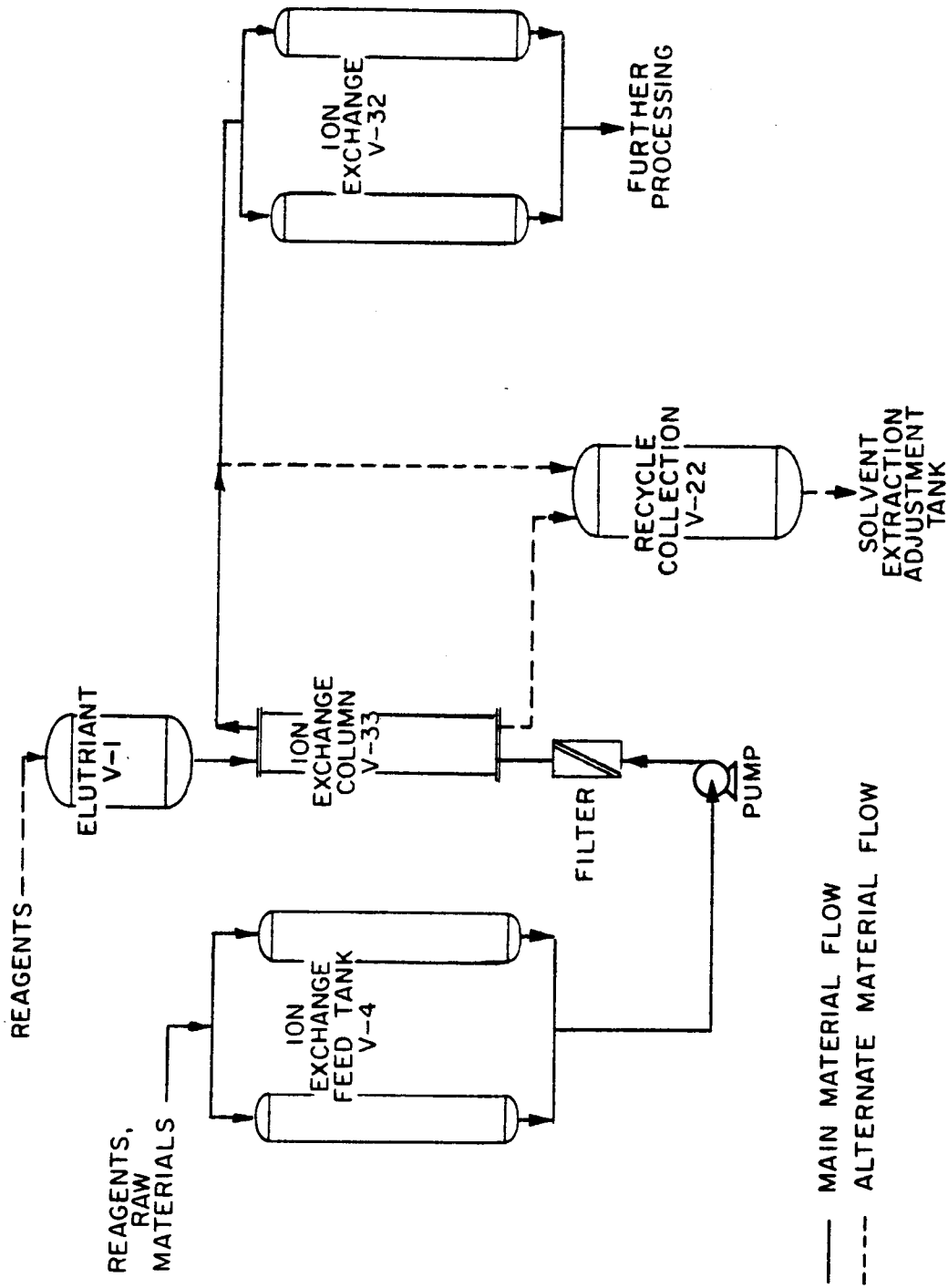


Figure 2. Flowsheet of an ion exchange system.

paralleling the pneumatic transmitters. The electronic transmitters provide a direct signal link to permit on-line (to the computer) volume determination.

Nondestructive analysis is used in the RPPP but, at present, only in determining uranium content of solid waste in 55-gallon drums.

The operations within the plant are essentially limited to handling thorium, uranium, and plutonium. Material accounting is correspondingly limited to maintaining inventories of those three elements and their accountable isotopes. Therefore, the models and estimations essentially address the same range of materials as the present accounting system. (Acid is also addressed but is not considered significant to the accountability aspects of this study.)

As the plant is a pilot facility, typical operations involve processing a category of source material, with a narrow range of characteristics (e.g., composition), for a relatively short period of time (i.e., 3 months to 5 years). At the end of an operating period, a different category of source material might be processed or a different type of product might be desired or both. Such changes in material characteristics necessitate operating condition changes, equipment redesign, or even new process development, design, and construction.

The character of pilot plant operation is a major consideration in the development of estimation routine strategies. It is significant to note that relatively short periods of operation and frequently extensive alterations to operating conditions and process equipment make it difficult to justify specialized modeling of unit operations as might be considered for a fixed, long-term process. (By contrast, NUMATH can

accommodate such alterations with relatively minor adjustments to a data file.) In addition, rigorous models tend to use extensive calculations to extract analytical or numerical solutions for unit operation simulations, making their use impractical on limited-memory minicomputers, especially when several other programs compete for memory space at the same time.

Features of NUMATH

NUMATH is a modularized, vessel-composition estimation program which uses nondestructive process measurements to estimate, with acceptable accuracy, in-process holdups (material retained within process vessels during or at the conclusion of steady-state operations) and end point (e.g., product, waste, etc.) vessel inventories until such time as confirmed inventories (inventories determined by both bulk quantity measurement and quantitative chemical analysis) can be established. Since the compositions are used for inventory estimation, the results are determined for and cataloged in container-oriented files. These estimated compositions represent material accumulated in applicable vessels--including consideration for material previously acknowledged in these vessels. The termination of any vessel's active involvement in the process prompts the program to collect pertinent data; to estimate the present inventory of every vessel (not designated as a source vessel--it is assumed that characteristics of material within source vessels do not change; only the bulk quantities of such vessels change in a depleting manner) which is involved in the unit operation based on each vessel's process measurements (i.e., volume and density), previous

vessel compositions (calculated or, if available, analyzed), unit operation characteristics (e.g., flow rates, vessel connections, transfer characteristics), and selected models; and, finally, to store the estimates in the physical inventory and other appropriate files in the system. Records in which estimates are stored are marked as containing estimated compositions until analyzed values supersede them. It is significant to note that all of these program activities are performed automatically--without any direct terminal operator interaction with NUMATH.

The entire NUMATH program is composed of over 10,000 lines of Fortran code which are overlayed to form a task that utilizes just over 16,000 words of active memory. Most of this code is involved in collecting applicable data, interpreting and cross referencing that data, and finally storing results in appropriate locations. The balance of the program is devoted to subroutines for supervising and calculating inventory estimates (Appendix A) for vessels involved in unit operations and is the focus of this document.

2. REVIEW OF LITERATURE

Specific and Modular Simulation Programs

Unit operation simulation programs may be classified, according to their structure and use, as either specific programs or modular programs.¹² Specific programs are rigidly structured programs designed to simulate a particular process or a particular plant. These specialized programs can be detailed, fully defined mathematical representations of physical plant models. The rigid, specialized structure of these programs promotes efficient simulation since they need not drag extraneous code and data into core with them. Conversely, the streamlined features of specialized programs render them inflexible and, hence, useless (without extensive modification) in simulating any process other than that for which they are designed.

The modular programs, on the other hand, are prepared to simulate a large number of processes or plants. This flexibility is usually made available at the expense of some of the detail and efficiency which can be obtained through specific programs. For the purpose of performing material balances, the dynamic layout of a pilot plant situation lends itself to the advantages of modular programs over those of specific programs. Therefore, this survey will emphasize modular programs.

The modular program gets its name from the technique used to simulate a plant or process. "Each chemical processing step is represented by a separate mathematical model called a 'unit module.' The unit modules are connected by data sets which represent material and energy flow between the units of the plant."¹³

An executive program supervises the program operations. It controls the order of calculations, the information flow between unit modules, and the access of information from a data base of physical and thermodynamic properties.¹²

Dynamic and Steady-State Simulation Programs

Simulation programs may be compiled for steady-state or dynamic process simulation. Dynamic simulation programs perform time-varying material and energy balances of plant operations. They can be very useful in studying plant start-up, shutdown, and transient conditions including problems of sensitivity and stability. The time-varying simulation of plant operations is obtained by numerical integration of the applicable systems of equations. To achieve the desired degree of accuracy (limit of integration error), the integration step size may need to be quite small, or complex numerical integration routines must be used. Such calculations require more time, sometimes by several orders of magnitude, than those for steady-state simulation.¹³ Additionally, dynamic simulation programs tend to resort to large equation systems, sometimes as large as 1000 differential equations. Consequently, the large amounts of computer time and space needed to solve the equation systems of time-varying simulation models render dynamic simulation of unit operations inappropriate for multiuser, mini-computer-based inventory estimation.

Commercially Available, Modular, Steady-State Simulation Programs

Modular, steady-state simulation programs have been under development since the middle 1950s. The simulators which enjoy acceptance

today represent legitimate tools for the process engineer, but their use is generally limited to the companies which developed them. The limited use can usually be attributed to (1) familiarity of the developer with the program, (2) potential difficulties in training the people who will use the program, or (3) potential problems in communicating to the developers difficulties in program operation or results interpretation.¹³

Despite the reluctance of industry to use programs not developed in-house, these modular, steady-state simulation programs have many attractive features for the design and process engineer: wide selections of models for different unit operations, extensive thermodynamic and physical properties data bases, equipment sizing and cost estimation, venture analysis, and others.¹³ Also, in general, the commercially available modular simulators have most of these features to promote universal applicability and wide acceptability among their potential users.

Since the simulator required for inventory estimation need only perform material balance calculations around unit operations, a significant portion of the software provided with most commercially available simulators would be superfluous. Of the subroutines specifically designed for process simulation, simulations of liquid-liquid extractions, stream mixing, stream splitting, absorption/stripping, chemical reaction, evaporation, and condensation are directly applicable to the subject plant's (and most nuclear fuel plants') operations. These routines typically represent 20% to 50% of the available modules for process simulation.¹³⁻¹⁵ The remaining simulation routines would not be utilized and, along with other superfluous code in commercially available simulation programs, would occupy precious data and code storage space.

Although the programs are modular in their use of various calculational routines, modularity need not extend to the realm of subroutine isolation or independence. That is, the deletion of a module because it is anticipated never to be directly needed as a simulation subroutine does not consider the possibility that the deleted module might be needed by some other module of recognized utility. These considerations make it risky, at best, to obtain a large program with the intention of culling the unnecessary modules so that it might fit on a computer with less memory than that for which it was designed.

The thermodynamic and physical properties data bases provided with commercially available programs tend to de-emphasize the compounds of actinide series elements. It is incumbent upon the user of such programs to provide any missing data necessary for proper simulation. If the necessary data are not directly available from the literature, then they must be estimated or measured in the laboratory.

An additional disadvantage of some commercially available programs is that, for the proprietary reasons, they are accessible only through the developing companies' computers¹⁴ and, therefore, require computer network or telephone communications capability. This requirement could become unnecessarily expensive for continuous, on-line estimation and, more seriously, would compromise the security necessary for computerized accountability of nuclear materials.

Simplified computer estimation of material distribution in unit operations has only recently been a subject of attention. With the rising popularity and affordability of minicomputers, more engineers are finding ready access to limited computing facilities. One modular,

steady-state flowsheet simulator (RUMBA) is the result of such computer availability.^{16,17} The RUMBA (Rudimentary Material Balance) program provides five modules to simulate chemical processes. The modules are addition (mixing of up to five inlet streams into one outlet stream), branching (fractional split of one inlet stream into two outlet streams of identical compositions), conversion (fractional conversion of a key component and the stoichiometric coefficients of all other components relative to the key from one inlet to one outlet stream), distribution (component distribution of one inlet stream to two outlet streams), and encircle (loop or recycle of the output of one module to the input of an upstream module). This program only 250 Fortran statements and can handle any number of streams, components, equipment units, and nested or intersecting loops.

Summary of Literature Review

RUMBA parallels NUMATH in the applicable model characteristics. However, four significant features of RUMBA and all previously discussed simulators render them inadequate for inventory estimation in the subject facility:

1. The results are stream compositions (not container compositions as in NUMATH) and, hence, integration would be required to yield container contents.
2. Since vessels themselves are unimportant (only streams are significant), there is no means of referencing vessels peripheral to the actual process vessels for the purpose of

including residual volumes into the holdup calculations and subsequently assigning the newly calculated compositions to their respective vessels.

3. The termination or rerouting of an existing stream or the inclusion of a new stream requires the availability of numerous flowsheet definition files (for each unit process) depicting all of the anticipated flowsheet configurations with appropriate labeling and decision capabilities to be able to recognize which file is representative of the present conditions.
4. No capability for verifying and adjusting estimated compositions is provided (NUMATH utilizes measured specific gravity to adjust estimated compositions to levels appropriate for the indicated process measurement).

It has been determined that the extensive software changes necessary to adapt any of the commercially available simulators to inventory estimation would be more costly than formulating a new program tailored to inventory estimation and thus would justify the need for a different kind of simulator.

It is appropriate to note that a specialized inventory estimator is being developed¹⁸ which promises to address container inventory estimation and estimate verification and adjustment based on some on-line material measurement. Although this program's goal is to estimate the contactor inventory within 5%, the program is inappropriate for NUMATH's intended use since it is specific to a certain process and is directed at estimating the inventory within the contactor vessel(s) only.

3. MODEL DEVELOPMENT

The inventories of individual vessels involved in or contributing to a unit operation may be estimated based on those vessels' functions in the unit operation. Simple models promote the definition of performance functions¹⁹ to characterize material distribution in the subject equipment. The general form of the performance equation is:

$$Y = P(X) \quad (3)$$

where

X = source materials vector,

Y = resultant materials vector,

P = performance function.

Based on data from plant operating history and the degree of accuracy required of the estimates (within 15% of analyzed values for fissile material and 25% for fertile material), the assumption has been made that the performance functions applicable to the operations in the subject plant are weakly dependent on the feed vectors and that the resultant material vectors may therefore be calculated without iteration. For steady-state operations, three basic models evolve from the above considerations: the blending model, the separation model, and the conversion model. Their implementation is directed toward inventory estimation as opposed to stream composition estimation normally found in simulators. The relationships utilized in each of these models are described below.

Blending Model

The blending model may be described as combining, with a perfect mixing model, bulk quantities (Q^s in liters, grams, liters per hour, or grams per hour) of materials of differing element (j) compositions (C_j^s in grams per liter or gram per gram) from several sources ($s = 1, 2, 3, \dots, n$):

$$\begin{array}{l} \text{total amount of} \\ \text{element } j \text{ combined} \end{array} = \sum^s Q^s C_j^s \quad (4)$$

and

$$\begin{array}{l} \text{total bulk quantity} \\ \text{of combined materials} \end{array} = \sum^s Q^s . \quad (5)$$

The element composition resulting in the subject vessel (v) may then be found from:

$$C_j^v = \frac{\sum^s Q^s C_j^s}{\sum^s Q^s} . \quad (6)$$

It should be noted that Q^s , the bulk quantity contributed from each source, may represent either the net quantity transferred or the bulk quantity flow rate depending on the subject vessel's transfer characteristics. This feature is provided to permit composition estimates for material residing only briefly in process vessels (e.g., continuously operated, flow-through contact columns and evaporators) in addition to composition estimates for material accumulating in process surge and storage vessels.

Nuclear material accounting requires maintenance of isotopic inventories in addition to elemental inventories. Isotopic contributions to the inventory are maintained in units of weight fraction--the basic units reported from isotopic analysis.

The isotopic weight fraction (F_i^V) resulting in the subject vessel may be developed in a manner similar to that of the resulting element composition:

$$\begin{array}{l} \text{total amount of} \\ \text{the } i^{\text{th}} \text{ isotope of} \\ \text{element } j \text{ combined} \end{array} = \sum^S Q^S C_j^S F_i^S, \quad (7)$$

where F_i^S is the weight fraction of the i^{th} isotope from the source s .

With the total amount of element j determined in Equation (4), F_i^V may be calculated as:

$$F_i^V = \frac{\sum^S Q^S C_j^S F_i^S}{\sum^S Q^S C_j^S}. \quad (8)$$

Separation Model

The separation model uses an equilibrium relationship, the "distribution-law" equation²⁰, to describe the resulting distribution of components between phases during solvent extraction, ion exchange, and centrifugation (where equilibrium changes occur):

$$C_j^V = D_j^S C_j^S, \quad (9)$$

where D_j^s is the distribution factor for element j from vessel s .

For several sources, the model may be developed in a manner similar to that of the blending model to yield:

$$C_j^v = \frac{\sum^s Q^s D_j^s C_j^s}{\sum^s Q^s}, \quad (10)$$

Similarly, the isotopic weight fraction resulting from such material distribution follows:

$$F_i^v = \frac{\sum^s Q^s D_j^s C_j^s F_i^s}{\sum^s Q^s D_j^s C_j^s}. \quad (11)$$

For the criteria discussed above, this model is valid over normal operating ranges of feed compositions and process conditions (e.g., flow rates and mixing energies). The distribution factors are empirically determined from process operating histories or from laboratory testing.

Conversion Model

An empirical conversion model is used to describe the change in composition during precipitation, calcination, and the resin form change during ion exchange (i.e., where completion or near-completion changes occur).

The conversion model is an empirical relation to adjust elemental compositions of material as it enters the reaction vessel:

$$c_j^v = A_j + \sum^s B_j^s c_j^s \frac{Q^s}{Q^v}, \quad (12)$$

where A_j and B_j^s are constants describing element j composition adjustments. Notice that B_j^s permits a partial composition adjustment of element j from vessel s , while the ratio of quantities of Q^s and Q^v describes a dilution effect. (For the flow mode, Q^v is replaced by Q^s to describe dilution.)

The relationship for adjusting isotopic composition is:

$$F_i^v = \frac{\sum^s B_j^s c_j^s \frac{Q^s}{Q^v} F_i^s}{\sum^s B_j^s c_j^s \frac{Q^s}{Q^v}}. \quad (13)$$

Notice that not all "B" constants for a given element should be set to zero so that the estimated isotopic fraction may be properly assigned. Similar to the distribution factors in Equations (9), (10), and (11), the conversion factors, A and B, may be empirically determined from process operating histories or from laboratory testing.

Specific Gravity Composition Adjustment

For any vessels having specific gravity (SpG) instrumentation, the estimated elemental compositions are adjusted to expected levels based on the measured specific gravity (see subroutine SPGCMP in Appendix A).

This adjustment is determined by applying a correction factor to the estimated compositions, C_j^V :

$$\text{adjusted composition} = \text{estimated composition} \cdot \text{factor}. \quad (14)$$

The empirical correction factor is determined by the ratio of an expected sum of compositions (based on the measured specific gravity) to the sum of compositions estimated by models mentioned above:

$$\text{factor} = \frac{\frac{(\text{SpG} - \text{minimum SpG})}{\sum_k (M_k W_k)} \sum_k \frac{M_k W_k^2}{M \text{SpG}_k}}{\sum_k M_k W_k}, \quad (15)$$

where

SpG = measured specific gravity,

k = elements (components) significantly affecting the specific gravity correction ($k=1,2,3,\dots,m$),

M_k = estimated molarity of element (or component) k,

W_k = molecular weight of the compound in which element k is found,

$M \text{SpG}_k$ = molarity-to-specific gravity conversion constant for element k.

This factor adjusts the compositions while preserving the molar ratios of the estimated species.

In the models noted above, composition (C), isotopic weight fraction (F), and quantity (Q) data are the most recent measured (or estimated) values obtained from the transfer packet (to be discussed in

Section 4); the distribution and conversion factors and the vessel interrelationships are obtained from a special file to be described below (Section 5 and Appendix C).

These three basic models may be used to estimate the inventory and distribution of elemental species (and their isotopic weight fractions) in any steady-state chemical process, under conditions mentioned above. Their use will be illustrated with the solvent extraction and ion exchange examples below.

4. EQUIPMENT AND NUMATH IMPLEMENTATION

Equipment

NUMATH has been developed and implemented on a Digital Equipment Corporation (DEC) PDP 11/70 minicomputer. This computer has 192K (1K = 1024) 16-bit words of memory. NUMATH was programmed in the Fortran IV-Plus²¹ programming language--an enhanced version of ANSI Fortran IV.

Over 100 independent programs have been developed for the nuclear material accounting system.²² Familiarity with certain features of the computerized material accounting system promotes an understanding of NUMATH's implementation:

1. Material is accounted for by containers or vessels (e.g., tanks, cans, bottles, hoppers, etc.). Records of containers (including compositions, net quantity, identification, and status information) are stored in the container data base (CDB).
2. Containers with multiple, immiscible phases (capable of bearing accountable quantities of nuclear material) exist as multiple containers (e.g., a solids dissolver would exist in the CDB as two containers: dissolver-solid and dissolver-liquid).
3. All transfers are coordinated by and cataloged in transfer packets. Transfer packets are composed of records of each container involved in the transfer (be it a complex unit operation transfer or a simple pump transfer from one vessel to another). Each record contains a "snapshot" of all CDB information on the container before the transfer and, when the information becomes available, after the transfer.

4. Multiple, distinct occurrences of any vessel's active involvement in a transfer results in multiple records in the transfer packet--one record for each active involvement.

Obviously, many other features (including on-line volume and specific gravity measurement) exist on the computer system; however, they are not central to NUMATH and, therefore, have not been discussed here.²²

NUMATH Implementation

NUMATH estimates material composition in vessels involved in unit operation transfers. NUMATH utilizes data files, unit operation definition files (see Section 5 and Appendixes B and C), unique to each operation. They contain information to define all of the vessels involved in a unit operation, their interrelationships, and the model references and parameters necessary to perform inventory estimation.

At the time of termination of any vessel's active involvement in the transfer, estimated compositions are calculated and stored in the posttransfer fields of the transfer packet and in the appropriate container record in the CDB. These estimated compositions permit estimation of material inventories in the involved vessels until such time as those vessels may be mixed, sampled, and analyzed (usually 4 to 8 hours after termination). The quantitative chemical analyses then replace estimated compositions in the transfer packet and the CDB.

The inventory of any unit operation within the subject plant may be estimated by a combination of one or more of the basic models described above. This concept may be best illustrated using a block diagram of a simplified separation process (Figure 3). This diagram

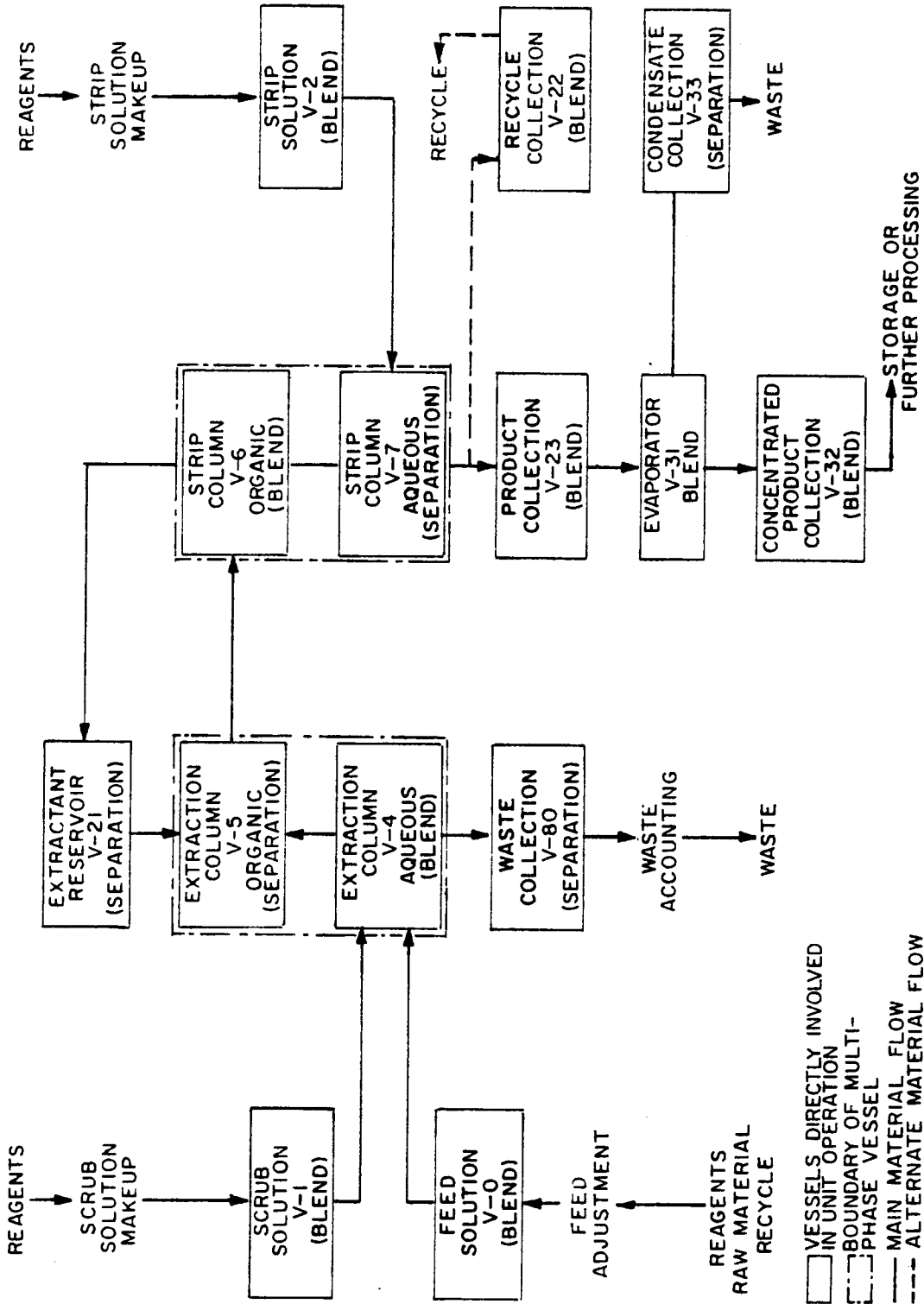


Figure 3. Block diagram of a single-cycle solvent extraction system.

depicts all vessels directly involved in a single-cycle solvent extraction separation in which uranium is recovered from a uranium-thorium mixture. The models used to estimate the contents (based on source materials) are shown in parentheses in each block. (Notice that only the blending and separation models were needed for this unit operation.) To accommodate the aqueous and organic phases coexistent in the contacting columns, the extraction column (which includes a scrubbing section) and the strip column have been represented as two vessels each. It is interesting to note that for extended operation, the surge capacity of this system (i.e., feed adjustment, waste accounting, and product or recycle) would require periodic replenishment or voiding, as applicable, and would involve multiple entries in the transfer packet for the effected vessels. A block diagram of the ion exchange system is provided in Figure 4.

NUMATH is not restricted to the three aforementioned models, but may be provided with any number of user-defined vessel models or, perhaps, rigorous estimators tailored to specific unit operation (notice in Appendix A the call within subroutine UOPCMP to subroutine ESTSDS--a solids dissolution estimator). Additionally, a capability has been provided for inventory estimation based on a model system not yet developed.

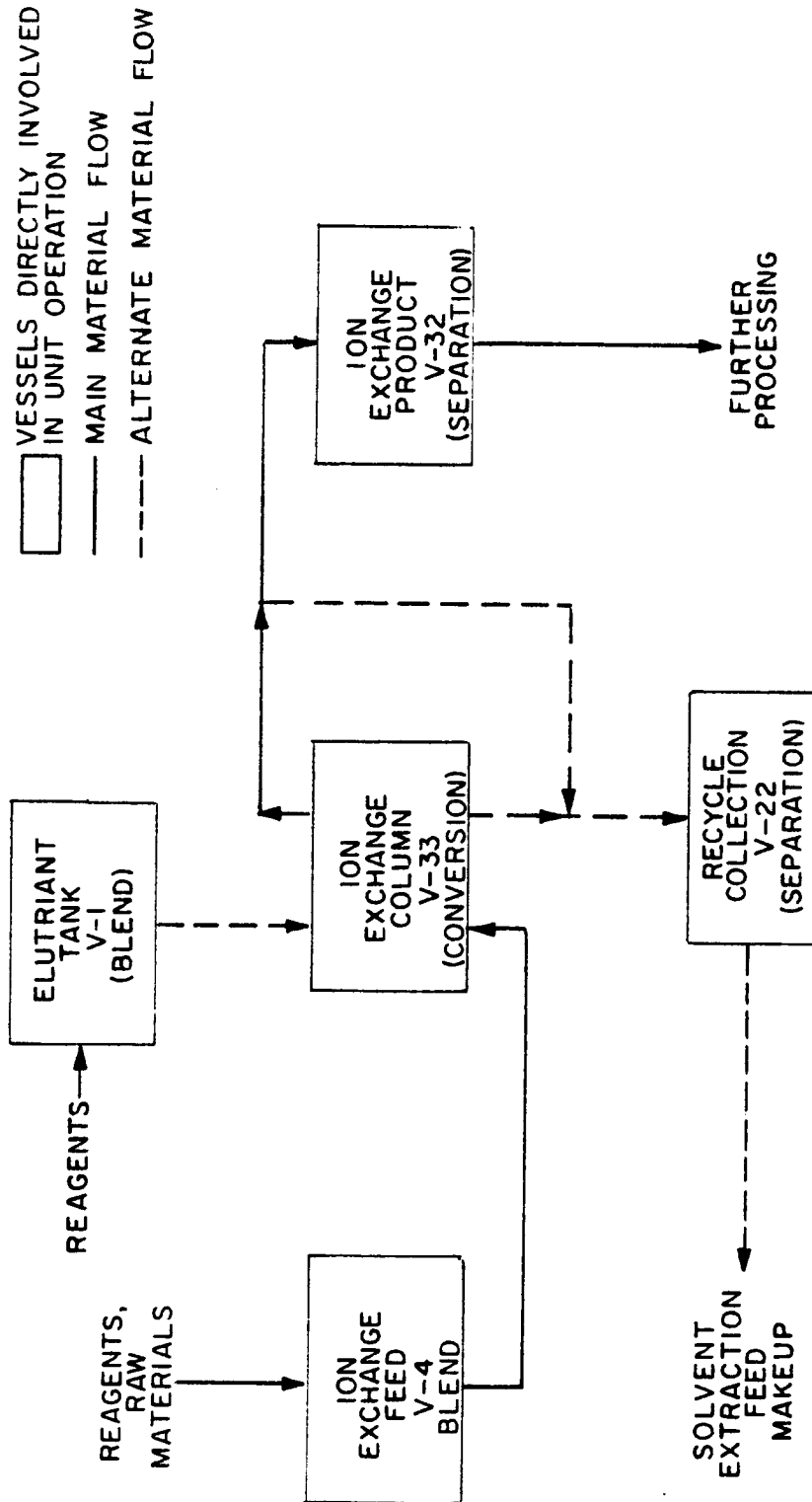


Figure 4. Block diagram of an ion exchange system.

5. SOFTWARE ORGANIZATION

Unit Operation Definition Files

Each unit operation or chemical process in the subject plant is characterized by a unique ASCII-formatted data file on the computer. These unit operation definition files are identical in structure and format (Appendix B). From these files, involved vessels and their transfer characteristics may be automatically cataloged in transfer packets.²² Other information in the files permits definition of interrelationships among vessels, model selections, and parameter assignments necessary for inventory estimation.

An explanatory sample unit operation definition file is provided in Figure C-1; the data type and common definitions for accessing information in such a file are shown in Figure C-3. Access to the information in this file would typically involve:

1. opening the file, after which the first data line (the file header) is read; these data include the unit operation name and the name of a specialized estimator, if applicable;
2. sequentially reading a vessel data record (the next 10 lines of data), which includes the identification and characterization of the principal (or "central") vessel of this record, identification of other vessels affecting the estimated contents of the central vessel, labels for referencing flow rates, subroutine references for estimating material compositions based on material characteristics alone (not yet implemented), and constants used in the estimating models; and

3. repeating step 2 until an end of file is indicated. Each repeat of step 2 refills with new values the common UOPVSL described in Figure C-3.

All information in a vessel data record is used to characterize a primary (or central) vessel. This characterization is prompted by the container-oriented inventory system. Consequently, during inventory estimation, a central vessel "pulls" material from contributing vessels in a manner consistent with the model and parameters specified.

The NUMATH user must be aware of the role of definition file data in the models discussed in Section 3. In the explanatory sample data file in Figure C-1 is a line of descriptive data labeled "Central Vessel Information." The first item on that line is the name of the central vessel and is noted in the models as superscript "v." The next line, entitled "Other Vessel Names," contains vessel names represented by superscript "s" in the models, which are usually summed over all "other" vessels noted on this line. (For collection-mode models, superscript "s" also includes previous material in the central vessel.) The "Flow Labels" listed on the following line are used for accessing flow rates applicable as alternative bulk quantities in flow-mode models. The coefficients for uranium, thorium, and plutonium appear in the models as the conversion and distribution factors A, B, and D. Guidelines for applying these factors are best left to the executable code in the model subroutines (Appendix A). Detailed guidelines for providing other data in the definition file are presented in Appendix C.

Since inventory estimation replaces compositions with updated values, care must be exercised in sequencing the vessel records so

that the updated compositions promote valid estimates. Usually, an order defined by material flow paths provides proper sequencing for the calculations; however, caution is recommended for paths in which internal recycle is encountered.

Alterations to any physical system in the plant might warrant comparable adjustments to relevant unit operation definition file(s). No changes should be required in the executable program or its subroutines.

NUMATH Software Interface

To isolate NUMATH from the other software with which it must interface (e.g., transfer packet programs and data files) and to promote NUMATH portability, a limited number of interfacing subroutines and a data common were established. All information external to the unit operation definition files is acquired through two subroutines (UOPFIL and UOPQTY) called in the UNTOPR subroutine (Appendix A). This information is assigned to appropriate variables defined in the UOPTPK common (Figure 5).

Inventory estimates result in updated values in the UOPTPK common. Upon completion of all estimating calculations for a given transfer packet, one subroutine (UOPMTY) stores the estimated values in the appropriate vessel records of the transfer packet and the CDB.

NUMATH Estimating Routines

After all applicable information has been gathered, a call to subroutine UOPCMP is made within the UNTOPR subroutine of NUMATH. UOPCMP coordinates all estimations in the following sequence:

```

C*****
C
C          'DM:[300,300] UDPTPK.COM'
C
C      COMMON TO HOLD TRANSFER PACKET DATA FOR UNIT OPERATIONS CALCULATIONS
C
C      PARAMETER UOMXVS = 40          !MAX # OF VESSELS IN A UNIT OPERATION
C
C      INTEGER UDTPKN                  !TRANSFER PACKET NUMBER
C      INTEGER UDOTYP                  !UNIT OPNS # (TFR TYPE CODE FROM TFR PKCT)
C      INTEGER UDNOVS                  !# OF VESSELS APPLICABLE TO THIS CALCULATION
C      INTEGER UDVSID(4,UOMXVS)       !VESSEL ID
C      INTEGER UDVSWD(UOMXVS)         !TFR PKCT VSL STATUS WORD
C      INTEGER UDITYP(3,UOMXVS)       !INITIAL CDB CONTAINER TYPE STATUS WORD
C      INTEGER UDFTYP(3,UOMXVS)       !FINAL CDB CONTAINER TYPE STATUS WORD
C      REAL UDICMP(21,UOMXVS)         !INITIAL COMPOSITIONS
C      REAL UDFCMP(21,UOMXVS)         !FINAL COMPOSITIONS
C      REAL UDIQTY(UOMXVS)            !INITIAL QTY
C      REAL UDINQY(UOMXVS)            !INTERMEDIATE QTY (AS OF LAST CALCULATION)
C      REAL UDFQTY(UOMXVS)            !FINAL QTY
C      REAL UDISPG(UOMXVS)            !INITIAL SP.G.
C      REAL UDFSPG(UOMXVS)            !FINAL SP.G.
C      REAL UDITMP(UOMXVS)            !INITIAL TEMPERATURE
C      REAL UDFTMP(UOMXVS)            !FINAL TEMPERATURE
C      REAL UDFLRT(UOMXVS)            !FLOW RATE OUT OF THIS VESSEL
C      REAL UDDATE(UOMXVS)            !RAD50 DATE OF LAST CALCULATION
C      REAL UDTIME(UOMXVS)            !RAD50 TIME OF LAST CALCULATION
C      REAL FLWTIM(UOMXVS)            !TIME (IN HOURS) SINCE LAST CALC
C      LOGICAL*1 FLWMDL(UOMXVS)       !FLOW MODEL INDICATOR FOR ...
C      LOGICAL*1 UDPRO(UOMXVS)        !... APPLICABILITY OF FLWRAT FOR TFR QTY
C      LOGICAL*1 UDESOK               !PROCESSED (OR CALCULATED) INDICATOR
C                                     !ESTIMATE OK
C
C      COMMON /UDPTPK/ UDTPKN,UDOTYP,UDNOVS,          !UNIT OPNS CHARACTERISTICS
C      1                UDVSID,UDVSWD,UDITYP,UDFTYP,  !VESSEL CHARACTERIZATION
C      2                UDICMP,UDFCMP,UDIQTY,UDINQY,UDFQTY,  !COMPOSITION & QTY DATA
C      3                UDISPG,UDFSPG,UDITMP,UDFTMP,  !SP.G., TEMPRTR
C      4                UDDATE,UDTIME,                !DATE & TIME
C      5                UDFLRT,FLWTIM,FLWMDL,          ! FLOW RATE DATA
C      6                UDPRO,UDESOK                  !PROCESSED INDICATOR & ESTIMATE OK
C
C*****

```

Figure 5. Data type and common definition for transfer packet data.

1. prompts the acquisition of a vessel record from the unit operation definition file; and if the central vessel appears in the UOPTPK common, continues with the remaining steps; if not, skips to Step 5;
2. establishes contributing vessel and flow label cross reference indexing (these cross references are cataloged in the common defined in Figure 6);
3. selects and executes appropriate estimating models (subroutines) which temporarily store the estimates in the BLEND common (see Figure 7) until they are copied to the UOPTPK common;
4. adjusts estimated compositions to measured specific gravity for those vessels with appropriate instrumentation; and
5. repeats steps 1 through 4 until all vessel records in the unit operation definition file have been addressed.

As described above, NUMATH utilizes three basic models--perfect mixing, separation, and conversion. It is significant to note, however, that certain process conditions warrant minor variations of applicable contributing vessel transfer quantities and material compositions for use in these models. For example, the perfect mixing model requires estimating modes for mixing flowing streams (where Q^S represents the source material flow rate), for collecting solutions from several vessels (where Q^S represents the source material transfer quantity), and for collecting solutions diluted by steam jet transfer techniques (where the compositions are adjusted by a jet dilution factor--see subroutine MDLJDL in Appendix A).

```

C*****
C
C
C      *PD:[300,300] UOCCOM.COM*
C
C      COMMON TO ASSIST IN PERFORMNG UNIT OPERATION CALCULATIONS
C      BY CATALOGING CROSS REFERENCE INDICES
C      FOR VESSEL NAMES AND FLOW LABELS.
C
C      THIS FILE MUST BE PRECEDED BY *PD:[300,300] UOPDFN.COM*.
C
C      PARAMETER FLBLMX = 10          !MAXIMUM # OF FLOW LABELS IN A UNIT OPERATION
C
C      VESSEL I. D. INFORMATION
C
C      INTEGER VSLCR5(4)              !CENTRAL VESSEL RAD-50 NAME
C      INTEGER VSLR50(4,UOVSMX)      !OVERLAY FOR VSL NAMES (RAD-50) OF UOP VSL ENTRY
C      INTEGER VSLSR5(4)              !SOURCE VESSEL R-50 NAME
C      INTEGER VSC1R5(4)              !FIRST CONTRIB VSL R-50 NAME
C      INTEGER VSC2R5(4)              !SECOND CONTRIB VSL R-50 NAME
C      INTEGER VSLQR5(4)              !RELATED QUANTITY VSL (E.G. FOR TWO PHASES)
C
C      INTEGER VSLNO(UOVSMX+1)        !OVERLAY FOR VESSEL INDEX NUMBERS
C      INTEGER VSLNUM                  !CENTRAL VESSEL NUMBER
C      INTEGER VNUM(UOVSMX)            !OVERLAY FOR VSL #'S OTHER THAN CENTRAL VSL
C      INTEGER SVSNUM                  !SOURCE VESSEL NUMBER
C      INTEGER CV1NUM                  !FIRST CONTRIBUTING VESSEL NUMBER
C      INTEGER CV2NUM                  !SECOND CONTRIBUTING VESSEL NUMBER
C      INTEGER QVSNUM                  !QUANTITY VESSEL NUMBER
C
C      FLOW RATE INFORMATION
C
C      INTEGER FLINDEX(UOFLMX)         !FLOW LABEL INDEX OF THIS VESSEL RECORD
C      INTEGER DFLNDX(UODFMX)         !DILUTION FLOW LABEL INDEX (SUBSET OF "FLINDEX")
C      INTEGER FLWLBL(6,FLBLMX)       !ASCII FLOW LABELS
C      REAL FLWRAT(FLBLMX)            !FLOW RATES
C
C      COMMON /UONTRY/ VSLCR5,VSLSR5,VSC1R5,VSC2R5,VSLQR5,      !VESSEL R-50 NAMES
C      1                VSLNUM,SVSNUM,CV1NUM,CV2NUM,QVSNUM,      !VESSEL INDEX NUMBERS
C      2                FLINDEX,FLWLBL,FLWRAT                    !FLOW RATE INFO
C
C      EQUIVALENCE (VSLR50(1,1),VSLCR5(1))                    !CENTRAL VESSEL OVERLAY
C      EQUIVALENCE (VSLNO(1),VSLNUM),(VNUM(1),SVSNUM)          !VESSEL INDEX NUMBERS OVERLAYS
C      EQUIVALENCE (FLINDEX(UOFLMX-UODFMX+1),DFLNDX(1))        !FLOW INDICES OVERLAY
C*****

```

Figure 6. Data type and common definition for cross reference indexes.

```

C*****
C
C          PD:[160,160]MIXCOM.COM
C
C          MIXING MODELS COMMON AREA
C
C          IT WAS DESIGNED TO BE USED IN PERFECT MIXING MODEL ESTIMATION (MDLPMX.FTN)
C          IT IS ALSO USED TO RECEIVE ESTIMATED COMPOSITIONS
C          IN OTHER SUBROUTINES CALLED IN NUMATH.
C
C          DEFINE DATA TYPES
C
C          REAL BLNDQY          !BLEND QUANTITY
C          REAL BLNDEI(21)      !BLEND ELEMENT & ISOTOPE VECTOR
C          REAL BLNDAC          !BLEND ACID CONCENTRATION
C          REAL BLNDISG         !BLEND SPECIFIC GRAVITY
C          REAL BLNDU           !BLEND URANIUM ELEMENT CONCENTRATION
C          REAL BLNDTH          !BLEND THORIUM ELEMENT CONCENTRATION
C          REAL BLNDPU          !BLEND PLUTONIUM ELEMENT CONCENTRATION
C
C          EQUIVALENCES
C
C          EQUIVALENCE (BLNDEI(1),BLNDAC)
C          EQUIVALENCE (BLNDEI(2),BLNDISG)
C          EQUIVALENCE (BLNDEI(3),BLNDU)
C          EQUIVALENCE (BLNDEI(10),BLNDTH)
C          EQUIVALENCE (BLNDEI(15),BLNDPU)
C
C          COMMON
C
C          COMMON /BLEND/ BLNDQY, BLNDEI
C
C*****

```

Figure 7. Data type and common definition for estimated compositions.

In the unit operation definition file, the designation of multiple vessels contributing to the central vessel's estimated composition provides flexibility in specifying alternate sources utilized in variations of flowsheet configurations. If one of the source vessels is not cataloged in the UOPTPK common, then it is assumed not to be presently involved in the transfer and is, therefore, ignored as a contributing factor in the estimation. This feature permits characterization of many variations of a flowsheet without the need for a unique unit operation definition data file for each variation.

Unit operation inventory estimation may be summarized with the following chronology and flowchart (Figure 8):

1. Upon termination of any vessel's activity in a transfer, the transfer termination program invokes NUMATH and informs it of the applicable transfer packet.
2. NUMATH then accesses the transfer packet and places in a working file the characteristics of any vessel which might be needed for vessel inventory estimation (i.e., any vessel which is presently active in the transfer or any vessel which was active but has not yet had its contents estimated).
Additionally, NUMATH would acquire any other information needed for inventory estimation (i.e., present bulk quantities, specific gravities, and any other relevant on-line measurements).
3. Next, NUMATH accesses the file describing the unit operation and sequentially addresses each vessel named therein. Any vessels named in the description file that also appear in the working file (UOPTPK) are estimated for composition by applying

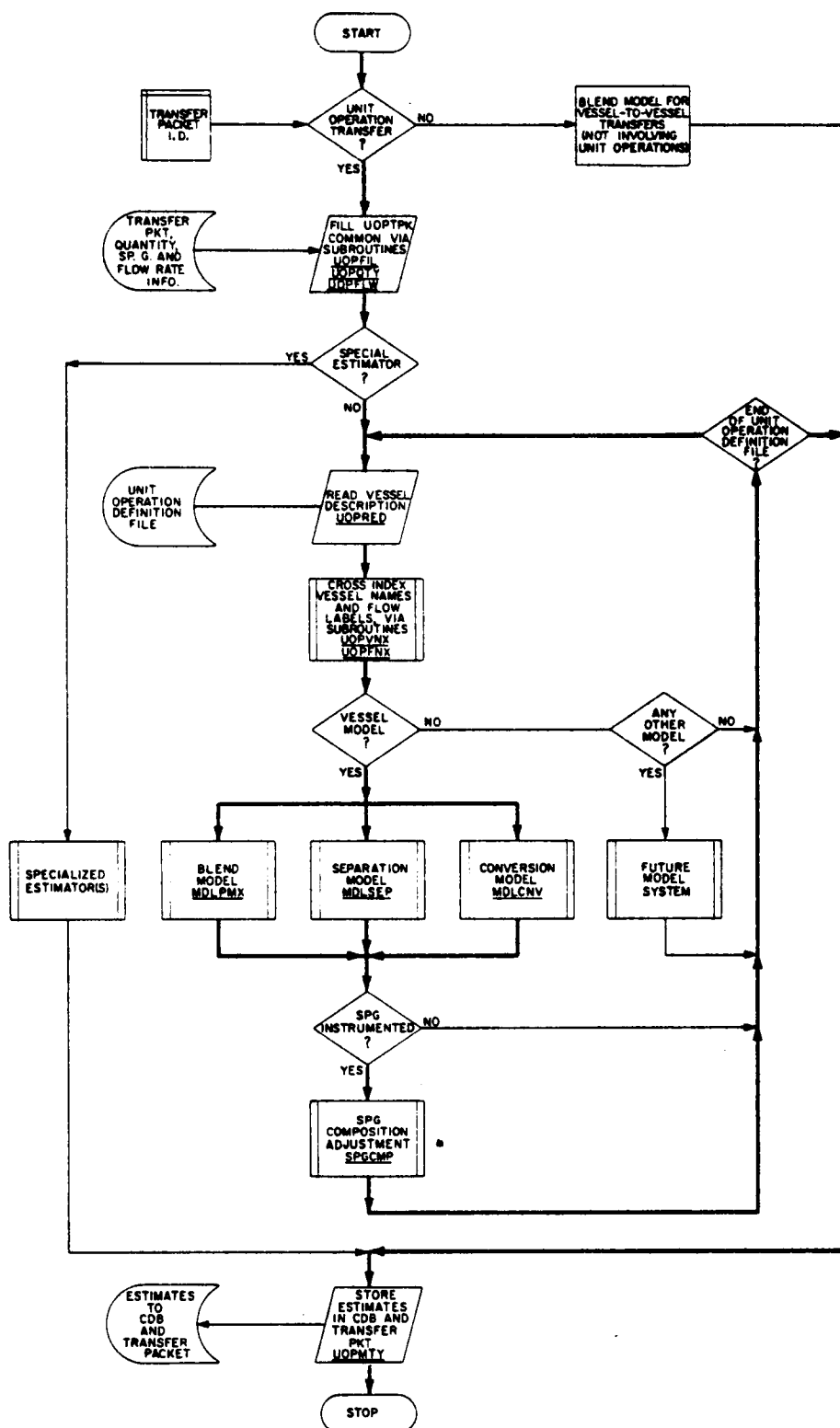


Figure 8. NUMATH flowchart.

factors from the definition file to the appropriate models. As noted above, any vessel continuously involved in an extensive transfer might be subjected to multiple inventory estimations during that transfer.

4. Finally, NUMATH inserts all estimated information into the appropriate records of the transfer packet and the container data base.

These estimates represent the composition of the material in each vessel involved in the transfer until representative samples are drawn and the analytical results supersede them.

The data processing depicted along the main (heavy) flowline in the NUMATH flowchart (Figure 8) is performed within the subroutines provided in Appendix A.

6. DATA COLLECTION AND MODEL PARAMETER FITTING

Data Collection

Solvent extraction and ion exchange run data were collected from chemical analyses reports and operating run sheets for use in determining material distribution and conversion factors and for use in simulated run evaluation of NUMATH. Ten solvent extraction runs (SX-57 through SX-66), in which UNH (uranyl nitrate hexahydrate) was separated from bulk thorium contaminant, were selected since they represented all historical runs from a recent program which utilized current procedures (changes were instituted prior to these runs to smoothe perturbations in the feed composition). Ten ion exchange runs (IX-180 through IX-189), in which residual thorium contamination was removed from the UNH, were selected since they represented all historical runs from a recent program which utilized the current charge of ion exchange resin (the current resin column was installed prior to IX-180).

The solvent extraction data (Table 1) included specific gravity (as measured by process instrumentation) and chemically analyzed composition data for the feed, extractant, product, and waste solutions, along with the flow rates (of which only the flow ratios have been provided) of the feed, extractant, scrub, and strip streams. The ion exchange data (Table 2) included specific gravity (as measured by process instrumentation) and chemically analyzed composition data for the feed and product solutions and resin loading data from laboratory development studies.²³ It should be noted that recycle solution composition data were not directly available from the historical records since these

TABLE 1
SINGLE-CYCLE SOLVENT EXTRACTION RUN DATA AND RESULTS

Run	Flow Ratios ^a	Information Source ^b	Solution Compositions (grams U or Th per liter)										NUMATH Material Balance ^c (% of measured inventory)	
			Feed		Extractant		Product		Waste					
			U	Th	SpG	U	Th	SpG	U	Th	U	Th	U	Th
SX-57	1.0/1.03/0.14/0.31	Measured NUMATH	7.19	135.6	0.89	0.173 0.118	0.26 0.15	1.354	249.9 248.3	0.0253 0.0241	1.360	112.0 118.8	99.3	106.1
SX-58	1.0/1.08/0.15/0.32	Measured NUMATH	7.53	140.5	0.88	0.0985 0.119	0.19 0.13	1.309	227.1 216.5	0.0288 0.0247	1.369	116.2 121.8	95.3	104.8
SX-59	1.0/1.06/0.14/0.32	Measured NUMATH	7.47	142.5	0.88	0.107 0.119	0.093 0.12	1.291	201.1 203.8	0.0300 0.0409	1.390	115.7 130.2	101.5	112.5
SX-60	1.0/1.06/0.14/0.31	Measured NUMATH	7.62	139.0	0.88	0.131 0.118	0.066 0.10	1.264 ^d	208.8 184.6	0.0395 0.0268	1.385	116.4 122.0	88.3	104.8
SX-61	1.0/1.06/0.14/0.32	Measured NUMATH	7.09	140.0	0.89	0.104 0.119	0.137 0.13	1.30	217.3 210.1	0.0324 0.0258	1.386	110.2 127.5	96.5	115.7
SX-62	1.0/1.08/0.15/0.32	Measured NUMATH	6.90	138.0	0.88	0.0684 0.108	0.108 0.13	1.30	217.1 209.8	0.0384 0.0240	1.378	110.8 120.0	96.4	108.3
SX-63	1.0/1.15/0.17/0.32	Measured NUMATH	6.20	135.0	0.88	0.111 0.0874	0.099 0.13	1.287	199.1 199.8	0.0353 0.0208	1.381	111.6 113.5	100.1	101.6
SX-64	1.0/1.11/0.15/0.32	Measured NUMATH	5.71	139.0	0.88	0.0961 0.0980	0.100 0.13	1.245	189.8 170.6	0.0329 0.0203	1.372 ^d	97.9 123.7	89.6	126.4
SX-65	1.0/1.10/0.14/0.32	Measured NUMATH	5.82	129.0	0.87	0.0987 0.0999	0.188 0.13	1.275	204.9 191.9	0.0374 0.0216	1.372	121.6 119.8	93.3	98.5
SX-66	1.0/1.20/0.16/0.36	Measured NUMATH	3.85 ^e	128.3	0.87	0.0764 0.0632	0.52 0.14	1.205	116.9 140.9	0.0118 0.0125	1.335	90.9 104.2	120.4	114.6

^aFlow ratios are listed as Feed/Extractant/Scrub/Strip.

^bInformation source for data include measured compositions from chemical analyses and specific gravities and flow rates from process instrumentation.

^cMaterial balances exclude recycle material.

^dSpecific gravity measurement of these solutions is suspect.

^eUranium feed composition outside normal feed range (4.0 to 8.0 grams U per liter).

TABLE 2
ION EXCHANGE RUN DATA AND RESULTS

Run	Information Source ^a	Solution Compositions (grams U or Th per liter)							NUMATH Material Balance ^b (% of measured inventory)	
		Feed		Ion Exchange Resin		Product				
		U	Th	U	Th	SpG	U	Th	U	Th
IX-180	Measured NUMATH	113.8	0.103	268.0 274.0	2.98 2.98	1.16	111.8 110.7	0.00 0.0	99.3	100.0
IX-181	Measured NUMATH	122.1	0.057	270.8 274.0	1.59 1.59	1.170	121.1 117.2	0.00 0.0	97.1	100.0
IX-182	Measured NUMATH	118.2	0.087	269.6 274.0	2.20 2.20	1.171	120.4 117.78	0.00 0.0	98.2	100.0
IX-183	Measured NUMATH	121.2	0.124	267.6 274.0	3.18 3.18	1.172	124.10 118.07	0.00 0.0	95.8	100.0
IX-184	Measured NUMATH	118.1	0.106	268.5 274.0	2.75 2.75	1.172	121.0 118.6	0.00 0.0	98.4	100.0
IX-185	Measured NUMATH	119.9	0.116	267.9 274.0	3.01 3.01	1.172	122.9 118.2	0.00 0.0	96.7	100.0
IX-186	Measured NUMATH	128.0	0.040	272.0 274.0	1.02 1.02	1.176	130.8 122.4	0.00 0.0	94.2	100.0
IX-187	Measured NUMATH	126.3	0.074	270.4 274.0	1.81 1.81	1.182	129.5 125.5	0.00 0.0	97.3	100.0
IX-188	Measured NUMATH	124.8	0.062	270.8 274.0	1.58 1.58	1.175	127.6 120.1	0.00 0.0	94.7	100.0
IX-189	Measured NUMATH	121.9	0.070	270.5 274.0	1.76 1.76	1.178	124.8 125.5	0.00 0.0	100.6	100.0

^aInformation source for data include measured compositions from chemical analyses, specific gravities from process instrumentation, and resin loadings from laboratory development studies.

^bMaterial balances exclude recycle material.

solutions represented material from several sources (the recycle collection tank is a multiservice vessel); additionally, recycle solutions were not strictly applicable to this study since the recycle solutions were collected during start-up and shutdown procedures and, therefore, reflect dynamic operating conditions as opposed to the steady-state operating conditions for which NUMATH was designed. In all cases, recycle amounted to less than 10% of the feed and typically represented less than 3% of the feed and should, therefore, have a minimal impact on this study.

Model Parameter Fitting

The historical solvent extraction and ion exchange run data (Tables 1 and 2) were evaluated to determine nuclear material distribution and conversion factors. Where inventories were measured (at outlet collection points), the distribution and conversion factors were determined directly from the measured outlet and inlet values. Where measured values were not available (as in some internal recycle solutions), the distribution and conversion factors were determined from a weighted, nonlinear, least squares fit of the entire system of analyzed exit material relative to the inlet material. For solvent extraction, the distribution factors reflect that fraction of the feed analyzed (or statistically determined) in the extractant, product, and waste solutions; and for ion exchange, the distribution and conversion factors reflect that fraction of the feed analyzed in the product and the degree of conversion of the resin from the acid form to the heavy metal form (as defined by laboratory development studies²³).

An example of directly determined distribution factors may be seen within the box in Figure C-2, where a segment of the simulation solvent extraction definition file (also shown in its entirety in Appendix B) depicts the distribution of material between the extraction column aqueous phase (V-4) and the extraction column organic phase (V-5). (Vessel labels are given in Figure 3.) It may be seen from the distribution factors that 99.35% of the uranium and 0.00301% of the thorium from the aqueous phase transfer to the organic phase. The uranium factor was determined from measured product collection (V-32) relative to waste collection (V-80) and feed (V-1) depletion. The thorium distribution was determined from the relative decontamination of uranium from thorium. Although the measured values were obtained at feed and product collection points, the distributions were assigned such that they more closely reflect material transfers within the physical system. This manipulation was possible since transfers requiring only trivial estimations (i.e., single stream blending) were encountered between the vessel in which the physical separation occurs and the vessel in which the material compositions are measured. A detailed presentation of the definition file data structure is provided in Appendix C.

7. DISCUSSION OF THE RESULTS

Trial NUMATH estimations were performed from simulation unit operation definition files (Appendix B) utilizing fictitious vessels assigned functions directly related to vessels in the real system. The fictitious vessels were necessary so the estimates would not disturb the measured inventories in the real system. Initial conditions (including feed compositions) were entered into applicable vessels, and the unit operations transfers were performed on the computer as they would be for actual runs. NUMATH was automatically invoked by the transfer operations. Estimated composition data were accumulated and tabulated (with the analyzed data) in Tables 1 and 2.

Although the measured and estimated compositions for individual solutions has been provided for comparison, the performance of NUMATH may be best evaluated by how well it estimates final inventories in relation to the measured final inventories. This evaluation has been included in the "Material Balance" columns of Tables 1 and 2 and is presented in graph form in Figure 9.

For the solvent extraction simulated runs, all but two of the material balances were within 11% of the measured material balance for uranium and within 16% of the measured material balance for thorium. Run SX-66 exceeded the 16% criterion established in Section 1 for fissile material balances; this disappointing result may be attributed to the effect of off-specification uranium feed composition (3.85 g/L in the feed is outside the normal range of 4.0 to 8.0 g/L) on solvent extraction performance. A suspiciously low specific gravity measurement

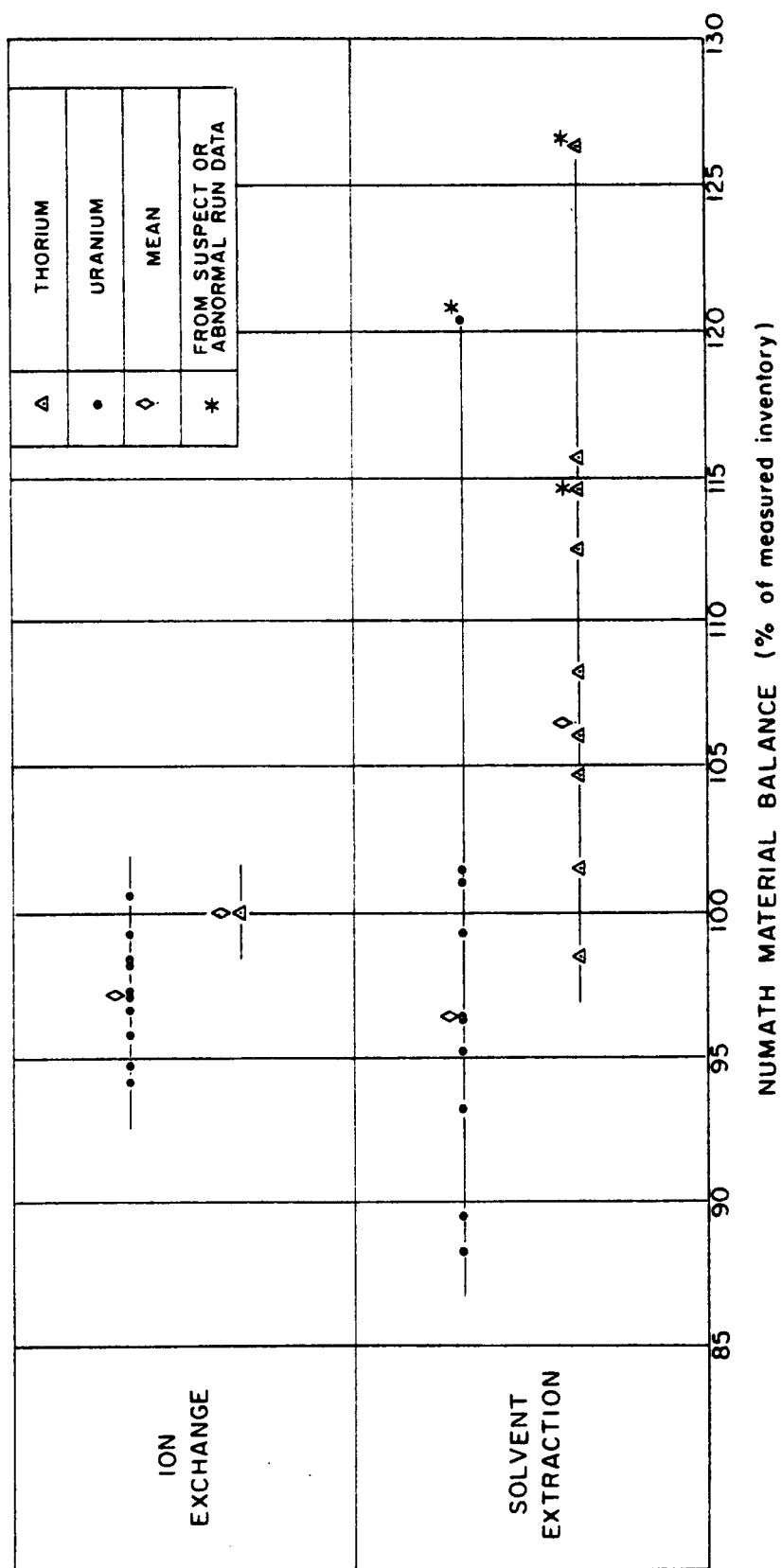


Figure 9. NUMATH performance relative to measured material balances.

of the product solution resulted in a low (but within the established criterion) uranium material balance in run SX-60. Conversely, the thorium material balance in run SX-64 fell marginally outside the $\pm 25\%$ criterion and significantly higher than any other result. This aberration was caused by a suspiciously high specific gravity measurement of the waste solution.

Ion exchange, a significantly simpler system, led to a much simpler unit operation definition files (Appendix B) and more accurate estimates. (Batch ion exchange operations made multiple unit operation definition files necessary--one for the purification step and one for each of two elution steps.) The simulated ion exchange runs yielded uranium material balances within 6% of the measured material balances; thorium was estimated precisely at the measured values. (Accurate thorium estimates are attributed to ion exchange operating procedures which ensure that all thorium in the feed is retained on the resin during product collection.) The isotopic inventories were estimated to the same relative accuracy as the estimated element inventories.

The estimated compositions appear to be biased $\sim 3\%$ low for uranium and $\sim 7.5\%$ high for thorium where specific gravity factored into the solution in which the major component was borne, indicating that the molarity-to-specific gravity conversion factors for uranium and thorium (which were determined from chemical analyses records²⁴ and applied in Equation 15) need improvement.

It should be noted that the data used for model simulation was also used for model parameter fitting. However, the data used encompasses operations planned in the near future. Therefore, the above comparisons should be valid.

Mention should be made of one vessel (V-33) which performs an accountability function in the solvent extraction system but was not included in Table 1. Vessel V-33 collects the condensate from the product concentrator. Since aqueous fissile and fertile materials have negligible vapor pressures at about 100°C, the condensate collected is essentially water with only minute contamination from entrainment. The instrument indicating the specific gravity was a pneumatic strip chart recorder with mechanical pen movement. The pen movement was restricted so that the lower limit reading indicated a specific gravity of 1.01 instead of 1.00. When the estimated compositions (typically <0.005 gram U per liter) were adjusted for the "measured" specific gravity, the resultant concentrations were grossly overestimated (>1 gram U per liter). To alleviate this problem, the distributions were changed to zero; this change should have minimum impact on the results of this study since the subject material typically constituted less than 0.01% of the material balance. (This condition has since been corrected--along with all other possible occurrences of this type--with on-line specific gravity instrumentation that is not limited by mechanical pen movements.)

8. CONCLUSIONS AND RECOMMENDATIONS

Conclusions

The following conclusions may be drawn from this study with regard to estimation of nuclear material residing in process vessels during process operations:

1. The NUMATH estimation of inventories yields material balances consistently within 11% (and typically within 7%) of measured values for fissile materials accounted for (i.e., uranium and certain of its isotopes) and within 16% for the fertile material (i.e., thorium and its isotopes) collected during steady-state process operation of normal ranges of feed. This performance is within the criteria established above.
2. The estimated inventories appear to be biased low for uranium and high for thorium where specific gravity measurements are factored into the calculations. (The molarity-to-specific gravity conversion factors were obtained from laboratory results.)
3. Caution must be exercised when attempting to employ a given unit operation definition file, including its distribution and conversion factors, for a transfer with characteristics (e.g., compositions and flow rates) outside the range for which the factors were determined.
4. For vessels accommodating very dilute solutions (e.g., minutely contaminated, aqueous, evaporator condensate) and utilizing specific gravity measurement from a pneumatic strip chart

recorder, material content may be grossly overestimated when the mechanical pen movement, prevented from indicating a true lower limit specific gravity of about 1.0, is read to be an inaccurately high specific gravity and, subsequently, factored into the NUMATH calculations.

Recommendations

The results of this study may be expanded to include evaluation of data and run simulation so that NUMATH performance is documented for other unit operations and chemical processes. Additionally, the estimates resulting from NUMATH may be improved, and the applicable range of a given set of factors in a unit operation definition file may be broadened by the following enhancements:

1. Perform additional study on the molarity-to-specific gravity conversion factors to correct an apparent bias in the constants.
2. Improve models to consider chemical and competing effects of associated components.
3. Develop equation systems in models to estimate compositions during non-steady-state conditions (i.e., during process start-up and shutdown and during stream perturbations).
4. Incorporate nondestructive analysis into NUMATH estimates.

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LIST OF REFERENCES

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APPENDIXES

APPENDIX A: FORTRAN PROGRAM AND SELECTED SUBROUTINES

Relevant Fortran source code has been provided in this appendix. The subroutines follow the main program in alphabetical order by subroutine name.


```

FORTRAN IV-PLUS V02-51C          10100146    06-MAR-81    PAGE 1
NUMATH.FTN /TR:BLOCKS/WR

0001      PROGRAM NUMATH
C
C      NUCLEAR MATERIAL HOLDUP ESTIMATOR TASK.
C
C      THIS PROGRAM ESTIMATES NUCLEAR MATERIAL HOLDUP
C      AFTER A TRANSFER TERMINATION.
C
C      TWO MAIN SEGMENTS ARE PROVIDED
C      1. PERFECT MIXING MODEL FOR TRANSFERS INVOLVING
C      SIMPLE MATERIAL MOVEMENT BETWEEN VESSELS
C      2. UNIT OPERATION TRANSFER ESTIMATION.
C
C      AUTHOR: A. N. KRICHINSKY
C
C      DATE: 12/12/78
C
C      IMPLICIT INTEGER(A-Z)
C      INCLUDE 'LL1C100,100J TFLUN.COM/NOLIST'
C      INCLUDE 'LL1C100,100J INVMGRUF.COM/NOLIST'
C
C      CONTINUE
C      ASSIGN LUNS
C      LUNDX=1
C      LUNTRV=2
C      LUNTRW=3
C      ERRLUN=7
C      CALL RECOEX(,MSGRUF)
C      CALL ASSIGN(5,'TT01')
C      CALL RLKRAK(1,ERR,0)
C      IF (ERR.NE.0) GO TO 90
C      IF (TTC.EQ.101) CALL ESTMIX(ERR) ! MIXING MODELS
C      IF (TTC.LE.100) CALL UNTOPR(ERR) ! UNIT OPERATIONS MODELS
C      IF (TFRSTF.EQ.6) CALL DIFENS(ERR) ! COMPUTE INVENTORY HUF FOR TRAN.
C      IF (ERR.NE.0) CALL NOTIFY
C      CONTINUE
C      PREPARE TO EXIT
C
C      CONTINUE
C      CALL RLSRAK
C      CALL CNTINU(MSGRUF)
C      CALL CLOSE(5)
C      GO TO 10
C      CALL NOTIFY
C      GO TO 91
C      END
0002
0003
0007
0021      10
0022      C
0023
0024
0025
0026
0027
0028
0029
0030
0031
0032      C
0033
0034      100
C
C      91
0035
0036
0037
0038
0039
0040
0041
0042      90
END

```



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FORTRAN IV-PLUS V02-51C
MOLCNUV.FTN /TR:BLOCKS/WR PAGE 1

0001 SUBROUTINE MOLCNUV(IERR)

      SUBROUTINE TO PERFORM COMPOSITION CONVERSIONS ESTIMATION.

      IT MAY TYPICALLY BE USED IN ESTIMATING ELEMENTAL COMPOSITIONS
      IN A COLLECTION VESSEL (NON-FLOW CASE) OR
      IN A CONTINUOUSLY FLOWING COLUMN (FLOW CASE).

      IT USES THE INFORMATION ASSOCIATED WITH UNIT OPERATIONS :
      FLOW LABELS AND THEIR ASSOCIATED FLOW RATES
      ARE USED (FOR FLOW CASE) IN CALCULATING
      DILUTION FACTORS FOR COMPOSITION ADJUSTMENT.
      FOR COLLECTION CASE, THE COLLECTING (CENTRAL) VESSEL IS
      ASSUMED TO HAVE ITS INITIAL CONTENTS AND
      QUANTITY INSERTED IN THE BLEND COMMON FIELDS
      BY CALLING MOLPMX WITH THOSE INITIAL CONDITIONS
      PRIOR TO CALLING THIS SUBROUTINE.
      COEFFICIENTS ARE EXPECTED FOR EACH ELEMENT
      (EACH ELEMENT SHOULD HAVE ONE COEFFICIENT
      FOR EACH SOURCE AND CONTRIBUTING VESSEL.
      ADDITIONALLY, THE LAST ELEMENT COEFFICIENT
      IS USED AS A CONSTANT COMPOSITION CONVERSION
      -- NOT A SCALER.)

      MODEL IS OF THE FORM:
      L(V,K) = A(K) + SUM(CIL(C,K)*R(C,K)*Q(C)/Q(V)) !FOR COLLECTING MODE
      L(V,K) = A(K) + SUM(CIL(C,K)*R(C,K)*Q(C)/SUM(C(C,C)) !FOR FLOWING MODE
      WHERE L = ELEMENTAL CONCENTRATION VECTOR
            A = CONVERSION CONSTANT
            R = TRANSFER QUANTITY OR FLOW RATE FROM VESSEL 'S'
            Q = TRANSFER QUANTITY OR FLOW RATE FROM VESSEL 'S'
            V = SUBJECT VESSEL SUBSCRIPT
            C = CONTRIBUTING VESSEL SUBSCRIPT
            K = ELEMENT (OR COEFFICIENT) SUBSCRIPT
            SUM(C) = SUM OVER ALL 'C' OF EXPRESSION IN 'C'

      ISOTOPES ARE ESTIMATED BY:
      I(V,J) = SUM(CIL(C,J)*L(C,K)*R(C,K)*Q(C)/SUM(C(C,C))
      /SUM(CIL(C,K)*R(C,K)*Q(C)/SUM(C(C,C))
      WHERE I = ISOTOPE COMPOSITION VECTOR
            J = ISOTOPE SUBSCRIPT

      INPUT: IERR = FLOW/COLLECTION INDICATOR
      (IERR<0 ---> FLOW MODE) IERR=0 ---> COLLECTION MODE)
      COMPOSITIONS, QUANTITIES, AND COEFFICIENTS IN UNIT OPS CALCULATION COMMONS

      OUTPUT: IERR = ERROR INDICATOR (IERR=0 ---> ALL OK)
      ESTIMATED COMPOSITIONS IN UNIT OPS CALCULATION COMMONS

      AUTHOR: A. M. KRICHINSKY

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FORTRAN IV-PLUS V02-51C          09:55112      06-MAR-81      PAGE 3
HDLCHV.FTN /TRIBLOCKS/WR

C
C
0204      IF (FLOW) GO TO 25
0206      TFRQTY = UOINQY(VNUM(LOOP)) - UOFTQY(VNUM(LOOP))
0208      IF (FLWMDL(VNUM(LOOP))) IFLOW MODEL IS APPLICABLE ...
1          OR, (TFRQTY, LE, 0.0)) ... OR NO PERCEIVED TFR QTY)
2          TFRQTY = UOFLRT(VNUM(LOOP)) * FLWTIN(VNUM(LOOP))
0209      IF (VNUM(LOOP) - EQ.QVSNUM)
1          TFRQTY = UOFTQY(VNUM(LOOP)) INQ QTY TFR JUST MAT'L TFR
0210      BLFCTR = BLNDQY
0211      BLFCTR = TFRQTY
0212      IF (.NOT. CTGER) UOOCF(LOOP) = 1.0      INQ QTY CORRECTION
0213      GO TO 30

C
C
C      FOR FLOW CASE, DETERMINE THE CONTRIBUTION FACTOR
C
0214      CONTINUE
0215      IF ((BLNDQY, GT, 0).AND.(FLINDX(LOOP), GT, 0)) GO TO 28
0216      BLFCTR = 1.0
0217      GO TO 30
C
0218      BLFCTR = FLWRAT(FLINDX(LOOP)) / BLNDQY
0219      IF (BLFCTR, LE, 0) GO TO 27

C
C
C      ACID CALCULATION
C
0220      ASSIGN 40 TO CNTNU
0221      LMNT = 1
0222      CFLMNT = 1
0223      GO TO 90

C
C
C      SPECIFIC GRAVITY CALCULATION
C
0224      ASSIGN 50 TO CNTNU
0225      LMNT = 2
0226      CFLMNT = 2
0227      GO TO 90

C
C
C      URANIUM CALCULATIONS
C
0228      ASSIGN 60 TO CNTNU
0229      LMNT = 3
0230      CFLMNT = 3
0231      START = 4
0232      STOP = 9
0233      GO TO 80

C
C
C      THORIUM CALCULATIONS
C
0234      ASSIGN 70 TO CNTNU
0235      LMNT = 10
0236      CFLMNT = 4
0237      START = 11
0238      STOP = 14
0239      GO TO 80
C

```



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FORTRAN IV-PLUS V02-51C      15:54136      05-MAR-81      PAGE 2
MDLJDL.FTN      /TR:BLOCKS/MR

0015      434      ASSIGN 435 TO CNTNU      !CONTINUE WITH URANIUM
0016      OUTCMP(2) = INCOMP(2) - (INCOMP(2)-1.0) * JTDLFC      !SF.G. ADJUST
0017      GO TO 435

C
0018      435      DILUTE URANIUM
0019      ASSIGN 436 TO CNTNU      !CONTINUE WITH THORIUM
0020      LMNT = 3      !URANIUM SUBSCRIPT
0020      GO TO 438

C
0021      436      DILUTE THORIUM
0022      ASSIGN 437 TO CNTNU      !CONTINUE WITH FLUTONIUM
0023      LMNT = 10      !THORIUM SUBSCRIPT
0023      GO TO 438

C
0024      437      DILUTE FLUTONIUM
0025      ASSIGN 439 TO CNTNU      !CONTINUE WITH MIXING MODEL
0026      LMNT = 15      !FLUTONIUM SUBSCRIPT
0026      GO TO 438

C
0027      438      OUTCMP(LMNT) = INCOMP(LMNT) * JTDLFC      !CALC DILUTED CONC
0028      IF (OUTCMP(LMNT).LT.0) IERR = -1      !NEGATIVE COMPOSITION DETECTED
0029      GO TO CNTNU

C
0030      439      RETURN
0031      END

```



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FURTRAN IV-PLUS V02-51C          10100123      06-MAR-81      PAGE 3
HDLPHX.FTN      /TRIBLOCKS/WR

C      80
0053      SUM = ARDEI(LMNT)*ADDOY + BLNDEI(LMNT)*BLNDY  !SUM OF ELEMENTAL CONTRIBUTIONS
0054      IF (SUM.LE.0) GO TO 90                          !IF ZERO, SKIP ISOTOPIC CALCULATIONS
0055      SRCFRC = ARDEI(LMNT) * ADDOY / SUM              !SOURCE CONTRIBUTION
0056      DSTFRC = BLNDEI(LMNT) * BLNDY / SUM             !DESTINATION CONTRIBUTION
0057      IF (SRCFRC.LT.0) SRCFRC = 0.0                  !DEFAULT FRACTION
0058      IF (DSTFRC.LT.0) DSTFRC = 0.0                  !DEFAULT FRACTION

C      C
C      CALCULATE NEW BLEND ISOTOPIC DISTRIBUTION
C
0059      IF (LMNT.LE.2) GO TO 90                          !NO ISOTOPES INVOLVED
0060      DO 85 LOOP=START,STOP
0061          BLNDEI(LOOP) = SRCFRC * ARDEI(LOOP) + DSTFRC * BLNDEI(LOOP)
0062          IF (BLNDEI(LOOP).LT.0) BLNDEI(LOOP) = 0.0
0063      CONTINUE
C      85
C      C
C      CALCULATE SOURCE & DESTINATION ELEMENT CONTRIBUTION FACTORS
C
C      90
0064      IF ((ADDOY+BLNDY).LE.0) GO TO 998              !NOTHING TO BLEND
0065      SRCCNT = ADDOY / (ADDOY + BLNDY)                !SOURCE ELEMENT CONTRIBUTION
0066      DSTCNT = BLNDY / (ADDOY + BLNDY)                !DESTINATION ELEMENT CONTRIBUTION
0067      IF (SRCCNT.LT.0) SRCCNT = 0.0                    !DEFAULT CONTRIBUTION
0068      IF (DSTCNT.LT.0) DSTCNT = 0.0                    !DEFAULT CONTRIBUTION

C      C
C      CALCULATE NEW BLEND ELEMENT CONCENTRATIONS
C
C      92
0069      BLNDEI(LMNT) = SRCCNT*ARDEI(LMNT)+DSTCNT*BLNDEI(LMNT)  !ELEMENTAL CONCENTRATIONS
0070      IF ((BLNDEI(LMNT).LT.0).AND.(LMNT.GT.1)) BLNDEI(LMNT) = 0.0
C
C      GO TO CNTNU
C
C      C
C      CALCULATE NEW BLEND QUANTITY
C
C      100
0072      BLNDY = ADDOY + BLNDY
C
C      998
0073      RETURN
C      0074      END

```



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FORTRAN IV-PLUS V02-51C                                PAGE 1
MDLSEP.FTN /TR:BLOCKS/MR                                09155146    06-MAR-81

0001 SUBROUTINE MDLSEP(IERR)

C
C
C SUBROUTINE TO PERFORM DISTRIBUTIVE SEPARATIONS ESTIMATION.
C
C IT MAY TYPICALLY BE USED IN ESTIMATING ELEMENTAL COMPOSITIONS
C IN A COLLECTION VESSEL (NON-FLOW CASE) OR
C IN A CONTINUOUSLY FLOWING COLUMN (FLOW CASE).
C
C IT USES THE INFORMATION ASSOCIATED WITH UNIT OPERATIONS :
C FLOW LABELS AND THEIR ASSOCIATED FLOW RATES
C ARE USED (FOR FLOW CASE) IN CALCULATING
C DILUTION FACTORS FOR COMPOSITION ADJUSTMENT,
C FOR COLLECTION CASE, THE COLLECTING (CENTRAL) VESSEL IS
C ASSUMED TO HAVE ITS INITIAL CONTENTS AND
C QUANTITY INSERTED IN THE BLEND COMMON FIELDS
C BY CALLING MDLPHX WITH THOSE INITIAL CONDITIONS
C PRIOR TO CALLING THIS SUBROUTINE.
C COEFFICIENTS ARE EXPECTED FOR EACH ELEMENT
C (EACH ELEMENT SHOULD HAVE ONE COEFFICIENT
C FOR EACH SOURCE AND CONTRIBUTING VESSEL).
C
C
C MODEL IS OF THE FORM:
C  $L(V,K) = \text{SUM}(C(L,C,K)*Q(C,K)*Q(C)/\text{SUM}(C(Q(C)))$ 
C WHERE L = ELEMENTAL CONCENTRATION VECTOR
C D = DISTRIBUTION COEFFICIENT DESCRIBING MASS TRANSFER FROM VESSEL 'C'
C Q = TRANSFER QUANTITY OR FLOW RATE FROM VESSEL 'S'
C (FOR COLLECTING SHARED QTY VSL, Q(C) = FINAL QTY)
C V = SUBJECT VESSEL SUBSCRIPT
C C = CONTRIBUTING VESSEL SUBSCRIPT
C K = ELEMENT (OR COEFFICIENT) SUBSCRIPT
C SUM(C) = SUM OVER ALL 'C' OF EXPRESSION IN 'C'
C
C ISOTOPES ARE ESTIMATED BY:
C  $I(V,J) = \text{SUM}(C(I(C,J))*L(C,K)*Q(C,K)*Q(C)/\text{SUM}(C(Q(C)))$ 
C WHERE I = ISOTOPE COMPOSITION VECTOR
C J = ISOTOPE SUBSCRIPT
C
C INPUT: IERR = FLOW/COLLECTION INDICATOR
C (IERR<0 ----> FLOW MODE, IERR>0 ----> COLLECTION MODE)
C COMPOSITIONS, QUANTITIES, AND COEFFICIENTS
C IN UNIT OPS CALCULATION COMMONS
C
C OUTPUT: IERR = ERROR INDICATOR (IERR=0 ----> ALL OK)
C ESTIMATED COMPOSITIONS IN UNIT OPS CALCULATION COMMONS
C
C
C AUTHOR: A. M. KRICHINSKY
C DATE: 12/14/78
C
C MODIFIED 04-DEC-80 BY A. M. KRICHINSKY

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FORTRAN IV-PLUS V02-51C          09155146      06-MAR-81          PAGE 2
HOLSEP.FTH      /TRIBLOCKS/WR

C      TO SUBSTITUTE ESTIMATED TFR QTY (FLOW RATE * TIME)
C      FOR CONTRIBUTING VESSELS HAVING FLOW MODELS ('HOLF--')
C      OR NO PERCEIVED TFR QTY (I.E., SIMULTANEOUS FLOW IN & OUT).
C
C      AND TO ESTABLISH ALL CASES OF 'BLECTR' & 'DLFCTR'
C      BETWEEN STATEMENT LABELS 1 & 30 (THEY WERE @ 80).
C
MODIFIED 23-DEC-80      BY A. M. KRICHINSKY
C      TO REMOVE QUANTITY ESTIMATION (AND PLACE IT IN UOFCMF)
C
0002      INCLUDE 'FBI[300,300] UOFTFK.COM/HOLIST'
0028      INCLUDE 'FBI[300,300] UOFCFN.COM/HOLIST'
0091      INCLUDE 'FBI[300,300] UOCCOM.COM/HOLIST'
0114      INCLUDE 'FBI[160,160] MIXCOM.COM/HOLIST'
0128      INCLUDE 'FBI[100,100] CTCOM.COM/HOLIST'
C
C      LOGICAL FLOW
C      INTEGER IERR
C      INTEGER CNTNU
C      INTEGER LNMT
C      INTEGER START, STOP
C      INTEGER CLMNT
C      REAL SRCFRC
C      REAL DSTFRC
C      REAL DLFCTR
C      REAL RLFCTR
C      REAL TFRQTY
C
C      FLOW INDICATOR
C      IERROR CODE ( 0 = OK )
C      !CONTINUATION STATEMENT LABEL
C      !ELEMENT # (H+ = 1, U = 3, TH = 10, PU = 15)
C      !START & STOP ISOTOPE SUBSCRIPTS
C      !COEFFICIENT ELEMENT #
C      !SOURCE ISO-DISTR WEIGHTING FACTR
C      !DEST ISO DISTR WEIGHTING FACTR
C      !SUM OF ELEMENTAL CONTRR TO BLEND
C      !DILUTION FACTOR
C      !BLEND CONTRIBUTING FACTOR
C      !COLLECTING TRANSFER QTY
C
C      FLOW = .FALSE.
C      IF (IERR.LT.0) FLOW = .TRUE.
C      IERR = 0
C      SUM = 0.
C
C      FOR THE FLOWING CASE, SUM THE DILUTING FLOW RATES
C
C      IF (.NOT.FLOW) GO TO 10
C      DO 1 LOOP=1,UOIFHX
C      IF (DFLNDX(LOOP).EQ.0) GO TO 1 !IF INDEX IS ZERO, SKIP IT.
C      BLNDQY = BLNDQY + FLOWRAT(DFLNDX(LOOP))
C      CONTINUE
C      RLFCTR = 1.0
C      !DEFAULT CONTRIBUTION FACTOR
C
C      SUM TRANSFER CONTRIBUTIONS
C
C      DO 100 LOOP=1,UOVSHX-1
C      IF (VNUM(LOOP).EQ.0) GO TO 100 !THERE IS NO VSL INDEX
C      FOR COLLECTING CASE, DETERMINE TRANSFER QTY AND CONTRIBUTION FACTORS.
C      IF (FLOW) GO TO 25

```

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FORTRAN IV-PLUS V02-S1C                                09:55:46    06-MAR-81    PAGE 3
HDLSEP.FTN /TRIRLOCKS/WR

0199 TFRQTY = UOINRY(VNUM(LOOP)) - UOQTY(VNUM(LOOP))
0200 IF (FLWML(VNUM(LOOP))) IFLOW MODEL IS AFFICABLE ...
1 .OR. (TFRQTY.LE.0.0)) !... OR NO PERCEIVED TFR QTY)
2 TFRQTY = UOFLRT(VNUM(LOOP)) * FLWML(VNUM(LOOP))
0201 IF (VNUM(LOOP).EQ.QVSNUM) TFRQTY = UOQTY(VNUM(LOOP)) !NO QTY TFR! JUST MAT'L TFR
0202 RLFCFTR = BLNDQY
0203 RLFCFTR = TFRQTY
0204 IF (.NOT.CTGER) UOOCF(LOOP) = 1.0 !NO QTY CORRECTION
0205 GO TO 30

C
C
C FOR FLOW CASE, DETERMINE THE CONTRIBUTION FACTOR
C
25 CONTINUE
0206 IF ((BLNDQY.GT.0).AND.(FLINDX(LOOP).GT.0)) GO TO 28
0207 RLFCFTR = 1.0 !DEFAULT DILUTION FACTOR
0208 GO TO 30
0209 C

C
28 RLFCFTR = FLWRAT(FLINDX(LOOP)) / BLNDQY
0210 IF (RLFCFTR.LE.0) GO TO 27
0211 C

C
C ACID CALCULATION
C
30 ASSIGN 40 TO CNTNU
0212 LMNT = 1 !CONTINUE WITH SP. G.
0213 CFLMNT = 1 !ACID SUBSCRIPT
0214 CFLMNT = 1 !ACID COEFF SUBSCRIPT
0215 GO TO 90

C
C SPECIFIC GRAVITY CALCULATION
C
40 ASSIGN 50 TO CNTNU
0216 LMNT = 2 !CONTINUE WITH URANIUM
0217 CFLMNT = 2 !SP. G. SUBSCRIPT
0218 CFLMNT = 2 !SP. G. COEFF SUBSCRIPT
0219 GO TO 90

C
C URANIUM CALCULATIONS
C
50 ASSIGN 60 TO CNTNU
0220 LMNT = 3 !CONTINUE WITH THORIUM
0221 CFLMNT = 3 !URANIUM
0222 CFLMNT = 3 !U COEFF SUBSCRIPT
0223 START = 4 !FIRST U ISOTOPE
0224 STOP = 9 !LAST U ISOTOPE
0225 GO TO 80

C
C THORIUM CALCULATIONS
C
60 ASSIGN 70 TO CNTNU
0226 LMNT = 10 !CONTINUE WITH PLUTONIUM
0227 CFLMNT = 10 !THORIUM
0228 CFLMNT = 4 !TH COEFF SUBSCRIPT
0229 START = 11 !FIRST TH ISOTOPE
0230 STOP = 14 !LAST TH ISOTOPE
0231 GO TO 80

C
C PLUTONIUM CALCULATIONS
C
70 ASSIGN 95 TO CNTNU
0232 LMNT = 15 !CONTINUE WITH NEXT VESSEL
0233 !PLUTONIUM

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01234567890123456789
01234567890123456789
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DM1:L300,300J5FGCHF.LST:1
DM1:L300,300J5FGCHF.LST:1
DM1:L300,300J5FGCHF.LST:1

16:15:16
16:15:16
16:15:16

5-MAR-81
5-MAR-81
5-MAR-81

** RSX-11M V3.1 **
** RSX-11M V3.1 **
** RSX-11M V3.1 **

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DM1:L300,300J5FGCHF.LST:1
DM1:L300,300J5FGCHF.LST:1
DM1:L300,300J5FGCHF.LST:1

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5-MAR-81
5-MAR-81
5-MAR-81

** RSX-11M V3.1 **
** RSX-11M V3.1 **
** RSX-11M V3.1 **

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DM1:L300,300J5FGCHF.LST:1
DM1:L300,300J5FGCHF.LST:1
DM1:L300,300J5FGCHF.LST:1

16:15:16
16:15:16
16:15:16

5-MAR-81
5-MAR-81
5-MAR-81

** RSX-11M V3.1 **
** RSX-11M V3.1 **
** RSX-11M V3.1 **

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FORTRAN IV-PLUS V02-51C 15156:19 05-MAR-81 PAGE 1
SFGCHP.FTN /TRIDBLOCKS/WR

0001 SUBROUTINE SFGCHP(EICMP,SFG,IECR)
C
C SUBROUTINE TO ADJUST THE ELEMENTAL COMPOSITIONS (EICMP)
C TO REFLECT THAT EXPECTED BASED UPON THE MEASURED SPECIFIC GRAVITY (SFG)
C
C INPUTS: EICMP = UNADJUSTED COMPOSITION VECTOR (ELEMENTS & ISOTOPES)
C SFG = MEASURED SPECIFIC GRAVITY
C
C OUTPUT: EICMP = ADJUSTED COMPOSITION VECTOR (ADJUSTMENT APPLIED TO ELEMENTS ONLY)
C IERR = ERROR INDICATOR (0 = ALL OK)
C
C ARGUMENTS: SEE INPUTS AND OUTPUTS
C
C AUTHOR: A. M. KRICHINSKY
C DATE: 5/30/79
C
C MODIFIED 11-NOV-80 BY A. M. KRICHINSKY
C TO CORRECT ANY COMPOSITIONS .LT. 0.0 TO .EQ. 0.0.
C AND TO EXIT IF SUM OF COMPOSITIONS IS 0.0.
C
C MODIFIED 10-DEC-80 BY A. M. KRICHINSKY
C TO CALCULATE AVERAGE ATOMIC WEIGHTS FROM ISOTOPIC INFO
C AND TO IMPROVE THE SUNCHP & TOTCHP CALCULATIONS.
C
C
0002 INTEGER IERR
0003 REAL EICMP(21)
0004 REAL OFFSET
0005 REAL ADOFST
0006 REAL ORDOST
0007 REAL SFG
0008 REAL SUNCHP
0009 REAL TOTCHP
0010 REAL RATIO
0011 REAL U, TH, FU
0012 REAL HNO3, UHM, THNO3, FUND3
0013 REAL HMLR, UMLR, THMLR, THULR
0014 REAL HSFG, USFG, THSFG, FUSFG
0015 REAL UAVI, THAVI, FUAVI
0016 REAL UI(419), TH(11114), FUI(16121)
0017 REAL UI232, UI233, UI234, UI235, UI236, UI238
0018 REAL TH1228, TH1229, TH1230, TH1232
0019 REAL FUI238, FUI239, FUI240, FUI241, FUI242, FUI244
0020 REAL UI101, TH101, FUI101
0021 REAL UIMSC, THIMSC, FUIIMSC
C
C EQUIVALENCE (UI(4),UI232), (UI(5),UI233), (UI(6),UI234),
C 1 (UI(7),UI235), (UI(8),UI236), (UI(9),UI238)
C EQUIVALENCE (TH(11),TH1228), (TH(12),TH1229),
C 1 (TH(13),TH1230), (TH(14),TH1232)
C EQUIVALENCE (FUI(16),FUI238), (FUI(17),FUI239), (FUI(18),FUI240),
C 1 (FUI(19),FUI241), (FUI(20),FUI242), (FUI(21),FUI244)
C
C

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FORTRAN IV-PLUS V02-51C          15156119      05-MAR-81      PAGE 2
SPGCMF.FTN      /TRIRLOCKS/WR

0025      DATA HND3 /63.013/
0026      DATA HSPG,USPG,THSPG,PUSPG /0.0308,0.318,0.358,0.396/
0027      DATA UI /232.037, 233.040, 234.041, 235.044, 236.046, 238.051/
0028      DATA THI /228.029, 229.032, 230.033, 232.038/
0029      DATA FUI /238.050, 239.052, 240.054, 241.057, 242.059, 244.064/
0030      DATA UAVI, THAVI, PUAVI /235.5, 232.0, 239.5/
0031      DATA AROFST, ORGOST /1.003, 0.86/      !SPG OFFSET (NO METAL BURDEN)
C
C
0032      IERR = 0      ! INITIALIZE ERROR INDICATOR FOR ALL OK
C
0033      OFFSET = AROFST      ! ASSUME AQUEOUS SOLUTION
0034      IF (SPG.LE.0.95) OFFSET = ORGOST      ! ASSUME SOLUTION IS EXTRACTANT
C
C
C      CALCULATE AVERAGE ATOMIC WEIGHTS FROM ISOTOPIC COMPOSITIONS
C
C URANIUM
      U = 0.0
      UITOT = 0.0
      DO 1 I = 4,9
        IF (EICMP(I).LT.0.0) EICMP(I) = 0.0
        U = U + UI(I) * EICMP(I)
        UITOT = UITOT + EICMP(I)
      1 CONTINUE
      IF (UITOT.GT.0.0) UITOT = 1.0
      UHSC = 1.0 - UITOT
      U = U + UAVI * UHSC
C
C THORIUM
      TH = 0.0
      THTOT = 0.0
      DO 2 I = 11,14
        IF (EICMP(I).LT.0.0) EICMP(I) = 0.0
        TH = TH + THI(I) * EICMP(I)
        THTOT = THTOT + EICMP(I)
      2 CONTINUE
      IF (THTOT.GT.0.0) THTOT = 1.0
      THHSC = 1.0 - THTOT
      TH = TH + THAVI * THHSC
C
C PLUTONIUM
      PU = 0.0
      PUTOT = 0.0
      DO 3 I = 16,21
        IF (EICMP(I).LT.0.0) EICMP(I) = 0.0
        PU = PU + PUI(I) * EICMP(I)
        PUTOT = PUTOT + EICMP(I)
      3 CONTINUE
      IF (PUTOT.GT.0.0) PUTOT = 1.0
      PUHSC = 1.0 - PUTOT
      PU = PU + PUAVI * PUHSC
C
C
C      CALCULATE MOLECULAR WEIGHTS AND MOLARITIES

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FORTRAN IO-PLUS V02-51C          15:56:19      05-MAR-81      PAGE 3
SFGCMP.FTN      /TRIBLOCKS/WR

0065      UNH = 156.04 + U          URANYL NITRATE (W.O. WATER'S)
0066      THN03 = 248.02 + TH      THORIUM NITRATE
0067      FUN03 = 248.02 + FU      PLUTONIUM NITRATE
      C

0068      IF (EICMP(1).LT.0) HMLR = 1.952*ARS(EICMP(1))
0069      IF (EICMP(1).GE.0) HMLR = EICMP(1)
0070      UMLR = EICMP(3) / U
0071      THLR = EICMP(10) / TH
0072      FUHLR = EICMP(15) / FU
      C

      SUM THE ESTIMATED MOLECULAR COMPOSITIONS
      C
      C
      C
0073      SUNCMP = HN03 * HMLR
      1      + UNH * UMLR
      2      + THN03 * THLR
      3      + FUN03 * FUHLR
      IF (SUNCMP.LE.0.0) GO TO 99
      C

0074      NOW CALCULATE EXPECTED TOTAL COMPOSITION BASED UPON SP.G.
      C
      C
      C
0075      SFGCOR = SP0 - OFFSET
0076      IF (SFGCOR.LT.0.0) SFGCOR = 0.0 !ASSUME NO H OR METAL BURDEN
0077      TOTCMP = (SFGCOR / SUNCMP) * (HMLR*HN03**2/HSFG
      1      + UMLR * UNH**2 / USFG
      2      + THLR * THN03**2 / THSFG
      3      + FUHLR * FUN03**2 / FUSFG)
      IF (SUNCMP.EQ.TOTCMP) GO TO 99
      C

      !FLUG IN MEASURED SP.G.
      !COMPOSITION ADJUSTMENT FACTOR FOR ...
      EICMP(2) = SFG
      EICMP(1) = EICMP(1) * RATIO
      EICMP(3) = EICMP(3) * RATIO
      EICMP(10) = EICMP(10) * RATIO
      EICMP(15) = EICMP(15) * RATIO
      GO TO 99
      C

0079      RETURN
0080      END
0081
0082
0083
0084
0085
0086
0087

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FORTRAN IV-PLUS V02-51C      15:57:05      05-MAR-81      PAGE 2
UNDOFR.FTN  /TRIBLOCKS/WR

0025      CALL OTCODE(9,MSGBUF(12),NANUOP(1))
0026      CALL UDOPFN(NANUOP,4,NDFILE,IERR)
0027      IF (IERR.NE.0) GO TO 903
0028      IF (NDFILE) GO TO 903
C
0029      CALL UDOPFLW(IERR)
0030      IF (IERR.NE.0) GO TO 903
0031      CALL UDOPCLS          ICLOSE UDP DEFN FILE TO START AT BEGINNG
C
0032      CALL UDOPFN(NANUOP,4,NDFILE,IERR)
0033      IF (IERR.NE.0) GO TO 903
0034      IF (NDFILE) GO TO 903
C
0035      CALL UDOPCHF(IERR)
0036      IF (IERR.NE.0) GO TO 903
0037      CALL UDOPCLS          IPERFORM CALCULATIONS
C
0038      CALL UDOPMTY(IERR)
0039      IF (IERR.NE.0) GO TO 903
C
C
C      EXIT
C
0040      IERR = 0
0041      CLOSE (UNIT=4)
0042      RETURN
0043      END

IINTERPRET UNIT OFN NAME TO ASCII
IOFEN THE FILE
ITHERE WAS NO UDP DEFN FILE
ICATALOG ALL FLOW RATES
IABORT
IEMPTY UDOPTPK COMMON TO CDB & IFR PKT

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FORTRAN IV-PLUS V02-51C          15:57:20    05-MAR-81          PAGE 1
UOPCHP.FTN /TRILLOCKS/WR

0001      SUBROUTINE UOPCHP(IERR)
C
C      THIS SUBROUTINE IS CALLED DIRECTLY FROM UNTOPR
C      TO SUPERVISE UNIT OPERATIONS ESTIMATING
C      VESSEL MODELLING, OR ELEMENT CALCULATIONS.
C
C      AUTHOR: A. M. KRICHINSKY
C      DATE: 12/6/78
C
C      MODIFIED: 04-DEC-80 BY: A. M. KRICHINSKY
C      TO SUBSTITUTE AN ESTIMATED TRANSFER QUANTITY
C      (I.E., FLOW RATE * TIME) FOR CONTRIBUTING VESSELS
C      HAVING FLOW MODELS ('MOLF--')
C      OR NO PERCEIVED QTY TFR (I.E., SIMULTANEOUS FLOW IN & OUT).
C
C      MODIFIED: 23-DEC-80 BY: A. M. KRICHINSKY
C      TO ADD QUANTITY CORRECTION/ESTIMATION TO UOPCHP
C      AFTER RETURN FROM VESSEL MODELS (STATEMENT LABEL 381).
C
C      INCLUDE 'PDI(100,100) INVMSBUF.COM/NOLIST'
C      INCLUDE 'PDI(300,300) UOPFNF.COM/NOLIST'
C      INCLUDE 'PDI(300,300) UOPTFK.COM/NOLIST'
C      INCLUDE 'PDI(300,300) UOCCOM.COM/NOLIST'
C      INCLUDE 'PDI(160,160) MIXCOM.COM/NOLIST'
C      INCLUDE 'PDI(100,100) VSWCOM.COM/NOLIST'
C      INCLUDE 'PDI(100,100) CTCOM.COM/NOLIST'
C
C      LOGICAL*1 CTRLZ
C      LOGICAL*1 NOFILE
C      LOGICAL*1 EOF
C      LOGICAL*1 FOUND
C      LOGICAL*1 NOVSL
C      LOGICAL*1 DATE(8), TIME(8)
C      INTEGER IERR
C      INTEGER CNTNU
C      INTEGER LWCNMF
C      INTEGER WCRSLT
C      INTEGER VESSEL
C      INTEGER NULL(2)
C      REAL TFRQTY
C      REAL TFRCHP(21)
C      REAL JTDLFC
C      REAL JTDLER
C
C      ICONTROL-Z INDICATOR
C      IUNIT OFN FILE DOES NOT EXIST INDICATOR
C      IEND OF FILE INDICATOR
C      IFOUND CENTRAL VESSEL IN LIST
C      ICENTRAL VESSEL NOT IN PACKET
C      IASCII DATE & TIME
C      IERROR CODE 0-OK
C      ICONTINUATION STATEMENT LABEL
C      IWORD COMPARISON FUNCTION
C      IWORD COMPARISON RESULT
C      IVESSEL SUBSCRIPT VARIABLE
C      INULL ENTRY LABEL
C      ITRANSFER QTY
C      ICONPOSITIONS OF TRANSFER QTY
C      IJET DILUTION FACTOR
C      IJET DILUTION FACTOR ERROR
C
C      IF A CHANGE IS MADE TO PARAMETERS 'MAXEST', 'MAXMDL', OR 'MAXCLC',
C      THE COMPUTED GO TO STATEMENTS (STATEMENT 25, 359, OR 727) AND
C      THE DATA STATEMENTS 'ESTMAT', 'MODEL', OR 'CALCLT' MUST ALSO BE CHANGED.

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FORTRAN IV-PLUS V02-51C          15157120      05-MAR-81          PAGE 2
UDFCNP.FTN /TRI/LOCKS/WR

0212 C      PARAMETER MAXEST = 1      IMAX # OF ESTIMATORS FOR ENTIRE UNIT OFN
0213 C      PARAMETER MAXMNL = 6      IMAX # OF MODELS FOR VESSEL MODELST
0214 C      PARAMETER MAXCLC = 1      IMAX # OF OTHER CALCULATORS
0215 C      INTEGER ESTMAT(5,MAXEST)    UNIT OFN ESTIMATION SUBR NAMES
0216 C      INTEGER MODEL(5,MAXMNL)    VESSEL MODEL SUBR NAMES
0217 C      INTEGER CALCLT(5,MAXCLC)    OTHER CALCULATION SUBR NAMES
0218 C      DATA ESTMAT /'ES','TS','IS','', ' ' / / ISTATIC DISSOLVER ESTIMATOR
0219 C      VESSEL MODELS CHARACTERIZED BY FLOW CONDITIONS SHOULD HAVE
0220 C      MODEL NAMES WITH FIRST FOUR LETTERS 'MULF--'.
0221 C      TO PERMIT SPECIAL QUANTIFYING OF TRANSFER AMOUNTS.
0222 C      DATA MODEL /
0223 C      1 'MD','LC','MX','', ' ' / COLLECTING PERFECT MIXING MODEL
0224 C      2 'MD','LF','MX','', ' ' / FLOWING PERFECT MIXING MODEL
0225 C      3 'MD','LC','CV','', ' ' / COLLECTING CONVERSION MODEL
0226 C      4 'MD','LF','CV','', ' ' / FLOWING CONVERSION MODEL
0227 C      5 'MD','LC','SP','', ' ' / COLLECTING SEPARATION MODEL
0228 C      6 'MD','LF','SP','', ' ' / FLOWING SEPARATION MODEL
0229 C      DATA CALCLT / 9,9,9,9,9 /
0230 C      DATA NULL /'N','N','A' /
0231 C      UDESOK = .TRUE.
0232 C      IERR = 0
0233 C      *****
0234 C      SPECIALIZED ESTIMATORS
0235 C      *****
0236 C      IS THERE AN OVERALL UNIT OPERATION ESTIMATOR ?
0237 C      WCRSLT = LWCOMP(UQUEST(1),NULL(1),2)
0238 C      IF (WCRSLT.EQ.0) GO TO 300      IND ESTIMATOR; TRY A VESSEL MODEL
0239 C      SELECT ESTIMATOR FOR ENTIRE UNIT OPERATION
0240 C      DO 22 LOOP=1,MAXEST
0241 C      WCRSLT = LWCOMP(UQUEST(1),ESTMAT(1,LOOP),5)
0242 C      IF (WCRSLT.EQ.0) GO TO 25      IF FOUND IT
0243 C      CONTINUE
0244 C      ESTIMATOR DOES NOT EXIST. ERROR LOG AND TRY VESSEL MODELS.
0245 C      GO TO 90
0246 C      GO TO THE ESTIMATOR
0247 C
0248 C
0249 C
0250 C
0251 C
0252 C
0253 C
0254 C
0255 C
0256 C
0257 C
0258 C
0259 C
0260 C
0261 C
0262 C
0263 C
0264 C
0265 C
0266 C
0267 C
0268 C
0269 C
0270 C
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0280 C
0281 C
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0290 C
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0298 C
0299 C
0300 C
0301 C
0302 C
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0310 C
0311 C
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0345 C
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0350 C
0351 C
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0360 C
0361 C
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0370 C
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0375 C
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0379 C
0380 C
0381 C
0382 C
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0384 C
0385 C
0386 C
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0390 C
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0397 C
0398 C
0399 C
0400 C

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FORTRAN IV-PLUS V02-51C          15157120    05-MAR-81          PAGE 3
UDPCHP,FTN      /TRIBLOCKS/MR

0231 25      GO TO (110) LOOP
0232      GO TO 90
0233 80      CALL UOFCLS
0234      RETURN
C
C      ERROR THE ESTIMATOR WHICH CANNOT BE FOUND
C
0235 90      CALL ERRLOG(7,UOTPKN,'K',0,
0236      1      'ESTIMATOR DOES NOT EXIST IN UOP DEFM FILE (TTY=FCNT #)')
C      GO TO 300
C=====
C
C      CALLS TO SPECIALIZED ESTIMATORS
C=====
C
C      DISSOLVER ESTIMATOR
C-----
C
0237 110     CALL ESTDS(IERR)
0238     IF (IERR.NE.0) GO TO 903
0239     GO TO 80
C
C      END OF SPECIALIZED ESTIMATORS
C=====
C
C      VESSEL MODELS
C=====
C
C      READ THE UNIT OPERATION DEFINITION FILE VESSEL ENTRY
C
0240 300     CALL UOPRED(EOP,IERR)
0241     IF (IERR.NE.0) GO TO 903
0242     IF (EOP) GO TO 990
0243     IF (UOUTYP.EQ.1) GO TO 300
C      IF FINISHED
C      TWO ESTIMATE ON SOURCE VSLs
C
C      LOCATE ALL THE VESSELS IN THIS VESSEL ENTRY
C
0244     CALL UOPVNX(FOUND,IERR)
0245     IF (IERR.NE.0) GO TO 300
0246     IF (.NOT.FOUND) GO TO 300
0247     IF (SVSNUM.EQ.0) GO TO 300
C      LOCATE ALL FLOW LABELS AND SET UP FLOW RATE CROSS REFERENCE INDEXING
C
0248     CALL UOPFNX(IERR)
0249     IF (IERR.NE.0) GO TO 300
C      SKIP THIS VESSEL
C
C      INITIALIZE BLEND FIELDS
C

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FORTRAN IV-PLUS V02-51C      15:57:20      05-MAR-81      PAGE 8
UDFCMP.FTM /TR:BLOCKS/WR

0352      C      IF (IERR.NE.0) GO TO 461
0353      C      GO TO 380
      C
      C
      C      THE FLOWING SEPARATION TRANSFER MODEL
      C      -----
      C
      C      THE FLOWING SEPARATION TRANSFER MODEL MAY ACCOMMODATE
      C      CONTRIBUTIONS FROM ALL VESSELS SPECIFIED
      C      IN THE VESSEL ENTRY OF THE UOP DEFINITION FILE.
      C
      C
      C      IERR = -1      ISET FLOW INDICATOR
0354      C      CALL MDLSEP(IERR)
0355      C      IF (IERR.EQ.0) GO TO 472
0356      C      UOESOK = .FALSE.
0357      C      IESTIMATE MAY NOT BE OK
      C
0358      C      GO TO 380
      C
      C
      C      END OF VESSEL MODELS
      C
      C*****
      C
      C      OTHER CALCULATIONS
      C      =====
      C
0359      C      DO 705 LOOP=1,UOLMHX      ISTEP THRU SUBROUTINE NAMES
0360      C      WCRSLT = LWCOMP(UOCLC(1,LOOP),NULL(1),2)
0361      C      IF (WCRSLT.EQ.0) GO TO 705      IWO CALCULATION SUBR
0362      C      DO 702 LOOP1=1,MAXCLC
0363      C      WCRSLT = LWCOMP(UOCLC(1,LOOP),CALCLT(1,LOOP1),5)
0364      C      IF (WCRSLT.EQ.0) GO TO 709
0365      C      CONTINUE
0366      C      CALL LOUWHF(UOCLC(1,LOOP),UOPNAM(1),IERR)      ILOG ENTRY NOT FOUND
0367      C      CONTINUE
      C
      C
      C      GO TO THE CALCULATION
      C
0368      C      GO TO (710) LOOP1
0369      C      GO TO 703
      C      =====
      C      ERROR LOG AND TRY ANOTHER ELEMENT
      C      =====
      C
      C      CALLS TO OTHER CALCULATION SUBROUTINES
      C      =====
      C
0370      C      GO TO 700
      C

```

```

FORTRAN IV-PLUS V02-51C      15:57:20      05-MAR-81      PAGE 9
UDPCNF.FTN /TR:BLOCKS/MR

0371      C      880      GO TO 300      !GET ANOTHER VESSEL
          C
          C
          C      END OF OTHER CALCULATIONS
          C*****
          C*****
          C
          C      PROGRAM EXITS
          C*****
          C
          C      ERROR DURING CALCULATIONS
          C      UDESOK = .FALSE.      !ESTIMATE MAY NOT BE OK
0372      C      903
          C
          C      NORMAL EXIT
          C
          C      990      RETURN
          C
0373      C
0374      C      END

```



```

FORTRAN IV-PLUS V02-51C          10137157    06-MAR-81          PAGE 1
UOFFIL.FTN /TRIBLOCKS/WR

0001      SUBROUTINE UOFFIL(IERR)
C
C      SUBROUTINE TO FILL 'UOFFTK' COMMON AREA WITH INFORMATION
C      APPLICABLE TO ESTIMATING UNIT OPERATIONS,
C      THE INFORMATION FILLING THE COMMON AREA IS OBTAINED FROM
C      THE TRANSFER PACKET FILE ASSOCIATED WITH THE TRANSFER.
C
C      AUTHOR:  A. M. KRICHINSKY
C
C      DATE:    10/28/78
C
C      INPUTS:  MESSAGE BUFFER DEFINED IN 'INVHSGRUF.COM'
C               TRANSFER PACKET INFORMATION
C
C      OUTPUTS: A COMMON AREA, 'UOFFTK', FILLED WITH AN ENTRY
C               FOR EACH APPLICABLE VESSEL IN THE PACKET.
C               ARGUMENT: IERR = ERROR CODE (0 = EVERYTHING OK)
C
C      MODIFIED: 21-MAY-80 BY A. M. KRICHINSKY
C               TO COPY TFR TERMINATION DATE & TIME INTO UOFFTK COMMON
C
C      INCLUDE 'FDI100,1001 INVHSGRUF.COM/NOLIST'
C      INCLUDE 'FDI100,1001 IPUSER.COM/NOLIST'
C      INCLUDE 'LLI100,1001TFLUN.EXP/NOLIST' 11/9/78
C      INCLUDE 'LLI100,1001TFFARN.EXP/NOLIST' 16/2/78
C      INCLUDE 'LLI100,1001TFFNDX.EXP/NOLIST' 16/2/78
C      INCLUDE 'LLI100,1001TFFHDR.EXP/NOLIST' 12/2/79
C      INCLUDE 'LLI100,1001TFFDAT.EXP/NOLIST' 16/2/78
C      INCLUDE 'FDI100,1001 VSMCON.COM/NOLIST'
C      INCLUDE 'FDI100,1001 CTCCOM.COM/NOLIST'
C      INCLUDE 'FDI300,3001 UOFFTK.COM/NOLIST'
C      INCLUDE 'FDI300,3001 UOFFEN.COM/NOLIST'
C
C      LOGICAL*1 ENDPKT          IEND OF TRANSFER PACKET INDICATOR
C      LOGICAL*1 VSLASC(12)      IASCII VESSEL NAME
C      LOGICAL*1 DATE(8), TIME(8) IEXECUT DATE AND TIME VECTORS
C      INTEGER IERR, IERROR      IEXECUTION ERROR CODES) 0 = OK
C      INTEGER CHITU             ICONTINUATION STATEMENT LABEL
C      INTEGER VRN               ITRANSFER PACKET NO. & TFR VESSEL REC NO
C      INTEGER OFCDH             ITERMINAL TO BE NOTIFIED FOR ILLEGAL ZEROS
C      INTEGER TIMOUT            ITIME OUT VARIABLE
C
C      DETERMINE IF PACKET ATTRIBUTES INDICATE THAT
C      UNIT OPERATIONS ESTIMATION IS WARRANTED.
C
C      IF (HSGRUF(6).GT.100) GO TO 9700
C      IF ((HSGRUF(5).NE.3).AND.(HSGRUF(5).NE.4)
C          .AND.(HSGRUF(5).NE.6)) GO TO 9800
C
C      !NON-PROCESSING TFR; RAIL OUT
C      !IF NOT TERMINATION OR COMPLETION
C      ! OR ROTH, RAIL OUT

```



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FORTRAN IV-PLUS V02-51C      10147105      06-MAR-81      PAGE 2
UOFLW.FTH      /TR:BLOCKS/MR

0130      IF (NUH.EQ.12) GO TO 45
0131      CALL LGUVNF(VSLCR5,UOPNAM,IERR)      !LOG VESSEL NOT FOUND
0132      GO TO 30      !TRY ANOTHER VSL ENTRY

C
0133      DO 50 LOOP1=1,UONOV5
45      WCRSLT = LWCOMP(VSLCR5,UOVSD(1,LOOP1),4)
0134      IF (WCRSLT.EQ.0) GO TO 60      !FOUND IT
0135      CONTINUE
0136      GO TO 30
50      !THIS VESSEL IS NOT INVOLVED IN CALCULATIONS

C
C      CALCULATE FLOW TIME SINCE LAST CALCULATION
C
0138      CONTINUE
0139      FLWTH(LLOOP1) = RLTAHR(UODATE(LLOOP1),UOTIME(LLOOP1))

C
C      SEE IF THIS FLOW LABEL SHOULD BE ADDED TO LIST
C
0140      WCRSLT = LWCOMP(UOCFLR(1),NULL(1),2)
0141      IF (WCRSLT.EQ.0) GO TO 90      !NO FLOW LABEL IN THIS ENTRY
0142      DO 70 LOOP1=1,FLWLNK      !IS IT IN THE LIST ?
0143      IF (FLWLBL(1,LOOP).EQ.0) GO TO 80      !NO MORE ENTRIES! ADD IT TO THE LIST
0144      WCRSLT = LWCOMP(UOCFLR(1),FLWLBL(1,LOOP),6)
0145      IF (WCRSLT.EQ.0) GO TO 30      !ALREADY HAVE IT
0146      CONTINUE
0147      GO TO 907      !INSUFFICIENT CAPACITY FOR FLOW LABELS

C
C
C      ADD FLOW LABEL AND FLOW RATE TO LIST
C
0148      CALL WCOPY(UOCFLR(1),FLWLBL(1,LOOP),6)      !CATALOG FLOW LABEL
0149      FLWRAT(LLOOP) = UOFLRT(LLOOP1)      !CATALOG FLOW RATE

C
C      ESTABLISH APPLICABILITY OF FLOW MODELS ('MULF---')
C
0150      CONTINUE
0151      FLWML(LLOOP1) = .FALSE.      !ASSUME FLOW MODEL NOT APPLICABLE
0152      WCRSLT = LWCOMP(MULF,UOVMDL,2)
0153      IF (WCRSLT.EQ.0) FLWML(LLOOP1) = .TRUE.      !FLOW MODEL IS APPLICABLE
0154      GO TO 30

C
C      DETERMINE ANY REQUIRED SOURCE FLOW RATES FROM DILUTIONS TO THESE VESSELS
C
C
C
C
100      CONTINUE
0155      CALL UOFPN(UOPNAM,4,NOFILE,IERR)
0156      IF (IERR.NE.0) GO TO 903
0157      IF (NOFILE) GO TO 903
0158      CALL UOFRED(EOF,IERR)
0159      IF (IERR.NE.0) GO TO 903
0160      IF (EOF) GO TO 903
0161      IS THIS VESSEL IN UOFTPK COMMON ? IF SO, GET INDEX NUMBER.
C
C

```

[illegible]


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FORTRAN IV-PLUS V02-51C          15159144    05-MAR-81    PAGE 1
UOFFNX.FTN /TRIBLOCKS/WR

0001      C
          C SURROUTINE UOFFNX(IERR)
          C SURROUTINE TO CROSS REFERENCE THE FLOW LABELS OF
          C A VESSEL ENTRY OF THE UNIT OFRTNS DEFN FILE WITH
          C A LIST OF ALL FLOW LABELS IN THE UNIT OFRTNS DEFN FILE.
          C
          C THE LINK BETWEEN THE TWO LISTS IS 'FLINDEX' WHICH HAS
          C ONE CROSS REFERENCING SUBSCRIPT VALUE ASSIGNED FOR
          C EACH LABEL OF THE VESSEL ENTRY.
          C
          C
          C AUTHOR: A. M. KRICHINSKY
          C DATE: 12/12/78
          C
          C INCLUDE 'D:\C100,100\ INVMSGRUF.COM\NOLIST'
          C INCLUDE 'D:\C300,300\ UOFFDN.COM\NOLIST'
          C INCLUDE 'D:\C300,300\ UOCCOM.COM\NOLIST'
          C
          C INTEGER IERR          !ERROR INDICATOR (0=OK)
          C INTEGER LWCOMP      !WORD COMPARISON FUNCTION
          C INTEGER WCRSLT      !WORD COMPARISON RESULT
          C INTEGER NULL(2)     !NULL ENTRY VECTOR
          C INTEGER WNZERO(4)   !VECTOR OF ZEROES
          C
          C DATA NULL /'N','A' //
          C DATA WNZERO /0,0,0,0,0,0/
          C
          C DO 40 LOOP=1,UOFFLNX
          C   FLINDEX(LOOP) = 0          !INITIALIZE THE INDEX
          C
          C   IS THIS LABEL NULL ?
          C     WCRSLT = LWCOMP(UOFFLRL(1,LOOP),NULL,2)
          C     IF (WCRSLT.EQ.0) GO TO 40    !YES IT IS
          C
          C   LOCATE FLOW LABEL IN THE LIST
          C     DO 30 LOOP1=1,FLBLNX
          C       IS THIS LIST ENTRY ZERO ?
          C       WCRSLT = LWCOMP(WNZERO(1),FLWLR(1,LOOP1),4)
          C       IF (WCRSLT.EQ.0) GO TO 40    !YES IT IS! NO MORE ENTRIES
          C       WCRSLT = LWCOMP(UOFFLRL(1,LOOP),FLWLR(1,LOOP1),4)
          C       IF (WCRSLT.EQ.0) GO TO 39    !FOUND IT IN THE LIST
          C     CONTINUE
          C     GO TO 40
          C   !FLOW NOT PRESENTLY ACTIVE
          C
          C   ASSIGN THE CROSS REFERENCE SUBSCRIPT
          C     FLINDEX(LOOP) = LOOP1
          C
          C   CONTINUE
          C
          C   RETURN
          C   END
0002
0016
0079
0102
0103
0104
0105
0106
0107
0108
0109
0110
0111
0112
0113
0114
0115
0116
0117
0118
0119
0120
0121
0122
0123

```



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FORTAN IV-PLUS V02-51C 10:40:19 06-MAR-81 PAGE 1
UOPNTY.FTN /TRLOCKS/WR

0001 C
      SUBROUTINE UOPNTY(IERR)
      SUBROUTINE TO UPDATE THE CDR & TFR PKT RECORDS
      (FOR ANY TERMINATED VESSELS)
      WITH RELATED INFORMATION HELD IN THE COMMON AREA 'UOPTPK'.

      AUTHOR: A. M. KRICHINSKY
      DATE: 10/28/78

      INPUTS: INFORMATION HELD IN 'UOPTPK' COMMON AREA

      OUTPUTS:
      UPDATED CDR RECORDS FOR EACH VESSEL WITH AN ENTRY IN 'UOPTPK'.
      TRANSFER PACKET VESSEL RECORDS UPDATED WITH PROCESSED RIT SET
      AND COMPOSITION VECTOR AND QUANTITY VARIABLE
      WHERE APPLICABLE
      ARGUMENT: IERR = ERROR CODE (0 = EVERYTHING OK)

      MODIFIED 18-DEC-80 BY A. M. KRICHINSKY
      TO CALCULATE NET TFR QTY AND ASSIGN IT TO 'ENETQ1' FOR
      TERMINATED VESSELS REQUIRING QTY ESTIMATN OR CORRECTN.

      INCLUDE 'PDIT300,300J UOPTPK.COM/NOLIST'
      INCLUDE 'PDIC123,123J CDR.COM/NOLIST'
      INCLUDE 'PDIC100,100J CTCCON.COM/NOLIST'
      INCLUDE 'PDIC100,100J TPUSER.COM/NOLIST'
      INCLUDE 'LLIC100,100JTFPLUM.EXP/NOLIST' 111/9/78
      INCLUDE 'LLIC100,100JTFPHARM.EXP/NOLIST' 16/2/78
      INCLUDE 'LLIC100,100JTFPHDX.EXP/NOLIST' 16/2/78
      INCLUDE 'LLIC100,100JTFPHOR.EXP/NOLIST' 12/2/79
      INCLUDE 'LLIC100,100JTFHAI.EXP/NOLIST' 16/2/78
      INCLUDE 'PDIC100,100J USWCOM.COM/NOLIST'

      INTEGER*2 VSLASC(6)
      LOGICAL*1 ENDPKT
      INTEGER IERR, IERROR
      INTEGER CHINU
      INTEGER LWCONF, WCHPRS
      INTEGER VRN
      INTEGER PACKET(S)
      REAL DAY1, DAY2
      REAL TIM

      DATA PACKET / 'TF','R','PA','CK','ET' /
      IERR = 0
      VRN = 0

      OPEN CDR AND TFR PKT TO UPDATE RECORDS

```

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FORTRAN IV-PLUS V02-S1C                                10140119      06-MAR-81      PAGE 2
UDPRTY.FTN /TRBLOCKS/WR

C
0221 CALL CORUP2(4,6,IERR)
0222 IF (IERR.NE.0) GO TO 9910

C
0223 CALL TINDFN(1,IERR)
0224 IF (IERR.NE.0) GO TO 9900

C
C=====
C
C FOR EACH VESSEL ENTRY IN 'UOPTPK' COMMON,
C READ THE TRANSFER PACKET ENTRY OF THAT VESSEL AND
C (WHERE THE VESSEL IS NOT STILL ACTIVE IN THE TRANSFER)
C READ THAT VESSEL'S RECORD IN THE CDR SO THAT
C IT MAY BE UPDATED WITH THE INFORMATION IN 'UOPTPK' COMMON.
C
C DO 200 LOOP=1,UONOV5
C
C CALL VSWNAM(UOVSWD(LLOOP))
C IF (VSWACT.NE.2) GO TO 100
C
C UPDATE THE CDR
C
C CALL CORGT2(UOVSID(1,LLOOP),NOREC,IERR)
C IF (IERR.NE.0) GO TO 9900
C IF (NOREC.EQ.0) GO TO 9100
C
C CALL CTCNAM(CTYPE)
C
C COPY FIELDS INTO CDR
C
C DO 20 LOOP1=1,21
C   IEICON(LLOOP1) = UOFCHP(LLOOP1,LLOOP)
C   CONTINUE
C IF (.NOT.CTOER) GO TO 22
C CQTY = UOFQTY(LLOOP)
C CQTY2 = UOFQTY(LLOOP)
C IF (UDESOK) CTCF = .TRUE.
C IF (.NOT.UDESOK) CTCF = .FALSE.
C CALL NAMCTC(CTYPE)
C
C CALL CORUP2(IERR)
C IF (IERR.NE.0) GO TO 9900
C
C UPDATE THE TRANSFER PACKET
C
C CONTINUE
C CALL TFRFED(UOTFKN,VRN,IERR,ENDPKT)
C IF (IERR.NE.0) GO TO 9900
C WCHPRS = LWCOMP(UOVSID(1,LLOOP),FVIDR1,4)
C IF (WCHPRS.EQ.0) GO TO 120
C IF (.NOT.ENDPKT) GO TO 100
C CALL LGUWVF(UOVSID(1,LLOOP),PACKET(1),IERR)

C
0243
0244
0245
0246
0247
0248
0249
! INTERPRET VESSEL STATUS WORD
! VESSEL NOT YET TERMINATED

! GET THE CDR VESSEL RECORD
! COULD NOT FIND VESSEL IN CDR
! INTERPRET CCONTAINER TYPE

! ELEMENT ISOTOPE VECTOR

! NO QTY CORRECTN OR ESTIMATE REQ'D
! CURRENT QTY
! ESTIMATED COMPOSITIONS PRESENT
! EST. COMPOS. NOT PRESENT
! RECODE CTYPE

! WRITE THE CDR VESSEL RECORD TO DISK

! IS THIS THE RIGHT VESSEL
! YES
! TRY AGAIN
! COULD NOT FIND IT IN THE PACKET

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FORTAN IV-PLUS V02-51C          16:01:00    05-MAR-81          PAGE 1
UDOPFN.FTN /TR:BLOCKS/WR

0001      C      SUBROUTINE UDOPFN(NAME,LUN,NOFILE,ERR)
          C      AUTHOR: L.R. LAYMAN
          C      FUNCTION: FORMAT A FILE NAME AND OPEN THE FILE
          C      FOR READING A UNIT OPERATION DEFINITION FILE.
          C      ARGUMENTS: NAME-- 9 CHARACTER FILE NAME IN ASCII.
          C      LUN-- LOGICAL UNIT NUMBER
          C      NOFILE--LOGICAL#1 VARIABLE SET TO .TRUE. IF FILE NO EXIT.
          C      IMPLICIT INTEGER(A-Z)

0002      C      MODIFIED: 12/3/79 BY: J.A. MCEEVERS
          C      ADDED "CALL ERSET" FOR ERROR 43 (BAD FILE NAME) TO COVER
          C      CASE OF A "-1" BEING ENTERED RATHER THAN A VALID UDOP NAME.
          C
          C      LOGICAL#1 INPUT(80)
          C      INCLUDE 'FD:1300,300JUDOPFN.COM/NOLIST'
          C
          C      LOGICAL#1 NAME(9),FSPEC(26)      19 CHAR. UDOP NAME & 26 CHAR FILE SPEC.
          C      LOGICAL#1 NOFILE
          C
          C      COMMON/UDOPLUN/UDOPLUN
          C      DATA FSPEC/'0','8','1','1','1','3','5','0','0','3','5','1','1','3',
          C      19,' ',' ','U','0','P','0/
          C      UDOPLUN=LUN

          C      INSERT USER SUPPLIED NAME IN FILE SPECIFIER.

0072      CALL BCOPY(NAME,FSPEC(13),9)
0073      NOFILE=.FALSE.  IASSUME FILE EXISTS
0074      CALL ERSET(29,.TRUE.,.FALSE.,.TRUE.,.FALSE.) ITURN OFF MESSAGE
0075      CALL ERSET(30,.TRUE.,.FALSE.,.TRUE.,.FALSE.) ITURN OFF MESSAGE
0076      CALL ERSET(43,.TRUE.,.FALSE.,.FALSE.,.FALSE.) ITURN OFF MESSAGE
0077      CALL ERSNS
0078      OPEN(UNIT=LUN,NAME=FSPEC,TYPE='OLD',ERR=100,SHARED,
          C      1 REASONLY,ACCESS='SEQUENTIAL')

          C      READ HEADER RECORD

0079      READ(LUN,40,END=200,ERR=100)INPUT
0080      FORMAT(80A1)
0081      CALL UNIFK(INPUT,UDOPNAM,80,10,2,LSBTYT)
0082      RETURN
0083      CALL ERSNS(ERNNO,FCSNO)
0084      IF(ERNNO.NE.30 .OR. FCSNO.NE.-29)GO TO 110 !ALREADY OPEN FOR WRITE
0085      CALL WFSHE      !WAIT FOR EVENT AND TRY AGAIN
0086      GO TO 10
0087      CONTINUE
0088      NOFILE=.TRUE.
0089      RETURN
0090      CALL ERKLOG(7,ERNNO,'F',FCSNO,
          C      1 'OPEN ERROR, ITV1 = ERROR NO., CODE1 = FCS NO.')
          C      ERR=-1
          C      RETURN
0091
0092
0093      IF (.NOT.(ERNNO.EQ.29 .OR. FCSNO.EQ.-26 .OR. ERNNO .EQ. 43))GO TO 105
0094      NOFILE=.TRUE.      !NO SUCH FILE
0095      RETURN

```

PAGE 2

FORTRAN IV-PLUS V02-51C 16101100 05-MAR-81
 UOFPN.FTN /TRIBLOCKS/WR

```

C----->
0096      ENTRY UOFCLS
0097      IF (UOFLUN.EQ.0) GO TO 190
0098      CLOSE(UNIT=UOFLUN)
0099      RETURN
0100      END
  
```

ILUN HAS NOT BEEN DEFINED


```

FORTRAN IV-FLUS  V02-51C      16101121      05-MAR-81      PAGE 1
U0F01Y.FIN      /TRIMBLOCKS/MR

SUBROUTINE U0F01Y(IERR)

  SURROUTINE TO OBTAIN THE PRESENT QUANTITIES OF ALL ACTIVE,
  NON-ON-LINE, INSTRUMENTED VESSELS IN THE UNIT OPERATIONS COMMON.

  AUTHOR:  A. M. KRICHINSKY
  DATE:    3/12/79

  INCLUDE 'PD:[1300,300]U0FIFK.COM/NDLIST',
  INCLUDE 'PD:[1100,100]VSWCOM.COM/NDLIST',
  INCLUDE 'PD:[1100,100]CTCCOM.COM/NDLIST',

  REAL LEVEL
  BYTE VSLASC(12)

  GET PRESENT QTY FOR EACH ACTIVE VESSEL

  DO 100 LOOP=1,U0NOVS
    CALL VSWNAM(U0VSUB(L00P))
    IF (VSWACT.NE.1) GO TO 100
    CALL CTCNAM(U0FTYF(1,L00P))
    IF (.NOT.CTOMLN) GO TO 5C
    VESSEL IS ON-LINE! GET QTY FROM VESCOM
    CALL QTYSL(L00VSIB(1,L00P),U0FQTY(L00P),U0FSPB(L00P),
     1 LEVEL,U0FTMF(L00P),IERR)
    GO TO 100

  VESSEL IS OFF-LINE! DETERMINE QTY FROM FLOW RATE
  FLOWHR = ULIARH(UPDATE(L00P),U0TIME(L00P))
  U0FQTY(L00P) = U0JNGY(L00P) - U0FLRT(L00P)*FLOWHR
  IF (U0FQTY(L00P).LT.0.0) U0FQTY(L00P) = 0.0
  IF (U0FQTY(L00P).LT.0.0) U0FQTY(L00P) = 0.0

  CONTINUE
  RETURN
  END

```



```

FORTRAN IV-PLUS 002-51C 10147137 06-MAR-81 PAGE 1
UDPRD.FTN /TRIBLOCKS/WR

0001 C SUBROUTINE UDPRD(EOF, IERR)
      C AUTHORS: AMK & LRL
      C FUNCTION: READ A VESSEL RECORD IN THE UNIT OPERATIONS
      C DEFINITION FILE SPECIFIED IN OPEN ROUTINE.

0002 C IMPLICIT INTEGER(A-Z)
0003 C INCLUDE 'PDIC300,300J UDPRDN.COM/NOLIST'

0066 LOGICAL*1 EOF, INPUT(80), TEMP(3)
0067 INTEGER*2 RECLTH, NAMLTH, NUMNAH, LSTRTY
0068 INTEGER*2 ERRBUF(30)
0069 COMMON/UDPLUN/UDPLUN
0070 EOF=.FALSE.
0071 DO 3 LOOP=1, UDPLVZ
0072 UDPLVZ(LLOOP)=0
0073 CONTINUE
0074 LSTRTY=0
0075 RECLTH=80
0076 NAMLTH=12
0077 NUMNAH=3

      C LAST BYTE CONVERTED BY UNPK SUBROUTINE
      C INPUT RECORD LENGTH IN BYTES
      C CHARACTERS PER NAME
      C NAMES PER RECORD

0078 C READ VESSEL I.D. RECORD
0079 1000 READ(UDPLUN, 1000, ERR=999, END=800) INPUT
      FDMAT(80A1)

0080 C UNPACK THREE 12 CHARACTER ASCII NAMES.
      CALL UNPK(INPUT, UDPLVZL, RECLTH, NAMLTH, NUMNAH, LSTRTY)

0081 C UNPACK 2 INTEGERS.
      ENCODE(3, 43, TEMP, ERR=7777)(INPUT(KK), KK=LSTRTY+1, LSTRTY+3)
0082 43 FORMAT(3A1)
0083 DECODE(3, 44, TEMP, ERR=8888) UDPLVYF, UDPLMTD
0084 44 FORMAT(2I2)

0085 C READ OTHER VESSEL NAMES.
      READ(UDPLUN, 1000, ERR=999, END=800) INPUT
0086 NAMLTH=12
0087 NUMNAH=4
0088 CALL UNPK(INPUT, UDPLVZL, RECLTH, NAMLTH, NUMNAH, LSTRTY)

0089 C READ FLOW LABELS RECORD.
      READ(UDPLUN, 1000, ERR=999, END=800) INPUT
0090 NAMLTH=12
0091 NUMNAH=6
0092 CALL UNPK(INPUT, UDPLVZL, RECLTH, NAMLTH, NUMNAH, LSTRTY)

0093 C READ CALCULATION SUBROUTINE NAMES
0094 READ(UDPLUN, 1000, ERR=999, END=800) INPUT
      NAMLTH=10
      CHARACTERS PER NAME

```

```

FORTRAN IV-PLUS V02-51C      10:47:37      06-MAR-81      PAGE 2
UDPRD.FTN      /TRIBLOCKS/WR

0095      NUNNAM=6      INAMES PER RECORD
0096      CALL UNPK(INPUT,UDCLC,RECLTH,NAHLTH,NUNNAM,LSBRT)

      C      READ 6 COEFFICIENT RECORDS.

0097      READ(UDPLUN,1005,ERR=999,END=800)UDCOF
0098      FORMAT(4F16.0)
0099      RETURN

0100      EOF=.TRUE.
0101      RETURN

      C      READ ERROR

0102      IERR=-1
0103      CALL NZERO(ERRBUF,30)      IZERO MESSAGE BUFFER
0104      ENCODE(60,199,ERRBUF,ERR=9999)UDPNAM,UDCVSL
0105      FORMAT('READ ERR ON ',5A2,'.UDF',1USL='',6A2,'. (TTY=LUN)')
0106      CALL ERRLOG(7,UDPLUN,'F',0,ERRBUF)
0107      RETURN
0108      IERR=-6
0109      RETURN
0110      IERR=-7
0111      CALL ERRLOG(7,0,'F',0,'ENCODE ERROR')
0112      RETURN
0113      IERR=-8
0114      CALL ERRLOG(7,0,'F',0,'DECODE ERROR')
0115      RETURN
0116      END

```



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FORTRAN IV-PLUS V02-51C          16102113    05-MAR-81          PAGE 1
UDFVNFX.FTN  /TR:BLOCKS/MR

0001      SUBROUTINE UDFVNFX(FOUND,IERR)
C
C      SUBROUTINE TO FIND ALL VESSELS INVOLVED IN A
C      UNIT OPERATION VESSEL ENTRY CALCULATION.
C      IT IS ASSUMED THAT THE UNIT OPERATION
C      DEFINITION FILE IS ALREADY OPEN.
C      ONCE THE CENTRAL VESSEL HAS BEEN FOUND,
C      "FOUND" IS SET TO .TRUE.
C
C      AUTHOR:  A. M. KRICHINSKY
C
C      DATE:  12/11/78
C
C
0002      INCLUDE 'F01[300,300] UOFTFK.COM/NOLIST'
0028      INCLUDE 'F01[300,300] UOPDFN.COM/NOLIST'
0091      INCLUDE 'F01[300,300] UOCCOM.COM/NOLIST'
0114      INCLUDE 'F01[100,100] VSWCOM.COM/NOLIST'
C
C
0122      LOGICAL*1 FOUND
0123      INTEGER IERR
0124      INTEGER NUM
0125      INTEGER LMCOMP
0126      INTEGER WCRSLT
0127      INTEGER WZZERO(3)
0128      INTEGER NULL(2)
C
C      CENTRAL VESSEL FOUND INDICATOR
C      ERROR INDICATOR (0-OK)
C      INCODDED CHARACTERS COUNTER
C      WORD COMPARISON FUNCTION
C      WORD COMPARISON RESULT
C      VECTOR OF ZEROES
C      NULL ENTRY IDENTIFIER
C
C129      DATA WZZERO /' ','0','0','0' /
C130      DATA NULL /'N','A' /
C
C      FIND THE CENTRAL VESSEL
C
C
0131      IERR = 0
0132      VSLNUM = 0
0133      FOUND = .FALSE.
C
C      INITIALIZE ERROR CODE
C      INITIALIZE CENTRAL VESSEL INDEX #
C      ASSUME WE CAN'T FIND IT
C
C134      DO 10 LOOP=1,3
0135          WCRSLT = LMCOMP(UOVCVSL(1),WZZERO(LOOP),1)
0136          IF (WCRSLT.EQ.0) GO TO 50
0137      CONTINUE
C
C      TEST FOR ZERO ENTRY
C      THE ENTRY IS ZERO! LOOK FOR MANUAL ENTRY
C
C138      CALL INCODE(12,UOVCVSL(1),VSLCR5(1),NUM) ! INCODE THE CENTRAL VSL NAME
0139      IF (NUM.EQ.12) GO TO 20
0140      CALL LOUVNF(UOVCVSL(1),UDPHAM(1),IERR) ! LOG AN INVALID VESSEL NAME
0141      RETURN
C
C142      DO 25 LOOP=1,UONOV5
0143          WCRSLT = LMCOMP(UOV5IN(1,LOOP),VSLCR5(1),4)
0144          IF (WCRSLT.EQ.0) GO TO 60
0145      CONTINUE
C
C      COMPARE IT WITH I.D.'S IN UOFTFK COMMON
C      VESSEL IS NOT INVOLVED IN CALCULATION
C
C      COULD NOT FIND CENTRAL VESSEL
C
0146      RETURN

```

```

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UOPVNX.FTN      /TR:BLOCKS/MR

C
C
C      FIND A MANUAL ENTRY
C
0147 50 DO 55 LOOP1=1,UDNOVS
0148     CALL VSMNH(UOVSWD(LOOP1))
0149     IF ((UOVSWD(LOOP1).GE.0).AND.
1      (.NOT.UOPRO(LOOP1)).AND.
2      (VSMYTF.EQ.UOVVTF).AND.
3      (VSMHET.EQ.UOHTH))
4      GO TO 60
0150 CONTINUE
0151 RETURN

C
C      FOUND CENTRAL VESSEL
C
0152 FOUND = .TRUE.
0153 VSLNUM = LOOP
0154 GO TO 100

C
C
C      FIND THE OTHER VESSELS INVOLVED IN CALCULATIONS
C
0155 DO 180 LOOP1=1,UOVSHX
0156     UNUM(LOOP) = 0
0157     WCRSLT = LMCOMP(UOVSL(1,LOOP),NULL,2)
0158     IF (WCRSLT.EQ.0) GO TO 180
0159     LOOP1 = 0
0160     DO 132 LOOP1=1,3
0161         WCRSLT = LMCOMP(UOVSL(1,LOOP),MDZERO(LOOP1),1)
0162         IF (WCRSLT.EQ.0) GO TO 150
0163         !IT IS ZERO. TRY MANUAL VSL
0164         CALL INCODE(12,UOVSL(1,LOOP),VSLR50(1,LOOP),NUM)
0165         IF (NUM.EQ.12) GO TO 133
0166         CALL LGUVHF(UOVSL(1,LOOP),UOPNH(1),IERR)
0167         IF (IERR.NE.0) RETURN
0168         DO 135 LOOP1=1,UDNOVS
0169             WCRSLT = LMCOMP(VSLR50(1,LOOP),UOVSLR(1,LOOP1),4)
0170             IF (WCRSLT.EQ.0) GO TO 160
0171         CONTINUE
0172         GO TO 180

C
C      FIND A MANUAL ENTRY
C
0173 DO 155 LOOP1=1,UDNOVS
0174     IF (UOVSWD(LOOP1).GE.0) GO TO 160
0175     CONTINUE
0176     GO TO 180

C
C      FOUND IT
C
0177 UNUM(LOOP) = LOOP1
0178 CONTINUE
0179 RETURN
0180 END

!CHECK VESSEL ATTRIBUTES
!INTERPRET VESSEL STATUS WORD
!IF IF USM IS POSITIVE (MANUAL ENTRY) AND
!NOT YET PROCESSED (CALCULATED) AND
!IS THE RIGHT TYPE (SRC,DSI,INTRH) AND
!HAS THE RIGHT IFR METHD
!THEN THIS IS THE NEXT VSL TO BE PROCESSED
!COULD NOT FIND ONE

!FOUND THE CENTRAL VESSEL
!ASSIGN CENTRAL VESSEL NUMBER
!NOW FIND THE RELATED VESSELS

!STEP THRU EACH OF THE OTHER VSLs
!ASSUME VESSEL NOT INVOLVED
!IS THE NAME NULL ?
!YES! SKIP IT

!TEST FOR ZERO ENTRY
WCRSLT = LMCOMP(UOVSL(1,LOOP),MDZERO(LOOP1),1)
!IT IS ZERO. TRY MANUAL VSL

!INCODE VSL NAME
!ERROR LOG INVALID ENTRY
!CHECK EACH VSL IN UOFTK COMMON
!COULD NOT FIND ONE! TRY ANOTHER VSL

!NO ACTIVE ENTRY! TRY ANOTHER VSL

!THIS IS A MANUAL ENTRY
!COULD NOT FIND ONE! TRY ANOTHER VSL

!ASSIGN VESSEL INDEX NUMBER

!NORMAL EXIT

```

APPENDIX B: UNIT OPERATION DEFINITION FILES

All unit operation definition files referred to in this report has been provided in this appendix. They include the explanatory sample unit operation definition file, the simulation solvent extraction definition file, and the simulation ion exchange definition files.

C THIS IS A EXPLANATORY UNIT OPERATIONS DEFINITION FILE.
 C IT IS TO BE USED AS INSTRUCTIONAL HELP IN CREATING
 C A UNIT OPERATIONS DEFINITION DATA FILE.
 C
 C THE ENTRIES BELOW ARE BRIEF DESCRIPTIONS OF DATA
 C TO BE INSERTED IN THE FILE.
 C
 C DESCRIPTIVE DATA LINES (LINES WITHOUT 'C' AT LEFT MARGIN)
 C BEGINNING AT 1ST TAB REPRESENT
 C THE BEGINNING OF A NEW LINE OF DATA.
 C DESCRIPTIVE DATA LINES BEGINNING AT 2ND OR 3RD TAB
 C ARE CONTINUATION OF PRECEEDING LINE.
 C
 C ALL DATA ENTRIES SHOULD BE FROM THE ASCII CHARACTER SET.
 C DATA FORMAT LIMITS ARE SPECIFIED WITHIN ANGLE BRACKETS '< >'.
 C
 C WHERE OPTIONAL INDICATORS, '(OPT)', OCCUR,
 C 'N/A' MUST BE INSERTED IF NO ENTRY IS APPLICABLE.
 C
 C THE FIRST LINE OF DATA BELOW, 'UNIT OPERATION INFO',
 C APPEARS ONLY ONCE PER DATA FILE.
 C ALL SUBSEQUENT LINES (10 LINES) OF DATA MAY APPEAR, AS A UNIT,
 C SEVERAL TIMES.
 C
 C IF ANY VESSEL NAMES ARE BLANK (' '), ZERO ('0'), OR THE LETTER O,
 C A MANUALLY ENTERED CENTRAL VESSEL NAME
 C WILL BE EXPECTED AT TRANSFER DEFINITION TIME.
 C
 C UNIT OPERATION INFO <2A12>:
 C NAME, ESTIMATOR SUBROUTINE NAME (OPT)
 C CENTRAL VESSEL INFO <3A12,2I2>:
 C NAME, LABEL (OPT)
 C (IF NAME IS ' ', '0', OR 'O',
 C LABEL IS DESCRIPTION OF MANNUALLY ENTERED VESSEL;
 C IF NOT, LABEL IS DESCRIPTION FOR FLOW RATE.),
 C MODEL (OPT),
 C POSITION TYPE (SOURCE=1,DISTINATION=2,INTERMEDIATE=3),
 C TRANSFER METHOD (PUMP=1,JET=2,PRESSURE=3,VACUUM=4,
 C AIR-LIFT=5,GRAVITY=6,MANUAL=7)
 C OTHER VESSEL NAMES <4A12>:
 C SOURCE VESSEL (OPT IF NO VESSEL MODEL IS APPLICABLE),
 C 1ST CONTRIBUTING VESSEL (OPT),
 C 2ND CONTRIBUTING VESSEL (OPT),
 C QTY INFLUENCING VESSEL (OPT)
 C FLOW LABELS (OPT) (AT LEAST ONE DILUTING VESSEL FLOW LABEL SHOULD
 C BE PRESENT TO CHARACTERIZE CENTRAL VESSELS
 C WITH SIMULTANEOUS IN/OUT FLOW) <6A12>:
 C SOURCE, 1ST CONTRIBUTING, 2ND CONTRIBUTING,
 C 1ST, 2ND, & 3RD DILUTING
 C CALCULATION SUBROUTINE NAMES (OPT) <6A10>:
 C ACID, TOTALS, URANIUM, THORIUM, PLUTONIUM, QUANTITY
 C COEFFICIENTS <6 RECORDS OF 4F16.0>:
 C ACID 1, 2, 3, 4
 C TOTALS 1, 2, 3, 4
 C URANIUM 1, 2, 3, 4
 C THORIUM 1, 2, 3, 4
 C PLUTONIUM 1, 2, 3, 4
 C QUANTITY 1, 2, 3, 4

SXSIM,N/A
 V-0,FEED,MDLCMX,1,1
 N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 V-1,SCRUB,MDLCMX,1,1
 N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 V-2,STRIP,MDLCMX,1,1
 N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 V-4,FEED + SCRUB,MDLFMX,3,1
 V-0,V-1,N/A,V-5
 FEED,SCRUB,N/A,FEED,SCRUB,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 V-5,N/A,MDLFSP,3,1
 V-21,V-4,N/A,V-21
 EXTRACTANT,FEED + SCRUB,N/A,EXTRACTANT,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0.0,0.002375,0,0
 0,0,0,0
 1.0,0.9935,0,0
 1.0,0.0000301,0,0
 1.0,1.0,0,0
 0,0,0,0.62
 V-6,N/A,MDLFMX,3,1
 V-5,N/A,N/A,V-21
 EXTRACTANT,N/A,N/A,EXTRACTANT,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0,0,0,0
 0,0,0,0

0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0.38
 V-7,N/A,MDLFSP,3,1
 V-6,V-2,N/A,V-6
 EXTRACTANT,STRIP,N/A,STRIP,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0.81,1.0,0,0
 0,0,0,0
 0.9999,1.0,0,0
 0.9999,1.0,0,0
 0,0,0,0
 0,0,0,0
 V-21,EXTRACTANT,MDLFSP,3,1
 V-6,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0.534,0,0,0
 0,0,0,0
 0.000095,0,0,0
 0.000095,0,0,0
 1.0,0,0,0
 0,0,0,0
 V-22,N/A,MDLCMX,3,1
 V-7,N/A,N/A,N/A
 N/A,N/A,N/A,STRIP,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 V-23,N/A,MDLCMX,3,1
 V-7,N/A,N/A,N/A
 N/A,N/A,N/A,STRIP,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 V-31,N/A,MDLCMX,3,1
 V-23,N/A,N/A,N/A
 N/A,N/A,N/A,STRIP,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0,0,0,0
 0,0,0,0

0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 U-32,N/A,MILCMX,2,1
 U-31,N/A,N/A,N/A
 N/A,N/A,N/A,STRIP,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 U-33,N/A,MILCSP,2,1
 U-31,N/A,N/A,N/A
 N/A,N/A,N/A,STRIP,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0,0,0,0,0
 0,0,0,0
 0,0,0,0,0
 0,0,0,0,0
 0,0,0,0,0
 0,0,0,0
 U-80,N/A,MILCSP,3,1
 U-4,N/A,N/A,N/A
 N/A,N/A,N/A,FEED + SCRUB,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 1.55,0,0,0
 0,0,0,0
 0.004,0,0,0
 0.99997,0,0,0
 0,0,0,0
 0,0,0,0

IXPURIFSM,N/A
 V-4,FEED,N/A,1,1
 N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 V-33,N/A,MILCCV,3,1
 V-4,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0,0,0,0
 0,0,0,0
 0.00001,0,0,274.0
 1.0,0,0,0
 1.0,0,0,0
 0,0,0,0
 V-22,N/A,MILCSP,2,1
 V-4,N/A,N/A,V-33
 N/A,N/A,N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 1.0,0,0,0
 0,0,0,0
 1.0,0,0,-1.0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 V-32,N/A,MILCSP,2,1
 V-4,N/A,N/A,V-33
 N/A,N/A,N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 1.0,0,0,0
 0,0,0,0
 1.0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0

IXACIDSIM,N/A
V-1,N/A,N/A,1,1
N/A,N/A,N/A,N/A
N/A,N/A,N/A,N/A,N/A,N/A
N/A,N/A,N/A,N/A,N/A,N/A
0,0,0,0
0,0,0,0
0,0,0,0
0,0,0,0
0,0,0,0
0,0,0,0
V-22,N/A,MILCSF,2,1
V-0,V-1,V-33,V-33
N/A,N/A,N/A,N/A,N/A,N/A
N/A,N/A,N/A,N/A,N/A,N/A
0.923,1.0,0,0
0,0,0,0
1.0,1.0,0.988,0
1.0,1.0,0.1,0
1.0,1.0,0.18,0
0,0,0,0
V-33,N/A,MILCCV,3,1
V-33,V-0,N/A,N/A
N/A,N/A,N/A,N/A,N/A,N/A
N/A,N/A,N/A,N/A,N/A,N/A
1.0,2.3777,0,0
0,0,0,0
0.0133,0,0,0
0.56,0,0,0
0.0111,0,0,0
0,0,0,0

IXACETSIM,N/A
 V-1,N/A,N/A,1,1
 N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 0,0,0,0
 V-23,N/A,MILCSF,2,1
 V-0,N/A,V-33,V-33
 N/A,N/A,N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 1.0,0,0,0
 0,0,0,0
 1.0,0,1.0,0
 1.0,0,0.999,0
 1.0,0,1.0,0
 0,0,0,0
 V-33,N/A,MILCCV,3,1
 V-33,V-0,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 N/A,N/A,N/A,N/A,N/A,N/A
 1.0,1.8,0,0
 0,0,0,0
 0,0,0,0
 0.0022,0,0,0
 0,0,0,0
 0,0,0,0

APPENDIX C. DETAILED DESCRIPTION OF SIMULATION SOLVENT EXTRACTION DEFINITION FILE SEGMENT

To familiarize users with the structure of the unit operation definition (UOD) file, a detailed description of a data file segment follows. An explanatory sample UOD file (Figure C-1) and a segment of the simulation solvent extraction definition file are provided (Figure C-2). Certain file conventions noted as comments in the first half of the explanatory sample (Figure C-1) are emphasized:

1. All data entries should be from the ASCII character set (data format limits are specified in angle brackets "<>").
2. Entry of specific items in certain fields is optional [indicated by "(OPT)"], however, these fields must have an "N/A" inserted when no specific item is applicable.
3. Provision has been made to accommodate central vessel names which are entered manually by terminal operators upon formation of the transfer packet for the unit operation. (Manual entry is in contrast to the automatic central vessel reference normally provided in the UOD file.) This provision is useful when a selection of several vessels not rigidly connected is encountered in material processing (e.g., fuel pellet trays, furnace boats, removable centrifuge bowl liners, etc.). Manually entered vessel names are indicated by a blank (" "), a zero ("0"), or a letter O ("O"). For manually entered vessel names, the "LABEL" entry is devoted to a short description of the vessel to be manually entered.

```

C      THIS IS A EXPLANATORY UNIT OPERATIONS DEFINITION FILE.
C      IT IS TO BE USED AS INSTRUCTIONAL HELP IN CREATING
C      A UNIT OPERATIONS DEFINITION DATA FILE.
C
C      THE ENTRIES BELOW ARE BRIEF DESCRIPTIONS OF DATA
C      TO BE INSERTED IN THE FILE.
C
C      DESCRIPTIVE DATA LINES (LINES WITHOUT 'C' AT LEFT MARGIN)
C      BEGINNING AT 1ST TAB REPRESENT
C      THE BEGINNING OF A NEW LINE OF DATA.
C      DESCRIPTIVE DATA LINES BEGINNING AT 2ND OR 3RD TAB
C      ARE CONTINUATION OF PRECEEDING LINE.
C
C      ALL DATA ENTRIES SHOULD BE FROM THE ASCII CHARACTER SET.
C      DATA FORMAT LIMITS ARE SPECIFIED WITHIN ANGLE BRACKETS '< >'.
C
C      WHERE OPTIONAL INDICATORS, '(OPT)', OCCUR,
C      'N/A' MUST BE INSERTED IF NO ENTRY IS APPLICABLE.
C
C      THE FIRST LINE OF DATA BELOW, 'UNIT OPERATION INFO',
C      APPEARS ONLY ONCE PER DATA FILE.
C      ALL SUBSEQUENT LINES (10 LINES) OF DATA MAY APPEAR, AS A UNIT,
C      SEVERAL TIMES.
C
C      IF ANY VESSEL NAMES ARE BLANK (' '), ZERO ('0'), OR THE LETTER O ('O'),
C      A MANUALLY ENTERED CENTRAL VESSEL NAME
C      WILL BE EXPECTED AT TRANSFER DEFINITION TIME.
C
C      UNIT OPERATION INFO <2A12>:
C      NAME, ESTIMATOR SUBROUTINE NAME (OPT)
C      CENTRAL VESSEL INFO <3A12,2I2>:
C      NAME, LABEL (OPT)
C          (IF NAME IS ' ', '0', OR 'O',
C           LABEL IS DESCRIPTION OF MANNUALLY ENTERED VESSEL;
C           IF NOT, LABEL IS DESCRIPTION FOR FLOW RATE.),
C          MODEL (OPT),
C          POSITION TYPE (SOURCE=1,DISTINATION=2,INTERMEDIATE=3),
C          TRANSFER METHOD (PUMP=1,JET=2,PRESSURE=3,VACUUM=4,
C          AIR-LIFT=5,GRAVITY=6,MANUAL=7)
C      OTHER VESSEL NAMES <4A12>:
C      SOURCE VESSEL (OPT IF NO VESSEL MODEL IS APPLICABLE),
C          1ST CONTRIBUTING VESSEL (OPT),
C          2ND CONTRIBUTING VESSEL (OPT),
C          QTY INFLUENCING VESSEL (OPT)
C      FLOW LABELS (OPT) (AT LEAST ONE DILUTING VESSEL FLOW LABEL SHOULD
C      BE PRESENT TO CHARACTERIZE CENTRAL VESSELS
C      WITH SIMULTANEOUS IN/OUT FLOW) <6A12>:
C      SOURCE, 1ST CONTRIBUTING, 2ND CONTRIBUTING,
C          1ST, 2ND, & 3RD DILUTING
C      CALCULATION SUBROUTINE NAMES (OPT) <6A10>:
C      ACID, TOTALS, URANIUM, THORIUM, PLUTONIUM, QUANTITY
C      COEFFICIENTS <6 RECORDS OF 4F16.0>:
C      ACID 1, 2, 3, 4
C      TOTALS 1, 2, 3, 4
C      URANIUM 1, 2, 3, 4
C      THORIUM 1, 2, 3, 4
C      PLUTONIUM 1, 2, 3, 4
C      QUANTITY 1, 2, 3, 4

```

Figure C-1. Explanatory sample unit operation definition file.

```

SXSIM,N/A
V-0,FEED,MDLCMX,1,1
N/A,N/A,N/A,N/A
N/A,N/A,N/A,N/A,N/A,N/A
N/A,N/A,N/A,N/A,N/A,N/A
0,0,0,0
0,0,0,0

.

.

.

0,0,0,0
0,0,0,0
V-4,FEED + SCRUB,MDLFMX,3,1
V-0,V-1,N/A,V-5
FEED,SCRUB,N/A,FEED,SCRUB,N/A
N/A,N/A,N/A,N/A,N/A,N/A
0,0,0,0
0,0,0,0
0,0,0,0
0,0,0,0
0,0,0,0
0,0,0,0
0,0,0,0
V-5,N/A,MDLFSP,3,1
V-21,V-4,N/A,V-21
EXTRACTANT,FEED + SCRUB,N/A,EXTRACTANT,N/A,N/A
N/A,N/A,N/A,N/A,N/A,N/A
0.0,0.002375,0,0
0,0,0,0
1.0,0.9935,0,0
1.0,0.0000301,0,0
1.0,1.0,0,0
0,0,0,0.62
V-6,N/A,MDLFMX,3,1
V-5,N/A,N/A,V-21
EXTRACTANT,N/A,N/A,EXTRACTANT,N/A,N/A

```

Figure C-2. Segment of simulation solvent extraction definition file.

The first line of an UOD file consists of two entries, each of which may be up to 12 characters long. In the sample file (Figure C-2), the first entry is the name of the unit operation, SXSIM, and is provided for file identity confirmation. The second entry is an optional name for a specialized unit operation estimator. No specialized estimator is applicable in the SXSIM UOD file; however, if a specialized estimator subroutine were available, its name should appear in the ESTMAT data statement within the UOPCMP subroutine (see Appendix A) along with the program routing (at statement label 25) and the call to the applicable subroutine (in the executable code portion of UOPCMP subroutine). The first line of the UOD file contains information about the file as a whole and is thus considered the UOD file header; as the file header, it occurs only at the beginning of the file.

The remaining lines of data describe the individual vessels involved in the unit operation. Ten lines of data are required (and must be supplied) to describe each vessel. The vessel described within a ten-line segment is considered the central vessel of that description; other peripheral vessels are optionally referenced in the description. In the sample file, a ten-line segment has been selected (see the boxed-in area in Figure C-2). This segment is the description of vessel V-5 (see Figure 3 for vessel labeling) in which the most significant (and one of the more complex) separation occurs--partitioning uranium from thorium [extractant, originating from the organic reservoir (V-21), contacts the uranium-thorium mixture in the aqueous phase of the column (V-4) and extracts the uranium to the organic phase of the column (V-5)].

The first line of this segment contains information pertaining exclusively to the characterization of the central vessel (V-5) in this ten-line description; this information is independent of the remaining nine lines of information, which consider interactions and contributions of vessels peripheral to the central vessel. The first item of this line is the central vessel name (V-5) and is followed by an optional dual-purpose label controlled by the central vessel name (see file convention 3 listed at the beginning of this appendix). Since all vessels involved in solvent extraction are rigidly connected (i.e., through process piping), all central vessel names may (and have been) predefined for automatic reference; therefore, this label is optionally used to describe the flow rate of solution *out of* the central vessel. Additionally, the flow label is used during transfer packet definition to prompt the terminal operators to enter the planned flow rate applicable to this vessel; therefore, to minimize the burden of data entry on terminal operators, a given flow label should be provided only once among all of the first lines of central vessel information in the UOD file. Since V-5 is the organic phase of the extraction column (and not the source of flow for that solution), the flow label EXTRACTANT is reserved for the source vessel of that solution, V-21.

The third item on the first line of this segment is an optional name of the vessel model which estimates material transfers *into* the central vessel. Material transfer into V-5 has been estimated by model MDLFSP, the flow-mode separation model. This model name (and any other model name to be used) must appear in the "MODEL" data statement within the UOPCMP subroutine (see Appendix A) along with the program routing

(at statement label 359), any data or vessel preparation (i.e., transfer quantity determination or processing the material already resident in the central vessel for collecting-mode models), and the call to the appropriate subroutine. Existing models and their applications are listed in Table C-1.

The remaining two items of central vessel information are integers. The first number describes the central vessel's position in the unit operation transfer as either (1) a source vessel, (2) a destination vessel, or (3) an intermediate vessel. For the purpose of inventory estimation, the most significant difference between these three positions is that destination and intermediate vessels are estimated for composition changes while source vessels are not. It is assumed that material characteristics within source vessels do not change; only the bulk quantity of material in such vessels change in a depleting manner. Hence, source vessels need not reference a model. Obviously, V-5 is indicated as an intermediate vessel (position category 3) in the sample segment in Figure C-2.

The second number describes the method of transferring material *out of* the central vessel. These methods include (1) pump, (2) jet, (3) pressure, (4) vacuum, (5) airlift, (6) gravity, and (7) manual. For the purpose of inventory estimation, there is a significant difference in the way data is handled for jet transfers relative to all other modes of transfer. In jet transfers utilizing the perfect mixing model (MDLCMX), the compositions of the central vessel contributing to another vessel are diluted by a jet dilution factor (see subroutine MDLJDL in Appendix A); for all other modes of transfer, the central vessel

TABLE C-1

IMPLEMENTED MODELS AND THEIR APPLICATION

Model (Subroutine Name)	Model Name		Description
	Collection Mode ^a	Flow Mode ^b	
Blend (MDLPMX)	MDLCMX	MDLFMX	Perfect mixing
Separation (MDLSEP)	MDLCSP	MDLFSP	Distributive separation
Conversion (MDLCNV)	MDLCCV	MDLFCV	Composition adjustment

^aCollection-mode models are used for estimating compositions in surge and storage vessels.

^bFlow-mode models are used for estimating compositions in flow-through vessels where material resides for a very short period.

compositions contribute to another vessel without a similar, across-the-board adjustment. Other transfer modes have been established to assist in future refinements of NUMATH. From the sample segment, it can be seen that the transfer of material out of V-5 is performed by pump (method number 1).

The second line of the vessel description contains names of vessels peripheral to the central vessel. The first three vessels (as applicable) are expected to contribute material to the central vessel in a manner consistent with the applicable model. Figure C-2 indicates that vessels V-21 (the organic reservoir) and V-4 (the aqueous phase of the extraction column) contribute material to V-5 (the organic phase of the extraction column). The fourth vessel influences the bulk quantity of material in the central vessel. For example, V-5 contains a volume of extractant proportional to the volume depletion in V-21. All vessel models (MDL___) require the first vessel on this line to be specified.

The third line of the vessel description contains labels describing flows affecting the composition of material transferred into the central vessel. They are used mainly to provide relative bulk quantity contributions applicable during flow-mode models. The first three labels describe the contribution of the first three vessels listed on the line above relative to the sum of the flow rates described in the second three labels. In Figure C-2, for example, V-5 gets material from V-4 corrected for the relative flow rate (FR) between the organic and aqueous phases by a "dilution" factor of $FR_{FEED} + SCRUB / FR_{EXTRACTANT}$. Similarly, V-5 gets material from V-21 corrected by a dilution factor of $FR_{EXTRACTANT} / FR_{EXTRACTANT} = 1.0$. As noted above, these labels are

used mainly during flow-mode estimation; however, it is advisable to provide at least one appropriate diluting flow label (i.e., in the second set of three labels) to characterize collecting central vessels with simultaneous inflow and outflow.

The fourth line of the vessel description is provided to list model systems not yet developed. Hence, this line always appears with "N/A" filling its spaces.

The remaining six lines of the vessel description contain factors to be used in the estimating models. The first five lines of factors and plutonium. Perfect mixing models (MDLFMX and MDLCMX) do not use any of these factors. However, the separation models (MDLFSP and MDLCSP) use the first three factors of each line--one for each of the three vessels contributing material to the central vessel. The conversion model uses all four factors. The general manner in which the separation and conversion models use these factors is best left to the description and code in the MDLSEP and MDLCNV subroutines (Appendix A). From the sample segment in Figure C-2, it can be seen that all (100.0%) of the uranium, thorium, and plutonium from V-21 transfer to V-5 while only 0.2375% of the acid, 99.35% of the uranium, 0.00301% of the thorium, and 100.0% of the plutonium transfer from V-4 to V-5. Factors in the final line of the ten-line vessel description are used to estimate bulk quantities of certain vessels tagged (in the transfer packet) as requiring quantity estimation. These factors are employed in the UOPCMP (see Appendix A) in a manner consistent with the code between statement labels 381 and 382.

To promote systematic access to and use of unit operation definition file data, special subroutines have been written and incorporated into NUMATH. These subroutines (in Appendix A) open (UOPOPEN), read data from (UOPRED), and close (entry UOPCLS in UOPOPEN) the file of interest. ASCII-formatted data is interpreted to internal computer data format (in Appendix A subroutines UNPK and UOPRED) after it has been read from the file. When a UOD file is opened, the file header is automatically read, interpreted, and held in the UOPHDR common (see Figure C-3). Central vessel information is read, interpreted, and held in the UOPVSL common (see Figure C-3). In the sequence in which the information appears in the UOD file, each call to the file "read" subroutine accesses a ten-line segment of central vessel information. Figure C-3 provides the data type definitions used in the program.

```

C*****
C
C          IM1:[300,300] UOPDFN.COM"
C
C  COMMON FOR ACCESSING INFORMATION IN THE UNIT OPERATION DEFINITION FILES.
C
C          PARAMETER UOPHSZ = 10          !HEADER COMMON SIZE IN WORDS
C          PARAMETER UOPVSZ = 134        !VESSEL COMMON SIZE IN WORDS
C          PARAMETER UOVSMX = 4          !MAXIMUM # OF VSLS (OTHER THAN CENTRAL VSL)
C          PARAMETER UODFMX = 3          !MAXIMUM # OF DILUTION FLOW LABELS PER VESSEL
C                                         (THIS IS A SUBSET OF "UOFLMX" BELOW)
C          PARAMETER UOFLMX = 6          !MAXIMUM # OF FLOW LABELS PER VESSEL
C                                         (OTHER THAN CENTRAL VSL FLOW LABEL)
C
C          UOFLMX MAY BE RECALCULATED BY:
C          UOFLMX = (UOVSMX-1) + UODFMX
C
C  HEADER VARIABLES DEFINITION
C
C          INTEGER UOPHOV(UOPHSZ)        !HEADER COMMON OVERLAY
C          INTEGER UOPNAM(5)             !UNIT OPN NAME
C          INTEGER UOUEST(5)             !UNIT OPN ESTIMATION SUBROUTINE NAME
C
C  VESSEL ENTRY VARIABLES DEFINITION
C
C          INTEGER UOPVOV(UOPVSZ)        !UOP VESSEL COMMON OVERLAY
C          INTEGER UOCVSL(6)             !CENTRAL VESSEL NAME
C          INTEGER UOCFLB(6)             !CENTRAL VESSEL FLOW LABEL
C          INTEGER UOVMDL(6)             !VESSEL MODEL SUBROUTINE NAME
C          INTEGER UOVTFP                !CENTRAL VESSEL TYPE (SOURCE, DEST., ETC.)
C          INTEGER UOTMTD                !TRANSFER METHOD (PUMP, JET, ETC.)
C
C  OTHER VESSEL NAMES INVOLVED WITH THIS CENTRAL VESSEL
C
C          INTEGER UOVSL(6,UOVSMX)       !SOURCE & CONTRIB. VSLS OVERLAY
C          INTEGER UOSVSL(6)             !SOURCE VESSEL NAME
C          INTEGER UO1VSL(6)             !FIRST CONTRIB VESSEL NAME
C          INTEGER UO2VSL(6)             !SECOND CONTRIB VESSEL NAME
C          INTEGER UOQVSL(6)             !QUANTITY REFERENCE VESSEL NAME
C
C  FLOW LABELS
C
C          INTEGER UOFLBL(6,UOFLMX)      !FLOW LABELS OVERLAY
C          INTEGER UOSVFL(6)             !SOURCE VESSEL FLOW LABEL
C          INTEGER UO1VFL(6)             !FIRST CONTRIB VESSEL FLOW LABEL
C          INTEGER UO2VFL(6)             !SECOND CONTRIB VESSEL VLOW LABEL
C          INTEGER UODFL(6,UODFMX)       !DILUTING FLOW LABELS OVERLAY
C          INTEGER UODFL1(6)             !FIRST DILUTING FLOW LABEL
C          INTEGER UODFL2(6)             !SECOND DILUTING FLOW LABEL
C          INTEGER UODFL3(6)             !THIRD DILUTING FLOW LABEL
C
C  ELEMENT CALCULATION SUBROUTINE NAMES
C
C          INTEGER UOCLC(5,6)            !ELEMENT CALCULATION SUBR NAMES OVERLAY
C          INTEGER UOHCLC(5)             !ACID CALCULATION SUBR NAME
C          INTEGER UOTOTC(5)             !TOTALS CALCULATION SUBR NAME
C          INTEGER UOUCLC(5)             !URANIUM CALCULATION SUBR NAME
C          INTEGER UOTCLC(5)             !THORIUM CALCULATION SUBR NAME
C          INTEGER UOPCLC(5)             !PLUTONIUM CALCULATION SUBR NAME
C          INTEGER UOQCLC(5)             !QUANTITY CALCULATION SUBR NAME

```

Figure C-3. Data type and common definitions for accessing information in a unit operation file.

```

C
C  MODELLING COEFFICIENTS
C
C      REAL UOCOF(UOVSMX,6)                      !COEFFICIENTS OVERLAY
C
C  ACID COEFFICIENTS
C      REAL UOHCF(UOVSMX)                        !ACID COEFFS OVERLAY
C      REAL UOHCF1, UOHCF2, UOHCF3, UOHCF4
C
C  TOTALS COEFFICIENTS
C      REAL UOTOT(UOVSMX)                        !TOTALS COEFFS OVERLAY
C      REAL UOTOT1, UOTOT2, UOTOT3, UOTOT4
C
C  URANIUM COEFFICIENTS
C      REAL UOUCF(UOVSMX)                        !URANIUM COEFFS OVERLAY
C      REAL UOUCF1, UOUCF2, UOUCF3, UOUCF4
C
C  THORIUM COEFFICIENTS
C      REAL UOTCF(UOVSMX)                        !THORIUM COEFFS OVERLAY
C      REAL UOTCF1, UOTCF2, UOTCF3, UOTCF4
C
C  PLUTONIUM COEFFICIENTS
C      REAL UOPCF(UOVSMX)                        !PLUTONIUM COEFFS OVERLAY
C      REAL UOPCF1, UOPCF2, UOPCF3, UOPCF4
C
C  QUANTITY COEFFICIENTS
C      REAL UORCF(UOVSMX)                        !QUANTITY COEFFS OVERLAY
C      REAL UORCF1, UORCF2, UORCF3, UORCF4
C
C
C      COMMON /UOPHDR/ UOPNAM, UOUEST              !HEADER COMMON
C
C
C      COMMON /UOPVSL/
C      1      UOCVSL,UOCFLB,UOVMDL,UOVTFP,UOTMTD,      !VESSEL COMMON
C      1      UOSVSL,UO1VSL,UO2VSL,UOQVSL,            !OTHER VESSEL NAMES
C      2      UOSVFL,UO1VFL,UO2VFL,UOIFL1,UOIFL2,UOIFL3, !FLOW LABELS
C      3      UOHCLC,UOTOTC,UOUCLC,UOTCLC,UOPCLC,UOQCLC, !CALCULATN SUBR NAMES
C      4      UOHCF1,UOHCF2,UOHCF3,UOHCF4,            !ACID COEFFS
C      5      UOTOT1,UOTOT2,UOTOT3,UOTOT4,            !TOTALS COEFFS
C      6      UOUCF1,UOUCF2,UOUCF3,UOUCF4,            !URANIUM COEFFS
C      7      UOTCF1,UOTCF2,UOTCF3,UOTCF4,            !THORIUM COEFFS
C      8      UOPCF1,UOPCF2,UOPCF3,UOPCF4,            !PLUTONIUM COEFFS
C      9      UORCF1,UORCF2,UORCF3,UORCF4            !QUANTITY COEFFS
C
C
C      EQUIVALENCE (UOPHOV(1),UOPNAM(1))              !HEADER OVERLAY
C      EQUIVALENCE (UOPVOV(1),UOCVSL(1))              !VESSEL OVERLAY
C      EQUIVALENCE (UOVSL(1),UOSVSL(1))              !OTHER VESSELS OVERLAY
C      EQUIVALENCE (UOFLBL(1),UOSVFL(1))              !FLOW LABELS OVERLAY
C      EQUIVALENCE (UOIFL(1),UOIFL1(1))              !DILUTION FLOW LABELS OVERLAY
C      EQUIVALENCE (UOCLC(1),UOHCLC(1))              !ELEMENT CALCULATN SUBR OVERLAY
C      EQUIVALENCE (UOCOF(1),UOHCF1)                  !COEFFICIENTS OVERLAY
C      EQUIVALENCE (UOHCF(1),UOHCF1)                  !ACID COEFFS OVERLAY
C      EQUIVALENCE (UOTOT(1),UOTOT1)                  !TOTALS COEFFS OVERLAY
C      EQUIVALENCE (UOUCF(1),UOUCF1)                  !URANIUM COEFFS OVERLAY
C      EQUIVALENCE (UOTCF(1),UOTCF1)                  !THORIUM COEFFS OVERLAY
C      EQUIVALENCE (UOPCF(1),UOPCF1)                  !PLUTONIUM COEFFS OVERLAY
C      EQUIVALENCE (UORCF(1),UORCF1)                  !QUANTITY COEFFS OVERLAY
C
C
C *****

```

Figure C-3. (Continued)

VITA

Alan Marshall Krichinsky was born in Baltimore, Maryland, on October 12, 1950. He attended public schools in Baltimore City and Baltimore County and graduated from Milford Mill High School, Baltimore County, Maryland, in June 1968.

Upon graduation from high school, he enlisted in the U.S. Naval Reserve intending to attend the U.S. Naval Academy through a Naval Reserve appointment. In November 1968, it was discovered that he did not physically qualify for the Academy and was subsequently permitted to become an inactive reservist to pursue his college education outside the military establishment.

In February 1969, he entered the University of Maryland, College Park, Maryland, and in August 1974 (including a one-year interlude to complete his active Naval Reserve service obligation) he earned his Bachelor of Science degree in Chemical Engineering.

In August 1974, he began work at the Oak Ridge National Laboratory, Oak Ridge, Tennessee. He entered the University of Tennessee Graduate School and began study toward the Master of Science degree in Chemical Engineering with a minor in Mathematics. This degree was awarded in June 1981.

The author is a member of the American Institute of Chemical Engineers and the Institute of Nuclear Materials Management. He is also one of the authors of the ANSI N15.19 standard on Volume Calibration Techniques for Nuclear Material Control.

He is married to the former Anna Mary Fine of Baltimore, Maryland, and has a three-year old son, Seth.