#138 ^{eps}
4/17/80

**CRYOGENIC DISTILLATION:
A FUEL ENRICHMENT SYSTEM FOR
NEAR-TERM TOKAMAK-TYPE
D-T FUSION REACTORS**

by

Balabhadra Misra and J. F. Davis

MASTER

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

**Prepared for the U. S. DEPARTMENT OF ENERGY
under Contract W-31-109-Eng-38**

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

The facilities of Argonne National Laboratory are owned by the United States Government. Under the terms of a contract (W-31-109-Eng-38) among the U. S. Department of Energy, Argonne Universities Association and The University of Chicago, the University employs the staff and operates the Laboratory in accordance with policies and programs formulated, approved and reviewed by the Association.

MEMBERS OF ARGONNE UNIVERSITIES ASSOCIATION

The University of Arizona	The University of Kansas	The Ohio State University
Carnegie-Mellon University	Kansas State University	Ohio University
Case Western Reserve University	Loyola University of Chicago	The Pennsylvania State University
The University of Chicago	Marquette University	Purdue University
University of Cincinnati	The University of Michigan	Saint Louis University
Illinois Institute of Technology	Michigan State University	Southern Illinois University
University of Illinois	University of Minnesota	The University of Texas at Austin
Indiana University	University of Missouri	Washington University
The University of Iowa	Northwestern University	Wayne State University
Iowa State University	University of Notre Dame	The University of Wisconsin-Madison

NOTICE

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government or any agency thereof, nor any of their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, mark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Printed in the United States of America
Available from
National Technical Information Service
U. S. Department of Commerce
5285 Port Royal Road
Springfield, VA 22161

NTIS price codes
Printed copy: A03
Microfiche copy: A01

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

ANL-78-96

ARGONNE NATIONAL LABORATORY
9700 South Cass Avenue
Argonne, Illinois 60439

CRYOGENIC DISTILLATION: A FUEL ENRICHMENT SYSTEM FOR
NEAR-TERM TOKAMAK-TYPE D-T FUSION REACTORS

by

Balabhadra Misra and J. F. Davis*

Chemical Engineering Division

February 1980

DISCLAIMER

This book was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof nor any of their employees makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

*Masters Thesis Student, Northwestern University.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

TABLE OF CONTENTS

	<u>Page</u>
ABSTRACT	1
I. INTRODUCTION	1
II. SPENT FUEL REPROCESSING	3
A. Preliminary Cleanup Steps	3
1. Debris Separation Step	3
2. Separation of Nonmetallic Elements from the Exhaust Stream Gases	3
B. Isotopic Separation and Enrichment by Cryogenic Distillation	5
III. DEVELOPMENT OF THE COMPUTER CODE FOR CRYOGENIC DISTILLATION BY A FOUR-COLUMN CASCADE	8
A. Format for Input Data	8
B. Program Limitations	12
C. Input Data for a Sample Problem	12
D. Output (Analytical Results)	14
IV. DISCUSSION OF RESULTS	14
A. Effect of Protium Fraction in Feed	14
B. Effect of Operating Pressure	19
C. Effect of Number of Theoretical Stages	19
D. Effect of Amount of Neutral Beam Recycle Going to Chemical Equilibrator	21
V. CONCLUSIONS	22
ACKNOWLEDGMENTS	22
REFERENCES	22
APPENDIX	24

LIST OF FIGURES

<u>No.</u>	<u>Title</u>	<u>Page</u>
1.	Schematic of Tokamak-Type Reactor Feed and Waste Streams	2
2.	Layout of Tritium Processing Systems for TNS	3
3.	TNS Cryogenic Distillation Cascade	7
4.	TNS Cryogenic Distillation Cascade (Alternate Scheme)	7

LIST OF TABLES

<u>No.</u>	<u>Title</u>	<u>Page</u>
1.	Composition and Mass Flow Rate of Main Exhaust Stream at 373 K	4
2.	Composition of a Typical Spent Fuel Mixture after Preliminary Cleanup	4
3.	Isotopic Composition of Spent Fuel for Distillation	5
4.	Input Data for Four-Column Cascade	13
5.	Analytical Results for Column 1 of Four-Column Cascade	15
6.	Analytical Results for Column 2 of Four-Column Cascade	16
7.	Analytical Results for Column 3 of Four-Column Cascade	17
8.	Analytical Results for Column 4 of Four-Column Cascade	18
9.	Cascade Parameter Study--Effect of Protium Fraction in Feed	19
10.	Cascade Parameter Study--Effect of Operating Pressure	20
11.	Cascade Parameter Study--Effect of Number of Theoretical Plates	20
12.	Cascade Parameter Study--Effect of Varying Amount of Neutral Beam Recycle Going to Equilibrator	21

CRYOGENIC DISTILLATION: A FUEL ENRICHMENT SYSTEM FOR NEAR-TERM TOKAMAK-TYPE D-T FUSION REACTORS

by

Balabhadra Misra and J. F. Davis*

ABSTRACT

The successful operation and economic viability of deuterium-tritium- (D-T-) fueled tokamak-type commercial power fusion reactors will depend to a large extent on the development of reliable tritium-containment and fuel-recycle systems. Of the many operating steps in the fuel recycle scheme, separation or enrichment of the isotopic species of hydrogen by cryogenic distillation is one of the most important. A parametric investigation was carried out to study the effects of the various operating conditions and the composition of the spent fuel on the degree of separation. A computer program was developed for the design and analysis of a system of interconnected distillation columns for isotopic separation such that the requirements of near-term D-T-fueled reactors are met. The analytical results show that a distillation cascade consisting of four columns is capable of reprocessing spent fuel varying over a wide range of compositions to yield reinjection-grade fuel with essentially unlimited D/T ratio.

I. INTRODUCTION

A number of design concepts for D-T-fueled fusion reactors have been presented.¹⁻⁴ They vary in duty cycles from a few pulses per year to prove the technological feasibility of controlled nuclear fusion [e.g., the Ignition Test Reactor (ITR)⁵] to experimental power reactors with many thousands of pulses per year [e.g., the ANL Experimental Power Reactor (ANL/EPR)¹]. Figure 1 shows a generalized picture of a tokamak-type fueling system which has two fuel sources: the main enriched fuel (cold injection) feed and the neutral beam (NB) injector feed. The principal sources of recyclable waste are the main exhaust gases from the plasma chamber and the neutral beam injector recycle (unused fuel). Tritium-bearing species from the waste consolidation system may also be recyclable.

Because of the inherent characteristics of tokamak-type reactors, such as very pure fuel requirements, low burnup rates, contamination of the unreacted fuel, radioactivity, and high fuel cost, it is essential that the unburned fuel in both the main exhaust stream and the neutral beam injector recycle be purified and reused. To accomplish this, the contaminants produced in the plasma chamber (by sputtering, transmutation, permeation, chemical reaction, etc.) must be removed from the spent fuel mixture before the fuel can be reinjected. In addition to removal of high-molecular-weight contaminant atoms, the purification of the hydrogen isotopes (H_2 , HD, HT, D_2 ,

*Masters Thesis Student, Northwestern University.

Fig. 1. Schematic of Tokamak-Type Reactor Feed and Waste Streams

DT, and T_2) into reinjectable forms must also be achieved. Not only must the protium atoms be removed from the fuel "ash," but the tritium and deuterium atom fractions of the wastes must be properly adjusted for both cold fuel (enriched fuel) and neutral beam reinjection.

Several cleanup and recycle schemes have been developed^{6,7} for near-term fusion reactors. Although no detailed information has been published regarding specific steps in these schemes, the consensus among analysts is that any fuel reconditioning process will involve a large number of steps such as debris separation, vapor recompression, helium removal, and nonmetallic-element separation, as well as isotope separation and enrichment. Of the several isotope separation schemes that have been considered, separation, or more properly, enrichment, by cryogenic distillation appears to be most promising. An examination of (1) the composition of the spent gases and (2) the required purity and composition of the injected gases shows that a complex separation scheme involving several distillation columns, arranged in a cascade, is needed.

A proposed plan of study for the D-T fuel cycle for TNS^{5,8} (The Next Step in the logical development of tokamak-type fusion reactors) and the subsequent upgrading of TNS is presented. Figure 2 presents generalized fuel recycle and reprocessing steps for a TNS-type reactor. This report discusses the possibility of incorporating cryogenic distillation into the TNS recycle scheme.

Fig. 2. Layout of Tritium Processing Systems for TNS

II. SPENT FUEL REPROCESSING

A. Preliminary Cleanup Steps

1. Debris Separation Step

The intense radiation environment anticipated for the first wall of an experimental fusion device is likely to cause sizable quantities of fine solid particles to be dislodged and carried out by the exhaust gases. Depending on the nature of these dispersoids, they must be removed either before or after the vacuum pumps by special cyclone separators or electrostatic precipitators (step 2, Fig. 2).

2. Separation of Nonmetallic Elements from the Exhaust Stream Gases

Three proposed design options of TNS⁵ are: (1) TNS-ITR, a small machine designed as an ignition test reactor, (2) TNS-UGO, a larger machine than ITR, designed with the capability of being upgraded to a power-producing

test reactor, and (3) TNS-UG, an upgraded version of TNS-UGO which could operate at higher duty cycle. Table 1 describes the estimated composition of the main exhaust streams from these reactors.

Table 1. Composition and Mass Flow Rate of Main Exhaust Stream at 373 K

Atomic Species	At. %	Flow rate, g/d			Principal Species
		INS-ITR	INS-UGO	INS-UG	
D	71-89	27.1	34.4	145.7	D ₂ , DT
T		40.7	51.6	218.5	T ₂ , DT
He	10-20	5.9	8.1	61.1	He
H	1.9	0.3	0.4	1.8	HD, HT, H ₂ O
C	0.12-1.0	0.1	0.1	0.5	CH ₄ , C ₂ H ₂
O	0.3	1.4	1.9	8.4	H ₂ O, CO, O ₂
N	0.010	0.25	0.35	1.5	N ₂ , NH ₃
Ar	<0.1	<1.2	<1.8	<7.0	Ar
Si	0.02	0.2	0.2	0.9	Silanes

The anticipated nonmetallic impurities in the exhaust gas from the plasma chamber include H₂, N₂, O₂, NH₃, H₂O, Ar, CO, CO₂, low-molecular-weight hydrocarbons, silanes, and unburned fuel containing up to 20 at. % helium. The current concepts for impurity removal (step 9 of Fig. 2) are aimed at removing these impurities by catalysts and/or getters designed to (1) crack hydrocarbons and other hydrogenous materials, (2) absorb CO, O₂, water vapor, N₂, etc., in a fixed form suitable for disposal, and (3) remove helium by selective adsorption (by palladium diffusers or a falling film separator). Thus, one can envision that following the preliminary cleanup (step 2, Fig. 2); the spent fuel must go through several stages of recompression (from a base pressure of ≤ 1 Pa to >200 kPa) and impurity removal (steps 3-9, Fig. 2.); a liquid fuel mixture containing the six isotopic species of hydrogen (*i.e.*, H₂, HD, HT, D₂, DT, and T₂) would result. Table 2 gives the composition of such a typical spent fuel mixture resulting from preliminary cleanup of the main exhaust stream.

Table 2. Composition of a Typical Spent Fuel Mixture after Preliminary Cleanup

	Isotopic Species					
	H	HD	HT	D ₂	DT	T ₂
At. %	2.0	1.25	1.25	23.75	47.5	23.75

B. Isotopic Separation and Enrichment by Cryogenic Distillation

There are a number of methods, such as cryogenic distillation, chromatography, electrolysis, laser-stimulated separation, and thermal diffusion that have been used for separation and enrichment of spent fuel (step 10, Fig. 2). Thus far, only cryogenic distillation has been shown applicable to amounts of material larger than laboratory-scale. Cost and reliability will ultimately dictate which method is adopted; however, the selection of the enrichment method will also depend on the purity requirements for the recycled fuel, the nature of the fuel injection system, and the amount of fuel involved.

Table 3 summarizes the estimated isotopic composition of the spent fuel from (1) the main exhaust stream and (2) the neutral beam injector recycle for three typical tokamak-type reactors. Considering these high spent-fuel flow rates even for a small experimental reactor, cryogenic distillation is considered to have the most potential as a practical, reliable, and economic method for main-stream enrichment.

Table 3. Isotopic Composition of Spent Fuel
for Distillation

Species, (at. %)	TNS-ITR	TNS-UGO	TNS-UG
<u>Main Exhaust Stream Flow Rates, g/d</u>			
D(49.4)	27.1	34.4	145.7
T(49.5)	40.7	51.6	218.5
H(1.1)	<u>0.3</u>	<u>0.4</u>	<u>1.8</u>
Total	68.1	86.4	366.0
<u>Neutral Beam Injector Recycle, g/d</u>			
D(99.9)	76.1	95.1	237.8
T(0.1)	<u>0.2</u>	<u>0.2</u>	<u>0.5</u>
Total	76.3	95.3	238.3

A detailed description of a computer program for design and analysis of multicomponent isotopic separations by cryogenic distillation is given in Ref. 9; descriptions of the development of distillation cascades for the ANL Experimental Power Reactor (ANL/EPR) and ANL Tokamak Experimental Test Facility (ANL/TETF) are given in Refs. 1 and 10. From the results presented in these publications, one finds that the size and the nature of the distillation cascade are essentially determined by the purity requirements for the recycled fuel and by the nature of the fuel injection system. For example, the size of the distillation cascade for a reactor having cold fuel injection, augmented by a neutral beam of deuterons, will be different from that of a reactor totally beam-driven by energetic deuterons and tritons. It may be noted that irrespective of the fuel injection scheme for D-T burning reactors, the

composition of the spent fuel will remain essentially unchanged. The enrichment system presented below assumes cold fuel (enriched fuel injection) augmented by a neutral beam of deuterons (see Fig. 1). Such an enrichment system must produce the following:

1. An essentially tritium-free stream of protium- and deuterium-bearing species for waste consolidation and disposal.
2. A deuterium stream with a deuterium content >98 at. % for reuse in neutral beam injection.
3. A tritium-rich stream ($T/D >1.1$) containing no ($<1\%$) protium for reuse in cold fuel injection. Another requirement for the enrichment scheme may be an additional stream of pure tritium.¹¹

The fuel reprocessing system must be capable of handling the main exhaust wastes and the recycle stream of contaminated deuterium from the neutral beam injector. The system must also be able to handle tritium-bearing species from the waste consolidation system as indicated in Fig. 1.

In order to develop an isotopic separation system, a four-column cascade, shown in Fig. 3, was analyzed. In this figure, the distillation feeds X and Y represent the main fuel recycle and the neutral beam injector recycle, respectively. The main fuel stream (X) shown includes the spent fuel from the fusion reactor and tritium-bearing species from the waste consolidation system. The output streams A, B, and C represent the enriched fuel return, the neutral injector feed, and the protium waste streams, respectively. Since for a typical D-T fueled reactor, stream "A" represents a major fraction of the recycled fuel, the physical sizes of columns 2, 3, and 4 were considered to be smaller (hence, they have a lower number of theoretical plates) than column 1. To reduce the amount of tritium-bearing species in stream C, it was found advantageous to use a chemical equilibrators where stream "Y" from the neutral beam injector is introduced. A variety of cascade arrangements are possible (for an example, see Fig. 4) for reprocessing the spent fuel. The computer program and the analytical results presented here are based on the cascade arrangement shown in Fig. 3.

Fig. 3. TNS Cryogenic Distillation Cascade

Fig. 4. TNS Cryogenic Distillation Cascade
(Alternate Scheme)

III. DEVELOPMENT OF THE COMPUTER CODE FOR CRYOGENIC DISTILLATION BY A FOUR-COLUMN CASCADE

A complete fuel recycle analysis should include not only the conditions under steady-state operation, but also conditions during transient, abnormal, or off-design events that occur during start-up, shutdown, and/or a power failure. Because the fuel reprocessing involves a large number of variables, the present analysis is divided into two phases. The first phase considers a parametric investigation under steady-state conditions, and the analytical results are presented herein. The results of the second phase, which considers transient conditions, are presented in a separate report.¹²

Using the computer program MISRA (Multicomponent Isotopic Separation and Recirculation Analysis⁹) as the basis, a second computer program has been developed for analyzing an interconnecting system of distillation columns designed to fulfill TNS requirements. The new program consists of the following three subroutines:

1. MISRA. This subroutine is essentially the same as the one presented in Ref. 9. It solves a set of linear, simultaneous equations by matrix inversion.
2. POLYFT. This subroutine is the same as the one in Ref. 9. It calculates a set of polynomial-fitting coefficients for the phase equilibrium constants by least-squares techniques.
3. EQLBTR. This subroutine solves a set of nonlinear equations used to calculate the equilibrium composition of an isotopic mixture after changing the temperature of and/or adding one or more constituents to the original fuel mixture.
4. AUX. This is an external function used in EQLBTR (see IMSL subroutine MINFT)..

FORTTRAN listings of the main program and the subroutines are given in the Appendix.

A. Format for Input Data

Since the computer program discussed herein is based on the MISRA program, the reader is requested to consult Ref. 9. The format statements for all READ and PRINT statements are as follows:

	<u>READ</u>	<u>PRINT</u>
Fixed Point Data	12I6	12I6
Floating Point Data	6D12.6	1P6D15.6
Title of Input Data	9A8	9A8

<u>Card No.</u>	<u>FORTRAN Name</u>	<u>Description</u>
1	TITLE	A set of alpha-numeric information to identify the input data.
2	M	Order of column vector B (in matrix $AX = B$). Also used to terminate calculations when $M \leq 0$.
	NC	Number of components of mixture to be distilled.
	NCL	Number of columns in distillation cascade.
	INPUT	Integer constant used to signal whether of not to print input data. $INPUT \leq 0$ skips printing of input data.
	IPRNT	Input constant designed to signal printing of polynomial fitting coefficients; $IPRNT \leq 0$ skips printout.
	KASE	Integer constant for stacked cases. Used when single column analysis is performed (<u>i.e.</u> , $NCL = 1$) for stacked cases.
	NTRL	Total number of iterations.
	ITR2	Number of iterative steps in MISRA.
	NPR	Integer constant having values of 1 to 5. Used to select the NPR^{th} value of pressure as the column operating pressure.
	IC2	Integer constant used to signal whether to use an initial set of temperatures as the first-guess values or to use the temperatures calculated from the previous case or column.
3	NM1	Order of matrix $AX = (NM1 \leq 20)$.
	M1	Number of rows of vector B ($M1 \leq 20$).
	IP	Number of columns of vector B ($IP \leq 2$).
	N1, NP1	Number of temperature/vapor pressure data points.
	NC1	Number of components.

<u>Card No.</u>	<u>FORTTRAN Name</u>	<u>Description</u>
3	NR1	Number of operating pressures.
	NJ	Number of iterative steps in EQLBTR.
4	XNB	Number of moles of D ₂ from neutral beam injector.
	TE	Equilibration temperature.
	RK	Equilibrium constant.
5	PT	A set of column operating pressures.
6	XF1	Composition of first feed mixture.
7	XF2	Composition of second feed mixture.
8	XF3	Composition of third feed mixture. (Note: If there is only one feed, use blank cards for 6 and 7. If there are only two feeds, use a blank card for 6.)
9-12	VT	A set of saturation temperatures.
13-16	VP(1)	Vapor pressure data corresponding to the above set of temperatures for H ₂ (Component 1).
17-20	VP(2)	Vapor pressure data corresponding to the above set of temperatures for HD (Component 2).
21-24	VP(3)	Vapor pressure data corresponding to the above set of temperatures for HT (Component 3).
25-28	VP(4)	Vapor pressure data corresponding to the above set of temperatures for D ₂ (Component 4).
29-32	VP(5)	Vapor pressure data corresponding to the above set of temperatures for DT (Component 5).
33-36	VP(6)	Vapor pressure data corresponding to the above set of temperatures for T ₂ (Component 6).

<u>Card No.</u>	<u>FORTRAN Name</u>	<u>Description</u>
-----------------	---------------------	--------------------

If NCL >1, this signals conditions for cascade analysis, and requires the following cards.

37	NPX	Number of theoretical stages of column 1.
	NF1X, NF2X, NF3X	Feed plate locations for column 1.
	NSX	Side-stream location for column 1.
38	D1X, D2X	Top-product and side-stream flow rates, respectively, for column 1.
	F1X, F2X, F3X	Feed rates for column 1.
	RFX	Reflux ratio for column 1.
39	WX	Bottom-product flow rate for column 1.
	TBX, TD	First-guess values for temperatures for the bottom plate and top plate, respectively, for column 1.
	XD2X	Moles of D ₂ used in equilibrators for column 1. (Note: Each column does not necessarily have a chemical equilibrators.)
	TOLX	Convergence tolerance for column 1.
(40, 41, 42), and (43, 44, 45) etc.		The values for the other columns corresponding to those given in cards 37-39.

Last Card		A blank card terminates the calculations.
-----------	--	---

If KASE = 1, it signals analysis of stacked cases (single column analysis after cascade).

40	TITLE	A set of alpha-numeric information to identify input data.
41	M, NC, etc.	Repeat of card 2.
42	NP, NF1, NF2, NF3, NS	Have the same meaning as the corresponding values with the X subscript (see card 37).
43	D1, D2, F1, F2, F3, RFX	Have the same meaning as the corresponding values with X subscript (see card 38).

<u>Card No.</u>	<u>FORTTRAN Name</u>	<u>Description</u>
44	W, TB, TD, XD2, TOL	Have the same meaning as the corresponding values with X subscript (see card 39).
45	Last Card	A blank card terminates the calculations.

NOTE: For stacked cases, use as many sets (cards 40-44) of data as desired.

From the description of the input data, it may be noted that the program is suitable for analyzing a set of interconnected distillation columns ($NCL < 5$) or a single column ($NCL = 1$) including stacked cases. Also, a set of parametric investigations for a single column can be carried out after the completion of the cascade analysis. In that case, the input data for the single column should follow the input data for the cascade.

B. Program Limitations

The current structure of the DIMENSION statements limits the program to the following: number of theoretical plates ($NP \leq 100$), number of components ($NC \leq 6$), number of operating pressures ($NPR \leq 5$), temperature/vapor pressure data points ($NP1 \leq 20$), and number of columns in a cascade ($NCL \leq 5$).

Since the above limits are not inherent limitations on the mathematical formulations, one can easily broaden the program to accept a larger number of input variables. However, the stability of the code and the convergence criteria must be checked to ensure that the computed results are consistent with the physical system. The other limitations are: (1) three feeds (F_1 , F_2 , F_3), (2) one side-stream product D_2 in addition to one top product (distillate D_1 , and (3) one bottom product (W). It should be noted that as NP increases, the computation time (for the same degree of convergence) increases significantly. For example, when NP was increased from 30 to 100, the computation time was increased by a factor of more than five.

C. Input Data for a Sample Problem

For a given feed mixture and a desired product purity, the simplest design procedure from a computational standpoint is to carry out a parametric investigation of the effects of the number of theoretical stages, reflux ratio, feed plate location, operating pressure, protium fraction in the feed, and the fraction of distillate going to the equilibrator. Of these parameters, the number of theoretical stages or plates has the greatest effect on the distillation. Using the results, one can then select a set of operating conditions which will give the desired product. Table 4 presents typical input data for the four-column cascade studied here.

Table 4. Input Data for Four-Column Cascade

INPUT DATA FOR 4-COLUMN CASCADE, JUNE 1977

1	6	4	1	1	0	10	3	3	0
20	20	5	1	20	6	5	5		
1.000000D-01		3.000000D 02			2.580000D 00		3.260000D 00		3.820000D 00
1.500000D 03		1.250000D 03			1.000000D 03		7.500000D 02		5.000000D 02

FEED COMPOSITION

0.0	8.700000D-03	0.0	9.900000D-01	1.300000D-03	0.0
2.000000D-03	2.700000D-02	1.100000D-02	2.620000D-01	4.280000D-01	2.700000D-01
1.638650D-07	3.657700D-04	1.000000D-06	2.504460D-01	4.942150D-01	2.553020D-01

OPERATING PARAMETERS FOR COLUMN NO.= 1

75	10	38	40	6				
2.600000D 01	0.0		0.0		9.000000D 01	1.200000D 01	1.500000D 01	
7.600000D 01	2.600000D 01	2.400000D 01	0.0		1.000000D-06			

OPERATING PARAMETERS FOR COLUMN NO.= 2

30	10	12	15	6				
1.400000D 01	0.0		0.0		1.000000D 01	2.600000D 01	1.500000D 01	
2.200000D 01	2.600000D 01	2.400000D 01	1.000000D-01		1.000000D-06			

OPERATING PARAMETERS FOR COLUMN NO.= 3

30	10	12	15	6				
4.000000D 00	0.0		0.0		0.0	1.400000D 01	1.500000D 01	
1.000000D 01	2.600000D 01	2.400000D 01	0.0		1.000000D-06			

OPERATING PARAMETERS FOR COLUMN NO.= 4

30	10	12	15	6				
1.000000D 01	0.0		0.0		0.0	2.200000D 01	1.500000D 01	
1.200000D 01	2.600000D 01	2.400000D 01	0.0		1.000000D-06			

D. Output (Analytical Results)

Tables 5-8 show typical computer output for columns 1-4, respectively, of a four-column cascade as given in Fig. 3, based on the input in Table 4. The composition of the six isotopomeric species at each theoretical stage, the temperature of the liquid mixture at each theoretical stage, the summation of mole fractions, along with other pertinent column operating parameters, are presented.

IV. DISCUSSION OF RESULTS

A parametric investigation to study the effect of the design (e.g., number of theoretical stages) and operating variables (e.g., column pressure, reflux ratio, feed plate location) on the composition of the various product streams was carried out. The effect of the concentration of the protium-bearing species in the plasma exhaust gases was also studied; this concentration can vary over a wide range depending on whether water (or steam), helium, or lithium is the first-wall heat-transport medium. In addition, the effect of varying the amount of neutral beam recycle going to the equilibrators was examined. In discussing the results, emphasis is placed on the composition of the three product streams, marked A, B, and C in Fig. 3.

The results of the parametric studies showed that the product compositions did not improve significantly above a reflux ratio of 5. Hence, analyses of all cases were carried out at a reflux ratio 5. The feed plate location was found to have only a minor influence on the product composition as long as the feed plates were located approximately at the lower one third of the column. The results of some of the parametric studies are presented below.

The actual sizes of the distillation columns were not determined since data on height equivalent to a theoretical plate (HETP), superficial vapor velocity, packing material characteristics, etc. were not available at the outset of the study. The sparse HETP data that are available ^{13,14} are considered to be of limited value in this application since they vary over a wide range. The experimental data from the Tritium System Test Assembly (TSTA)⁷ at Los Alamos are expected to provide the basis for a more practical assessment of the cascade design for cryogenically distilling isotopes of hydrogen.

A. Effect of Protium Fraction in Feed

Table 9 shows how the composition of the product streams is affected by the protium content in the feed stream. [For the sake of simplicity, the feed stream from the waste consolidation system has been combined with the feed stream from the main exhaust fuel reprocessing system to form a single feed (see Fig. 1).] By examining the composition of the product streams, for the three cases analyzed, it can be concluded that the distillation cascade shown in Fig. 3 is capable of producing the required recycle streams as specified in Section II-B, even though the feed stream may contain as much as 7.5 at. % protium. For example (1) the ratio of T/D for the bottom product of column 1 is about 1.1 (except for the first case), (2) at. % D for the top product of column 4 is greater than 98% and (3) the top product from column 3 contains essentially H and D with only 1-2 at. % T.

Table 5. Analytical Results for Column 1 of Four-Column Cascade (Input given in Table 4)

CRYOGENIC DISTILLATION OF HYDROGEN ISOTOPES FOR DFME/TSTA,...B. MISRA..., JUNE 1977

ANALYTICAL RESULTS AT PT= 1.500D 03 TORR AFTER 10 ITERATIONS FOR COLUMN NO: 1
 NUMBER OF THEORETICAL STAGES: 75 REFLUX RATIO L/D1= 1.500D 01
 FIRST FEED PLATE LOCATION: 10 2ND FP LOCATION: 38 3RD FP LOCATION= 40
 FEED RATES: 0.0 9.00D 01 1.20D 01 DISTILLATE: 2.60D 01 BOTTOMS: 7.60D 01

FEED COMP. N-H2	HD	HT	N-D2	DT	N-T2	APH	APD	APT
2.000000D-03	2.700000D-02	1.100000D-02	2.620000D-01	4.280000D-01	2.700000D-01	2.100D 00	4.895D 01	4.895D 01
2.534413D-14	1.286257D-06	8.413705D-05	9.001460D-01	9.826373D-02	1.504886D-03	4.271D-03	9.493D 01	5.068D 00

SUMMATION OF LIQUID MOLE FRACTIONS.....(FROM L TO R IN ASCENDING ORDER OF PLATE NUMBER)

9.999990D-01	9.999991D-01	9.999992D-01	9.999993D-01	9.999993D-01	9.999993D-01
9.999992D-01	9.999992D-01	9.999992D-01	9.999991D-01	9.999990D-01	9.999989D-01
9.999989D-01	9.999988D-01	9.999987D-01	9.999986D-01	9.999985D-01	9.999984D-01
9.999984D-01	9.999983D-01	9.999982D-01	9.999982D-01	9.999981D-01	9.999981D-01
9.999981D-01	9.999981D-01	9.999981D-01	9.999981D-01	9.999982D-01	9.999982D-01
9.999983D-01	9.999984D-01	9.999986D-01	9.999987D-01	9.999989D-01	9.999990D-01
9.999992D-01	9.999994D-01	9.999994D-01	9.999995D-01	9.999995D-01	9.999995D-01
9.999995D-01	9.999996D-01	9.999996D-01	9.999996D-01	9.999996D-01	9.999996D-01
9.999996D-01	9.999996D-01	9.999995D-01	9.999995D-01	9.999995D-01	9.999995D-01
9.999994D-01	9.999994D-01	9.999993D-01	9.999992D-01	9.999992D-01	9.999991D-01
9.999990D-01	9.999989D-01	9.999988D-01	9.999988D-01	9.999987D-01	9.999986D-01
9.999985D-01	9.999985D-01	9.999984D-01	9.999984D-01	9.999984D-01	9.999984D-01
9.999985D-01	9.999986D-01	9.999987D-01			

EQUILIBRIUM STAGE TEMPERATURES, DEG.K..(FROM L TO R IN ASCENDING ORDER OF PLATE NUMBER)

2.611417D 01	2.615889D 01	2.618979D 01	2.621169D 01	2.622774D 01	2.624002D 01
2.624989D 01	2.625829D 01	2.626584D 01	2.627299D 01	2.628003D 01	2.628719D 01
2.629464D 01	2.630248D 01	2.631082D 01			
2.680574D 01	2.681668D 01	2.682932D 01	2.684397D 01	2.686100D 01	2.688083D 01
2.690400D 01	2.693108D 01	2.696277D 01	2.699976D 01	2.704277D 01	

PLATE NO.	N-H2	HD	HT	N-D2	DT	N-T2	APH	APD	APT
1	6.923187D-03	9.346334D-02	3.805179D-02	8.470846D-01	1.446471D-02	1.128880D-05	7.268D 00	9.010D 01	2.627D 00
2	1.850753D-03	4.968430D-02	2.823115D-02	8.987392D-01	2.147110D-02	2.350702D-05	4.081D 00	9.343D 01	2.487D 00
3	1.076607D-03	3.733430D-02	2.442012D-02	9.117038D-01	2.543252D-02	3.268319D-05	3.195D 00	9.431D 01	2.496D 00
4	7.131139D-04	2.894927D-02	2.128801D-02	9.192469D-01	2.975793D-02	4.478419D-05	2.583D 00	9.486D 01	2.557D 00
5	5.428931D-04	2.329556D-02	1.874543D-02	9.228613D-01	3.449405D-02	6.073314D-05	2.156D 00	9.518D 01	2.668D 00
6	4.631149D-04	1.949949D-02	1.669788D-02	9.235692D-01	3.968858D-02	8.173816D-05	1.856D 00	9.532D 01	2.827D 00
7	4.255141D-04	1.695599D-02	1.505731D-02	9.220620D-01	4.538976D-02	1.093755D-04	1.643D 00	9.532D 01	3.033D 00
8	4.075453D-04	1.525191D-02	1.374660D-02	9.188023D-01	5.164591D-02	1.456960D-04	1.491D 00	9.523D 01	3.284D 00
9	3.987045D-04	1.410777D-02	1.270055D-02	9.140947D-01	5.850495D-02	1.933602D-04	1.380D 00	9.504D 01	3.580D 00
10	3.941016D-04	1.333564D-02	1.186527D-02	9.081354D-01	6.601375D-02	2.558089D-04	1.299D 00	9.478D 01	3.920D 00
11	3.914575D-04	1.280972D-02	1.119680D-02	9.010472D-01	7.421734D-02	3.374773D-04	1.239D 00	9.446D 01	4.304D 00
12	3.897060D-04	1.244600D-02	1.065965D-02	8.929028D-01	8.315779D-02	4.440620D-04	1.194D 00	9.407D 01	4.735D 00
13	3.883449D-04	1.218851D-02	1.022534D-02	8.837420D-01	9.287296D-02	5.828506D-04	1.160D 00	9.363D 01	5.213D 00
14	3.871348D-04	1.199999D-02	9.871128D-03	8.735837D-01	1.033949D-01	7.631272D-04	1.132D 00	9.313D 01	5.740D 00
15	3.859595D-04	1.185567D-02	9.578918D-03	8.624346D-01	1.147482D-01	9.966652D-04	1.110D 00	9.257D 01	6.316D 00
65	1.016888D-11	3.323192D-06	1.831825D-04	3.575467D-01	4.731859D-01	1.690809D-01	9.325D-03	5.941D 01	4.058D 01
66	5.296197D-12	2.436099D-06	1.563024D-04	3.455361D-01	4.815379D-01	1.727673D-01	7.937D-03	5.863D 01	4.136D 01
67	2.751415D-12	1.778215D-06	1.325611D-04	3.320862D-01	4.902609D-01	1.775185D-01	6.717D-03	5.772D 01	4.227D 01
68	1.425030D-12	1.291133D-06	1.116156D-04	3.170789D-01	4.991364D-01	1.836718D-01	5.645D-03	5.666D 01	4.333D 01
69	7.352843D-13	9.312230D-07	9.316389D-05	3.004926D-01	5.078381D-01	1.916652D-01	4.705D-03	5.543D 01	4.456D 01
70	3.775611D-13	6.659094D-07	7.694048D-05	2.819606D-01	5.159025D-01	2.020593D-01	3.880D-03	5.399D 01	4.600D 01
71	1.926135D-13	4.708895D-07	6.271300D-05	2.616818D-01	5.226975D-01	2.155575D-01	3.159D-03	5.230D 01	4.769D 01
72	9.734400D-14	3.280448D-07	5.027872D-05	2.395351D-01	5.273937D-01	2.337295D-01	2.530D-03	5.032D 01	4.967D 01
73	4.848297D-14	2.238795D-07	3.946163D-05	2.155486D-01	5.289457D-01	2.554660D-01	1.984D-03	4.800D 01	5.200D 01
74	2.355515D-14	1.483497D-07	3.010941D-05	1.898322D-01	5.260940D-01	2.840431D-01	1.513D-03	4.529D 01	5.471D 01
75	1.091983D-14	5.398609D-08	2.209025D-05	1.626030D-01	5.174061D-01	3.199687D-01	1.109D-03	4.213D 01	5.787D 01

*** I M S L (UEFTST) *** TERMINAL ZSYSTM 1 (IER = 129)
 *** I M S L (UEFTST) *** TERMINAL ZSYSTM 1 (IRP = 129)

Table 6. Analytical Results for Column 2 of Four-Column Cascade (Input given in Table 4)

CRYOGENIC DISTILLATION OF HYDROGEN ISOTOPES FOR DFME/TSTA,....B. MISRA...., JUNE 1977

ANALYTICAL RESULTS AT PT= 1.250D 03 TORR AFTER 10 ITERATIONS FOR COLUMN NO: 2
 NUMBER OF THEORETICAL STAGES: 30 REFLUX RATIO L/D1= 1.500D 01
 FIRST FEED PLATE LOCATION: 10 2ND FP LOCATION: 12 3RD FP LOCATION= 15
 FEED RATES: 0.0 1.00D 01 2.65D 01 DISTILLATE: 1.41D 01 BOTTOMS: 2.20D 01

FEED COMP. N-H2	HD	HT	N-D2	DT	N-T2	APH	APD	APT
2.486777D-05	8.507170D-01	3.024668D-02	1.188458D-01	1.655711D-04	9.386678D-08	4.405D 01	5.443D 01	1.521D 00
6.077361D-03	1.271435D-01	3.320802D-03	8.159347D-01	4.682039D-02	7.033172D-04	7.131D 00	9.029D 01	2.577D 00

SUMMATION OF LIQUID MOLE FRACTIONS.....(FROM L TO R IN ASCENDING ORDER OF PLATE NUMBER)

9.965653D-01	9.956333D-01	9.947545D-01	9.940620D-01	9.936754D-01	9.936579D-01
9.939944D-01	9.946018D-01	9.953641D-01	9.961700D-01	9.969356D-01	9.976112D-01
9.980841D-01	9.985093D-01	9.988666D-01	9.990531D-01	9.992189D-01	9.993613D-01
9.994804D-01	9.995783D-01	9.996576D-01	9.997212D-01	9.997718D-01	9.998118D-01
9.998431D-01	9.998673D-01	9.998856D-01	9.998990D-01	9.999080D-01	9.999131D-01

EQUILIBRIUM STAGE TEMPERATURES, DEG.K..(FROM L TO R IN ASCENDING ORDER OF PLATE NUMBER)

2.419131D 01	2.427859D 01	2.437792D 01	2.448727D 01	2.460223D 01	2.471701D 01
2.482572D 01	2.492370D 01	2.500820D 01	2.507843D 01	2.513514D 01	2.517995D 01
2.525443D 01	2.531275D 01	2.535764D 01	2.539525D 01	2.542536D 01	2.544929D 01
2.546823D 01	2.548320D 01	2.549508D 01	2.550458D 01	2.551232D 01	2.551878D 01
2.552441D 01	2.552956D 01	2.553460D 01	2.553985D 01	2.554567D 01	2.555245D 01

PLATE NO.	N-H2	HD	HT	N-D2	DT	N-T2	APH	APD	APT
1	1.158195D-02	8.508725D-01	2.456292D-02	1.093918D-01	1.560974D-04	8.986362D-08	4.493D 01	5.349D 01	1.236D 00
2	4.634746D-03	7.512414D-01	3.184453D-02	2.118305D-01	4.483661D-04	3.830924D-07	3.979D 01	5.903D 01	1.622D 00
3	3.046650D-03	6.847039D-01	3.451672D-02	2.770243D-01	7.077148D-04	7.321204D-07	3.646D 01	6.230D 01	1.771D 00
4	2.100057D-03	6.116153D-01	3.622917D-02	3.489804D-01	1.073768D-03	1.344059D-06	3.280D 01	6.592D 01	1.876D 00
5	1.538906D-03	5.359989D-01	3.683962D-02	4.240509D-01	1.569257D-03	2.375695D-06	2.898D 01	6.972D 01	1.933D 00
6	1.205922D-03	4.622151D-01	3.635344D-02	4.980075D-01	2.214004D-03	4.051362D-06	2.521D 01	7.349D 01	1.941D 00
7	1.006326D-03	3.940962D-01	3.491964D-02	5.669464D-01	3.024725D-03	6.685077D-06	2.168D 01	7.701D 01	1.909D 00
8	8.842689D-04	3.342831D-01	3.278359D-02	6.280215D-01	4.016815D-03	1.071392D-05	1.854D 01	8.015D 01	1.851D 00
9	8.075344D-04	2.839997D-01	3.022170D-02	6.797470D-01	5.207361D-03	1.674916D-05	1.587D 01	8.282D 01	1.781D 00
10	7.577943D-04	2.432365D-01	2.748591D-02	7.218759D-01	6.618247D-03	2.565254D-05	1.366D 01	8.501D 01	1.714D 00
11	7.246282D-04	2.111480D-01	2.477242D-02	7.550377D-01	8.278602D-03	3.864643D-05	1.190D 01	8.674D 01	1.662D 00
12	7.020152D-04	1.864658D-01	2.221386D-02	7.803344D-01	1.022642D-02	5.747040D-05	1.053D 01	8.808D 01	1.632D 00
13	6.951635D-04	1.450058D-01	1.938557D-02	8.218836D-01	1.294231D-02	8.753945D-05	8.305D 00	9.026D 01	1.628D 00
14	6.834228D-04	1.135927D-01	1.669716D-02	8.527731D-01	1.612244D-02	1.311417D-04	6.593D 00	9.190D 01	1.657D 00
15	6.715306D-04	9.032739D-02	1.424584D-02	8.747195D-01	1.984174D-02	1.939707D-04	5.302D 00	9.309D 01	1.726D 00
16	3.577408D-04	7.030285D-02	1.313923D-02	8.956909D-01	2.031293D-02	1.963083D-04	4.212D 00	9.419D 01	1.694D 00
17	1.894022D-04	5.431924D-02	1.201609D-02	9.124879D-01	2.078890D-02	1.985000D-04	3.338D 00	9.508D 01	1.661D 00
18	9.978575D-05	4.171955D-02	1.091000D-02	9.257727D-01	2.129724D-02	2.007472D-04	2.643D 00	9.579D 01	1.631D 00
19	5.236755D-05	3.188389D-02	9.844018D-03	9.361461D-01	2.187026D-02	2.033222D-04	2.093D 00	9.635D 01	1.607D 00
20	2.739770D-05	2.426407D-02	8.832834D-03	9.441227D-01	2.254642D-02	2.066097D-04	1.658D 00	9.679D 01	1.590D 00
21	1.429843D-05	1.839561D-02	7.884770D-03	9.501217D-01	2.337246D-02	2.111753D-04	1.316D 00	9.713D 01	1.585D 00
22	7.446868D-06	1.389661D-02	7.003561D-03	9.544683D-01	2.440621D-02	2.178735D-04	1.046D 00	9.739D 01	1.593D 00
23	3.871554D-06	1.045970D-02	6.189755D-03	9.573983D-01	2.572038D-02	2.280159D-04	8.330D-01	9.757D 01	1.619D 00
24	2.009342D-06	7.841351D-03	5.441782D-03	9.590639D-01	2.740728D-02	2.436334D-04	6.645D-01	9.769D 01	1.667D 00
25	1.040868D-06	5.850895D-03	4.756742D-03	9.595387D-01	2.958475D-02	2.678845D-04	5.306D-01	9.774D 01	1.744D 00
26	5.378306D-07	4.340317D-03	4.130966D-03	9.588189D-01	3.240363D-02	3.056870D-04	4.237D-01	9.773D 01	1.858D 00
27	2.768302D-07	3.195488D-03	3.560411D-03	9.568223D-01	3.605683D-02	3.646941D-04	3.379D-01	9.766D 01	2.018D 00
28	1.415452D-07	2.328845D-03	3.040927D-03	9.533830D-01	4.079031D-02	4.567941D-04	2.685D-01	9.750D 01	2.237D 00
29	7.149132D-08	1.673470D-03	2.568441D-03	9.482417D-01	4.691594D-02	6.003987D-04	2.121D-01	9.726D 01	2.534D 00
30	3.525387D-08	1.178377D-03	2.139085D-03	9.410329D-01	5.482572D-02	8.239005D-04	1.659D-01	9.691D 01	2.931D 00

Table 7. Analytical Results for Column 3 of Four-Column Cascade (Input given in Table 4)

CRYOGENIC DISTILLATION OF HYDROGEN ISOTOPES FOR DFME/TSTA,....B. MISRA...., JUNE 1977

ANALYTICAL RESULTS AT PT= 1.000D 03 TOPR AFTER 10 ITERATIONS FOR COLUMN NO: 3
 NUMBER OF THEORETICAL STAGES: 30 REFLUX RATIO L/D1= 1.500D 01
 FIRST FEED PLATE LOCATION: 10 2ND FP LOCATION: 12 3RD FP LOCATION= 15
 FEED RATES: 0.0 0.0 1.40D 01 DISTILLATE: 4.00D 00 BOTTOMS: 1.00D 01

FEED COMP. N-H2	HD	HT	N-D2	DT	N-T2	APH	APD	APT
1.158195D-02	8.508725D-01	2.456292D-02	1.093918D-01	1.560974D-04	8.986362D-08	4.493D 01	5.349D 01	1.236D 00

SUMMATION OF LIQUID MOLE FRACTIONS....(FROM L TO R IN ASCENDING ORDER OF PLATE NUMBER)

9.999976D-01	9.999987D-01	9.999993D-01	9.999998D-01	1.000000D 00	1.000000D 00
1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	9.999998D-01	9.999996D-01
9.999993D-01	9.999990D-01	9.999985D-01	1.000000D 00	1.000002D 00	1.000005D 00
1.000007D 00	1.000009D 00	1.000011D 00	1.000013D 00	1.000013D 00	1.000013D 00
1.000011D 00	1.000008D 00	1.000004D 00	9.999987D-01	9.999952D-01	9.999951D-01

EQUILIBRIUM STAGE TEMPERATURES, DEG.K..(FROM L TO R IN ASCENDING ORDER OF PLATE NUMBER)

2.306670D 01	2.308524D 01	2.309683D 01	2.310424D 01	2.310921D 01	2.311287D 01
2.311596D 01	2.311903D 01	2.312253D 01	2.312693D 01	2.313276D 01	2.314068D 01
2.315158D 01	2.316663D 01	2.318735D 01	2.318976D 01	2.319158D 01	2.319301D 01
2.319422D 01	2.319535D 01	2.319659D 01	2.319816D 01	2.320039D 01	2.320380D 01
2.320919D 01	2.321792D 01	2.323216D 01	2.325533D 01	2.329273D 01	2.335190D 01

PLATE NO.	N-H2	HD	HT	N-D2	DT	N-T2	APH	APD	APT
1	4.061852D-02	9.580378D-01	1.187111D-03	1.541564D-04	6.780625D-09	1.288369D-13	5.202D 01	4.792D 01	5.936D-02
2	1.757752D-02	9.802013D-01	1.851098D-03	3.700124D-04	2.510720D-08	7.353967D-13	5.086D 01	4.905D 01	9.256D-02
3	1.224271D-02	9.849412D-01	2.260786D-03	5.552219D-04	4.651934D-08	1.686096D-12	5.058D 01	4.930D 01	1.130D-01
4	9.007155D-03	9.874342D-01	2.734791D-03	8.237825D-04	8.528836D-08	3.831079D-12	5.041D 01	4.945D 01	1.367D-01
5	7.049523D-03	9.884531D-01	3.284082D-03	1.213182D-03	1.554360D-07	8.665586D-12	5.029D 01	4.954D 01	1.642D-01
6	5.866421D-03	9.884347D-01	3.921019D-03	1.777622D-03	2.822742D-07	1.955227D-11	5.020D 01	4.960D 01	1.961D-01
7	5.151327D-03	9.875934D-01	4.659451D-03	2.595304D-03	5.114414D-07	4.404582D-11	5.013D 01	4.964D 01	2.330D-01
8	4.718271D-03	9.859873D-01	5.514721D-03	3.778749D-03	9.250894D-07	9.909631D-11	5.005D 01	4.968D 01	2.758D-01
9	4.454580D-03	9.835510D-01	6.503519D-03	5.489241D-03	1.670760D-06	2.226644D-10	4.995D 01	4.973D 01	3.253D-01
10	4.291921D-03	9.801049D-01	7.643441D-03	7.956711D-03	3.012588D-06	4.995513D-10	4.982D 01	4.980D 01	3.823D-01
11	4.188659D-03	9.753474D-01	8.952065D-03	1.150644D-02	5.421332D-06	1.118533D-09	4.963D 01	4.992D 01	4.479D-01
12	4.119122D-03	9.688323D-01	1.044524D-02	1.659358D-02	9.730744D-06	2.497794D-09	4.938D 01	5.010D 01	5.227D-01
13	4.067066D-03	9.599364D-01	1.213420D-02	2.384492D-02	1.740449D-05	5.557401D-09	4.901D 01	5.038D 01	6.076D-01
14	4.021698D-03	9.478224D-01	1.402089D-02	3.410405D-02	3.098042D-05	1.230247D-08	4.849D 01	5.080D 01	7.026D-01
15	3.975246D-03	9.314102D-01	1.609112D-02	4.846863D-02	5.478341D-05	2.704570D-08	4.777D 01	5.142D 01	8.073D-01
16	2.892229D-03	9.323676D-01	1.616420D-02	4.852117D-02	5.480914D-05	2.705444D-08	4.772D 01	5.147D 01	8.110D-01
17	2.102750D-03	9.329971D-01	1.625852D-02	4.858674D-02	5.483371D-05	2.706179D-08	4.767D 01	5.151D 01	8.157D-01
18	1.527641D-03	9.333524D-01	1.638442D-02	4.868069D-02	5.486246D-05	2.706885D-08	4.764D 01	5.154D 01	8.220D-01
19	1.108897D-03	9.334531D-01	1.655564D-02	4.882745D-02	5.490414D-05	2.707710D-08	4.761D 01	5.156D 01	8.305D-01
20	8.041045D-04	9.332828D-01	1.679070D-02	4.906736D-02	5.497501D-05	2.708913D-08	4.758D 01	5.157D 01	8.423D-01
21	5.823006D-04	9.327796D-01	1.711471D-02	4.946830D-02	5.510733D-05	2.711029D-08	4.755D 01	5.159D 01	8.585D-01
22	4.209045D-04	9.318169D-01	1.756164D-02	5.014516D-02	5.536720D-05	2.715303D-08	4.751D 01	5.161D 01	8.808D-01
23	3.034615D-04	9.301706D-01	1.817714D-02	5.129291D-02	5.589206D-05	2.724785D-08	4.745D 01	5.164D 01	9.116D-01
24	2.179879D-04	9.274616D-01	1.902170D-02	5.324173D-02	5.697002D-05	2.747221D-08	4.735D 01	5.170D 01	9.539D-01
25	1.557599D-04	9.230632D-01	2.017369D-02	5.654814D-02	5.920677D-05	2.802620D-08	4.718D 01	5.181D 01	1.012D 00
26	1.104299D-04	9.159535D-01	2.173078D-02	6.214136D-02	6.387377D-05	2.943099D-08	4.689D 01	5.201D 01	1.090D 00
27	7.738253D-05	9.044946D-01	2.380651D-02	7.154782D-02	7.362097D-05	3.304349D-08	4.642D 01	5.238D 01	1.194D 00
28	5.326786D-05	8.861316D-01	2.651541D-02	8.720575D-02	9.388829D-05	4.236407D-08	4.564D 01	5.303D 01	1.330D 00
29	3.566393D-05	8.570656D-01	2.993530D-02	1.128278D-01	1.355401D-04	6.623977D-08	4.435D 01	5.414D 01	1.504D 00
30	2.283455D-05	8.121098D-01	3.403203D-02	1.536159D-01	2.192887D-04	1.262437D-07	4.231D 01	5.598D 01	1.713D 00

Table 8. Analytical Results for Column 4 of Four-Column Cascade (Input given in Table 4)

CRYOGENIC DISTILLATION OF HYDROGEN ISOTOPES FOR DFME/TSTA,....B. MISRA...., JUNE 1977

ANALYTICAL RESULTS AT PT= 7.500D 02 TORR AFTER 10 ITERATIONS FOR COLUMN NO: 4
 NUMBER OF THEORETICAL STAGES: 30 REFLUX RATIO L/D1= 1.500D 01
 FIRST FEED PLATE LOCATION: 10 2ND FP LOCATION: 12 3RD FP LOCATION= 15
 FEED RATES: 0.0 0.0 2.20D 01 DISTILLATE: 1.00D 01 BOTTOMS: 1.20D 01

FEED COMP. N-H2	HD	HT	N-D2	DT	N-T2	APH	APD	APT
3.525387D-08	1.178377D-03	2.139085D-03	9.410329D-01	5.482572D-02	8.239005D-04	1.659D-01	9.690D 01	2.931D 00

SUMMATION OF LIQUID MOLE FRACTIONS....(FROM L TO R IN ASCENDING ORDER OF PLATE NUMBER)

1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00
1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00
1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00	1.000000D 00
1.000000D 00	1.000000D 00	9.999999D-01	9.999999D-01	9.999999D-01	9.999999D-01	9.999999D-01	9.999999D-01	9.999999D-01
9.999998D-01	9.999998D-01	9.999998D-01	9.999997D-01	9.999997D-01	9.999996D-01	9.999996D-01	9.999996D-01	9.999996D-01

EQUILIBRIUM STAGE TEMPERATURES, DEG.K..(FROM L TO R IN ASCENDING ORDER OF PLATE NUMBER)

2.361786D 01	2.361982D 01	2.362134D 01	2.362260D 01	2.362373D 01	2.362481D 01	2.362591D 01	2.362709D 01	2.362837D 01
2.362591D 01	2.362709D 01	2.362837D 01	2.362960D 01	2.363142D 01	2.363327D 01	2.363539D 01	2.363781D 01	2.364060D 01
2.363539D 01	2.363781D 01	2.364060D 01	2.364113D 01	2.364168D 01	2.364229D 01	2.364301D 01	2.364389D 01	2.364499D 01
2.364301D 01	2.364389D 01	2.364499D 01	2.364639D 01	2.364819D 01	2.365052D 01	2.365355D 01	2.365750D 01	2.366263D 01
2.365355D 01	2.365750D 01	2.366263D 01	2.366931D 01	2.367796D 01	2.368916D 01	2.369576D 01	2.370331D 01	2.371186D 01

PLATE NO.	N-H2	HD	HT	N-D2	DT	N-T2	APH	APD	APT
1	7.755853D-08	2.591077D-03	4.613785D-03	9.904466D-01	2.347286D-03	1.089218D-06	3.603D-01	9.929D 01	3.482D-01
2	1.535418D-08	1.155464D-03	3.061715D-03	9.922348D-01	3.545516D-03	2.481879D-06	2.109D-01	9.946D 01	3.306D-01
3	8.219488D-09	8.177671D-04	2.552594D-03	9.923381D-01	4.287913D-03	3.651662D-05	1.685D-01	9.949D 01	3.424D-01
4	5.360731D-09	6.096489D-04	2.166128D-03	9.920731D-01	5.145822D-03	5.321708D-06	1.388D-01	9.950D 01	3.661D-01
5	4.215133D-09	4.814126D-04	1.872858D-03	9.915010D-01	6.137005D-03	7.705269D-06	1.177D-01	9.948D 01	4.013D-01
6	3.755676D-09	4.023939D-04	1.650328D-03	9.906544D-01	7.281804D-03	1.110607D-05	1.026D-01	9.945D 01	4.477D-01
7	3.570923D-09	3.536850D-04	1.481449D-03	9.895454D-01	8.603471D-03	1.595640D-05	9.176D-02	9.940D 01	5.058D-01
8	3.496073D-09	3.236322D-04	1.353228D-03	9.881717D-01	1.012853D-02	2.287108D-05	8.384D-02	9.934D 01	5.764D-01
9	3.465118D-09	3.050547D-04	1.255797D-03	9.865192D-01	1.188718D-02	3.272377D-05	7.804D-02	9.926D 01	6.604D-01
10	3.451607D-09	2.935281D-04	1.181658D-03	9.845644D-01	1.391367D-02	4.675465D-05	7.376D-02	9.917D 01	7.594D-01
11	3.444927D-09	2.863263D-04	1.125117D-03	9.822751D-01	1.624674D-02	6.672220D-05	7.057D-02	9.905D 01	8.753D-01
12	3.440801D-09	2.817685D-04	1.081848D-03	9.796113D-01	1.893000D-02	9.511641D-05	6.818D-02	9.892D 01	1.010D 00
13	3.437488D-09	2.788178D-04	1.048564D-03	9.765248D-01	2.201235D-02	1.354576D-04	6.637D-02	9.877D 01	1.167D 00
14	3.434256D-09	2.768332D-04	1.022759D-03	9.729595D-01	2.554822D-02	1.927136D-04	6.498D-02	9.859D 01	1.348D 00
15	3.430774D-09	2.754168D-04	1.002526D-03	9.688504D-01	2.959778D-02	2.738807D-04	6.390D-02	9.838D 01	1.557D 00
16	1.568291D-09	1.933907D-04	8.615346D-04	9.686752D-01	2.995533D-02	2.745407D-04	5.275D-02	9.838D 01	1.570D 00
17	7.168135D-10	1.357582D-04	7.396077D-04	9.683341D-01	3.051500D-02	2.755667D-04	4.377D-02	9.837D 01	1.590D 00
18	3.275853D-10	9.526919D-05	6.341739D-04	9.677983D-01	3.119508D-02	2.771829D-04	3.647D-02	9.834D 01	1.619D 00
19	1.496821D-10	6.682683D-05	5.430024D-04	9.670249D-01	3.208548D-02	2.797493D-04	3.049D-02	9.831D 01	1.659D 00
20	6.837943D-11	4.684870D-05	4.641603D-04	9.659538D-01	3.325133D-02	2.838466D-04	2.555D-02	9.826D 01	1.714D 00
21	3.122957D-11	3.281724D-05	3.959738D-04	9.645034D-01	3.477739D-02	2.904111D-04	2.144D-02	9.819D 01	1.788D 00
22	1.425786D-11	2.296340D-05	3.369943D-04	9.625652D-01	3.677384D-02	3.009538D-04	1.800D-02	9.810D 01	1.886D 00
23	6.506314D-12	1.604424D-05	2.859686D-04	9.599966D-01	3.938346D-02	3.179112D-04	1.510D-02	9.797D 01	2.015D 00
24	2.967027D-12	1.118652D-05	2.418134D-04	9.566113D-01	4.279050D-02	3.452078D-04	1.265D-02	9.780D 01	2.186D 00
25	1.351666D-12	7.776755D-06	2.035925D-04	9.521680D-01	4.723148D-02	3.891518D-04	1.057D-02	9.759D 01	2.411D 00
26	6.147865D-13	5.384018D-06	1.704977D-04	9.463564D-01	5.300790D-02	4.598538D-04	8.794D-03	9.729D 01	2.705D 00
27	2.788721D-13	3.705605D-06	1.418323D-04	9.387806D-01	6.050039D-02	5.734536D-04	7.277D-03	9.690D 01	3.089D 00
28	1.258787D-13	2.528908D-06	1.169970D-04	9.289416D-01	7.018333D-02	7.555746D-04	5.976D-03	9.640D 01	3.591D 00
29	5.627950D-14	1.704616D-06	9.547792D-05	9.162186D-01	8.263764D-02	1.046601D-03	4.859D-03	9.575D 01	4.241D 00
30	2.466773D-14	1.127884D-06	7.683663D-05	8.998547D-01	9.855771D-02	1.509576D-03	3.898D-03	9.491D 01	5.083D 00

Table 9. Cascade Parameter Study--Effect of Protium Fraction in Feed (all compositions given in at. %)

Composition of Spent Fuel			Column Number ^a	Composition of Product Stream ^a					
H	D	T		Top ^b			Bottom ^b		
				H	D	T	H	D	T
2.1	48.95	48.95	1	7.26	90.34	2.39	3.4E-3	48.84	51.09
			2	13.60	83.06	3.33	0.16	99.20	0.74
			3	46.81	51.75	1.13	0.23	95.61	4.20
			4	0.55	98.88	0.55	1.1E-2	97.59	2.40
3.75	48.13	48.13	1	11.63	85.92	2.48	1.7E-3	47.97	52.02
			2	19.99	76.81	1.88	0.12	99.07	0.84
			3	51.65	46.11	1.30	0.17	95.60	4.33
			4	0.42	99.08	0.50	9.7E-3	97.41	2.58
7.50	46.25	46.25	1	18.89	77.71	3.43	1.0E-3	45.73	54.24
			2	28.42	66.92	4.63	0.15	99.32	0.60
			3	56.35	40.40	2.15	0.22	92.84	7.03
			4	0.53	98.76	0.70	1.2E-2	96.52	3.47

^aNumber of theoretical stages for the four columns of the cascade are, respectively, 75, 30, 30 and 30. The operating pressures are, respectively, 200, 167, 133 and 100 kPa. Reflux ratio = 5 for each column.

^bThe terms "top" and "bottom" refer to the product streams as depicted in Fig. 3 from each column.

B. Effect of Operating Pressure

In practice, the first column of a distillation cascade should be operated at the highest selected pressure, with each succeeding downstream column operating at a progressively lower pressure. However, because of the need for interconnecting feed and product streams between the columns, selection of a set of pressures is not straightforward. The effect of the operating pressure on the product streams in the range of 100-200 kPa was found to be minor (see Table 10).

C. Effect of Number of Theoretical Stages

From a parametric investigation to study the effect of the number of theoretical stages for the distillation cascade as shown in Fig. 3, one finds that the first column of the distillation cascade is the most important in the design of the entire cascade. All three cases in Table 11 meet the distillation requirements. That is, from the table one can see for the three cases analyzed that (1) the T/D ratio for stream A is >1.1, (2) at. % D for stream B is >98, and (3) the tritium content of stream C is of the order of only 2%. Thus, it is seen that when the total number of theoretical plates is about 200 and the first column contains greater than 50 theoretical stages and the other columns contain about 30-50 theoretical stages each, the enrichment scheme will meet the recycle requirements.

Table 10. Cascade Parameter Study--Effect of Operating Pressure^a

Case	Column Pressure, kPa				Composition of Product Stream, at. %			
	Col. 1	Col. 2	Col. 3	Col. 4	Isotope	A	B	C
I	200	167	133	100	H	0.04	0.14	49.6
					D	45.5	99.3	47.8
					T	54.4	0.59	2.9
II	200	200	200	200	H	0.04	0.19	50.0
					D	45.5	98.7	47.9
					T	54.4	1.21	2.3
III	100	100	100	100	H	0.01	0.07	50.0
					D	44.6	99.7	48.1
					T	55.3	0.33	2.1

^aNumber of theoretical plates = 75, 30, 30, 30 for columns 1, 2, 3, and 4, respectively.

Feed composition = 2.1 at. % H, 48.95 at. % D, 48.95 at. % T.

NB to equilibrator = 1% of feed to column 1.

Reflux ratio = 5 for each column.

Table 11. Cascade Parameter Study--Effect of Number of Theoretical Plates^a

Case	Number of Theo. Plates				Composition of Product Stream, at. %			
	Col. 1	Col. 2	Col. 3	Col. 4	Isotope	A	B	C
I	75	30	30	30	H	10 ⁻³	0.1	51.4
					D	43.6	99.8	48.4
					T	56.4	0.16	0.42
II	75	50	50	50	H	10 ⁻³	0.03	51.4
					D	43.7	99.9	47.9
					T	56.3	0.04	0.8
III	50	50	50	50	H	0.01	0.04	50.9
					D	44.1	99.9	47.2
					T	55.9	0.06	2.1

^aOperating pressures = 220, 167, 133, and 100 kPa for the four columns, respectively.

Feed composition = 2.1 at. % H, 48.95 at. % D, 48.95 at. % T.

NB to equilibrator = 1% of feed to column 1.

Reflux ratio = 5 for each column.

D. Effect of Amount of Neutral Beam Recycle Going to Chemical Equilibrator

As discussed in Ref. 10, the use of a chemical equilibrator is essential to reduce the tritium content in the protium stream that goes either to the waste consolidation system or to the disposal system. In the analysis of the four-column cascade, the contaminated deuterium stream (from the neutral beam injector) was split into two streams--one going to the equilibrator along with the top product stream from column 1 and the other going as a separate feed stream to column 2. Table 12 shows the results of varying the amount of neutral beam injector recycle which goes to the equilibrator. It can be seen that the addition of neutral beam injector deuterium stream to the product stream from column 1 is not required to obtain the desired product compositions.* The desired equilibration among the isotopic species can be achieved in the equilibrator by simple warming of the top product from column 1 from the operating temperatures of 20-25 K to room temperature (300 K) in the presence of a suitable catalyst (e.g., platinum) to speed up the reaction.

Table 12. Cascade Parameter Study--Effect of Varying Amount of Neutral Beam Recycle Going to Equilibrator^a

Case	Amount of Neutral B. Recycle to Equilibrator, mol % of feed to Col. 1	Composition of Product Stream, at. %			
		Isotope	A	B	C
I	1.0	H	0.01	0.04	50.9
		D	44.1	99.9	47.2
		T	55.9	0.06	2.1
II	4.0	H	0.01	0.03	48.8
		D	44.1	99.9	49.2
		T	55.9	0.05	1.92
III	8.0	H	0.01	0.02	42.3
		D	44.1	99.9	56.3
		T	55.9	0.04	1.31

^aComposition of feed to column 1 = 2.1 at. % H, 48.95 at. % D, 48.95 at. % T.
Operating pressures = 200, 167, 133, and 100 kPa for the four columns, respectively.
Number theoretical plates = 75, 30, 30, 30 for the four columns, respectively.
Reflux ratio = 5 for each column.

*Analyses with no NB deuterium going to the equilibrator gave similar product compositions.

V. CONCLUSIONS

It has been shown that a four-column cryogenic distillation cascade system should be effective for the isotope separation and enrichment of spent fuel from a tokamak-type D-T fusion reactor. The system was found capable of producing (1) a tritium-free stream of protium- and deuterium-bearing species for waste disposal, (2) a stream of >98% deuterium for reuse in neutral beam injection, and (3) a protium-free stream containing $T/D > 1.1$ for reuse in cold fuel injection.

A computer program was developed to simulate the effects of varying certain design (e.g., number of theoretical plates) and operating (e.g., pressure, reflux ratio, and feed composition) parameters on the composition of the distillates. It was found that the feed stream may contain as much as 7.5 at. % protium and still meet the system requirements. The effect of operating pressure was found to be small within the range of 100-200 kPa. The results also showed that the requirements are met when there are a total of about 200 theoretical plates, and the first column contains greater than 50 theoretical stages and the other columns contain 30-50 plates each. Finally, it was shown that the recycle deuterium stream from the neutral beam injector need not pass through the chemical equilibrator before distillation; the desired isotopic equilibration can be achieved by simple warming of the product from column 1 to room temperature in the equilibrator in the presence of a suitable catalyst.

Since no exhaustive study was made to assess the effects of varying the design and operating parameters on the three product streams, no single system can yet be described to best meet all the TNS recycle requirements.

The experimental data from the Tritium System Test Assembly (TSTA) at Los Alamos Scientific Laboratory are expected to provide the basis for a more practical assessment of the potential of a multi-column cascade design for isotope separation and enrichment.

ACKNOWLEDGMENTS

The authors express their appreciation to Dr. Victor A. Maroni for helpful and stimulating discussions during the development of the computer program and its application to the enrichment system.

REFERENCES

1. W. M. Stacey, Jr. et al., Tokamak Experimental Reactor Conceptual Design, Argonne National Laboratory Report ANL/CTR-76-3 (August 1976).
2. Experimental Power Reactor Conceptual Design Study, General Atomic Company Report GA-A14000 (July 1976).
3. Oak Ridge Tokamak Experimental Power Reactor Study, Oak Ridge National Laboratory Reports ORNL/TM-5572 through ORNL/TM-5577 (1976).

4. B. Badger et al., UWMAK-III, a Non-Circular Tokamak Power Reactor Design, University of Wisconsin, UWFD-112 (1976).
5. GAC-ANL TNS Scoping Studies, Argonne National Laboratory Report ANL/FPP-77-6, Vol. V (January 1978).
6. F. A. Cafasso et al., Mound Facility and Argonne National Laboratory Joint Proposal for a Tritium Safety System Test Facility, (August 1976); Mound Facility Report MLM-2500 (February 1978).
7. J. L. Anderson and R. H. Sherman, Tritium System Test Assembly Design for Major Device Fabrication Review, Los Alamos Scientific Laboratory Report LA-6855-P (June 1977).
8. Oak Ridge TNS Program: System Description Manual, ORNL Report ORNL/TM-6721 (May 1978).
9. B. Misra and V. A. Maroni, Multicomponent Isotopic Separation and Recirculation Analysis, Argonne National Laboratory Report ANL-76-92 (1977).
10. B. Misra and V. A. Maroni, Isotopic Enrichment of Plasma Exhausts from Controlled Thermonuclear Reactors by Cryogenic Distillation, Nucl. Technol. 35, 40 (1977).
11. J. R. Bartlilt et al., Proc. of the Third Topical Meeting on The Technology of Controlled Nuclear Fusion, May 9-11, 1978, Santa Fe, New Mexico, Vol. 2, p. 778.
12. J. F. Davis et al., Dynamics and Control of a Packed Distillation Column for Isotopic Enrichment of Plasma Exhausts from Controlled Thermonuclear Reactors, accepted for publication, Nuclear Technology.
13. T. M. Flynn et al., Adv. Cryog. Eng. 3, 58 (1960); ibid., 4, 464 (1961).
14. B. S. Johnson and F. Rust, Low Temperature Still for Separation of Hydrogen Isotopes, Savannah River Plant Report DP 732 (October 1962).

APPENDIX

FORTRAN Listings


```

C      MULTISTAGE DISTILLATION CASCADE
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION APH(100), APD(100), APT(100), APHF(3), APDF(3), APTF(3),
1PHITP(100), T(100), TC1(100), TC2(100), TC3(100), TC4(100),
2TC5(100), XF1(6), XF2(6), XF3(6), XF10(6), XF20(6), XF30(6),
3XF40(6), XC(100,6), XC1(100,6), XC2(100,6), XC3(100,6), XC4(100,6)
4,XC5(100,6), Y(1,6), Y1(1,6), Y2(1,6), Y3(1,6), Y4(1,6), Y5(1,6)
      DIMENSION D1X(6), D2X(6), F1X(6), F2X(6), F3X(6), TBX(6), TDX(6),
2RFX(6), WX(6), NPX(6), NF1X(6), NF2X(6), NF3X(6), NSX(6), XMD2(6)
      DIMENSION C1(6), C2(6), C3(6), C4(6), C5(6), CX1(5,6), CX2(5,6),
1CX3(5,6), CX4(5,6), CX5(5,6), PT(5), VT(20), VP(20,6)
      DIMENSION RK(6), XE(6), XF0(6), RK0(6), TITLE(9), TOLX(6)
      COMMON/MISRA1/F3, XD2, XF3, XE, RK, XF0, RK0, NJ, IPRNT
      COMMON/MISRA2/D1, D2, F1, F2, RFX, TB, TD, VO, W, NP, M, INPUT,
1 NF1, NF2, NF3, NC, NS, NTRL, NR, IC2, ITR2
      COMMON/MISRA3/APH, APD, APT, C1, C2, C3, C4, C5, APHY, APDY, APTY,
1PHITP, T, XF1, XF2, XC, Y, TOL
      COMMON/MISRA4/CX1, CX2, CX3, CX4, CX5, PT, VT, VP, NM1, M1, N1,
1NP1, IP, NC1, NR1
      READ 1200, TITLE
      READ 1500, M, NC, NCL, INPUT, IPRNT, KASE, NTRL, ITR2, NPR, IC2
      IF (M.LE.0) GO TO 1100
      READ 1500, NM1, M1, N1, IP, NP1, NC1, NR1, NJ
      READ 1700, XNB, TE, ( RK(I), I = 1, 3 )
      READ 1700, ( PT(L), L = 1, NR1 )
      READ 1700, ( XF1(I), I = 1, NC )
      READ 1700, ( XF2(I), I = 1, NC )
      READ 1700, ( XF3(I), I = 1, NC )
      READ 1700, ( VT(I), I = 1, NP1 )
      DO 10 K = 1, NC
10 READ 1700, ( VP(I,K), I = 1, NP1 )
      DO 20 I = 1, NC1
      READ 1500, NPX(I), NF1X(I), NF2X(I), NF3X(I), NSX(I)
      READ 1700, D1X(I), D2X(I), F1X(I), F2X(I), F3X(I), RFX(I), WX(I),
1TBX(I), TDX(I), XMD2(I), TOLX(I)
20 CONTINUE
      IF ( NCL .GT. 1 ) KASE = 0
      IF ( INPUT .LE. 0 ) GO TO 45
      PRINT 1200, TITLE
      PRINT 1500, M, NC, NCL, INPUT, IPRNT, KASE, NTRL, ITR2, NPR, IC2
      PRINT 1500, NM1, M1, N1, IP, NP1, NC1, NR1, NJ
      PRINT 2000, XNB, TE, ( RK(I), I = 1, 3 )
      PRINT 2000, ( PT(L), L = 1, NR1 )
      PRINT 2100
      PRINT 2000, ( XF1(I), I = 1, NC )
      PRINT 2000, ( XF2(I), I = 1, NC )
      PRINT 2000, ( XF3(I), I = 1, NC )
      DO 30 I = 1, NC1
      PRINT 1950, I
      PRINT 1500, NPX(I), NF1X(I), NF2X(I), NF3X(I), NSX(I)
      PRINT 2000, D1X(I), D2X(I), F1X(I), F2X(I), F3X(I), RFX(I), WX(I),
1TBX(I), TDX(I), XMD2(I), TOLX(I)
30 CONTINUE
      PRINT 2025
      DO 40 I = 1, NP1
40 PRINT 1750, VT(I), ( VP(I,K), K = 1, NC )
45 CONTINUE
      CALL POLYFT
      IF ( IPRNT .LE. 0 ) GO TO 60
      PRINT 2360
      PRINT 2370

```

```

DO 50 L = 1, NR1
DO 50 K = 1, NC
50 PRINT 1775, PT(L), CX1(L,K), CX2(L,K), CX3(L,K), CX4(L,K),
1CX5(L,K)
60 CONTINUE
DO 70 I = 1, NC
XF0(I) = XF1(I)
XF10(I) = XF1(I)
XF20(I) = XF2(I)
XF30(I) = XF3(I)
XF40(I) = XF3(I)
70 CONTINUE
NR = 0
NF0 = 1
IC1 = 0
IC2 = 0
IC3 = 0
IC4 = 0
IC5 = 0
ITR = 1
75 CONTINUE
IF ( KASE .LE. 0 ) GO TO 80
READ 1200, TITLE
READ 1500, M, NC, NCL, INPUT, IPRNT, KASE, NTRL, ITP2, NPR, IC2
IF ( M .LE. 0 ) GO TO 1100
READ 1500, NP, NF1, NF2, NF3, NS
READ 1700, D1, D2, F1, F2, F3, RFX, W, TB, TD, XD2, TOL
READ 1700, ( XF1(I), I = 1, NC )
READ 1700, ( XF2(I), I = 1, NC )
READ 1700, ( XF3(I), I = 1, NC )
PRINT 1300, TITLE
PRINT 1500, NP, NF1, NF2, NF3, NS
PRINT 1500, M, NC, NCL, INPUT, IPRNT, KASE, NTRL, ITR2, NPR, IC2
PRINT 2000, D1, D2, F1, F2, F3, RFX, W, TB, TD, XD2, TOL
PRINT 2100
PRINT 2000, ( XF1(I), I = 1, NC )
PRINT 2000, ( XF2(I), I = 1, NC )
PRINT 2000, ( XF3(I), I = 1, NC )
ITR = 1
VO = (1.0D00 + RFX ) * D1
PR = PT(NPR)
NPRO = NPR
KASE = 1
80 CONTINUE
GO TO 110
100 CONTINUE
NR = 0
ITR = ITR + 1
IF ( ITR .GT. NTRL ) KASE = 1
IF ( ITR .GE. 2 ) IPRNT = 0
IF ( ITR .GE. 2 ) IC2 = 1
IF ( ITR .GT. NTRL ) GO TO 75
110 CONTINUE
NR = NR + 1
NPR = NR
IF ( NR .GT. NCL ) GO TO 100
IF ( NCL .EQ. 1 ) NPF = NPRO
DO 115 L = NPR, NPR
DO 115 K = 1, NC
C1(K) = CX1(L,K)
C2(K) = CX2(L,K)
C3(K) = CX3(L,K)

```

```

      C4(K) = CX4(L,K)
      C5(K) = CX5(L,K)
115  CONTINUE
      IF ( NCL .EQ. 1 ) GO TO 120
      NP = NPY(NR)
      NP1 = NP1X(NR)
      NP2 = NP2X(NR)
      NP3 = NP3X(NR)
      NS = NSX(NR)
      D1 = D1X(NR)
      D2 = D2X(NR)
      F1 = F1X(NR)
      F2 = F2X(NR)
      F3 = F3X(NR)
      PR = PT(NR)
      RFX = RFX(NR)
      TD = TDX(NR)
      TE = TBX(NR)
      TOL = TOLX(NR)
      VO = ( 1.0D00 + RFX ) * D1
      W = WX(NR)
      XD2 = XMD2(NR)
120  CONTINUE
      IF ( IPRNT .EQ. 0 ) GO TO 125
      PRINT 2200, NR, PR
      PRINT 2300, (( C1(K), C2(K), C3(K), C4(K), C5(K)), K = 1, NC )
125  CONTINUE
      GO TO ( 130, 190, 240, 280, 360 ), NR
130  CONTINUE
      IF ( NCL .EQ. 1 ) GO TO 165
      IF ( IC1 .EQ. 0 ) GO TO 145
      DO 140 I = 1, NC
140  XP3( I ) = XC4( NPX(4), I )
145  CONTINUE
      DO 160 I = 1, NC
160  XF2(I) = XF20(I)
165  CONTINUE
      IF ( IC1 .EQ. 0 ) GO TO 175
      DO 170 J = 1, NP
170  T(J) = TC1(J)
175  CONTINUE
      IC1 = 1
      CALL MISRA
      IF ( NCL .EQ. 1 ) IC2 = 1
      GO TO 500
190  CONTINUE
      DO 200 I = 1, NC
      XF2(I) = XF0(I)
200  XF3(I) = Y1(1,I)
      IF ( IC2 .GT. 0 ) GO TO 215
      DO 210 J = 1, NP
      TC2(J) = TC1(J)
      TC3(J) = TC1(J)
      TC4(J) = TC1(J)
210  TC5(J) = TC1(J)
215  CONTINUE
      IF ( IC2 .EQ. 0 ) GO TO 222
      DO 220 I = 1, NC
220  XF2(I) = XC3( NPX(3), I )
222  CONTINUE
      DO 225 J = 1, NP
225  T(J) = TC2(J)

```

```

      CALL EQLBTR
      PRINT 2325
      PRINT 2350, TR, XD2
      PRINT 2000, ( XR(I), I = 1, NC )
      PRINT 2000, ( RK0(I), I = 1, NC )
      DO 230 I = 1, NC
230  IF ( XF3(I) .LT. 0.0D00 ) XF3(I) = 1.0D-06
      F30 = F3
      F3 = F30 + XNB-XD2
      DO 235 I = 1, NC
235  XF3(I) = F30 * XF3(I) / F3
      XF3(4) = (F30 * XF3(4) + XNB - XD2) / F3
      D1 = D1 + XNF
      CALL MISRA
      GO TO 500
240  CONTINUE
      DO 250 I = 1, NC
250  XF3(I) = Y2(1,I)
      IC3 = 1
      DO 260 J = 1, NP
260  T(J) = TC3(J)
      CALL MISRA
      GO TO 500
280  CONTINUE
      DO 290 I = 1, NC
290  XF3(I) = XC2( NFX(2), I )
      DC 350 J = 1, NP
350  T(J) = TC4(J)
      IC4 = 1
      CALL MISRA
      GO TO 500
360  CONTINUE
      DO 370 I = 1, NC
370  XF3(I) = Y4(1,I)
      IF ( IC5 .EQ. 0 ) GO TO 410
      DO 400 J = 1, NP
400  T(J) = TC5(J)
410  CONTINUE
      IC5 = 1
      CALL MISRA
500  CONTINUE
      APHF(1) = (XF1(1) + 0.5 * XF1(2) + 0.5 * XF1(3)) * 1.0D02
      APDF(1) = (0.5 * XF1(2) + XF1(4) + 0.5 * XF1(5)) * 1.0D02
      APTF(1) = (0.5 * XF1(3) + 0.5 * XF1(5) + XF1(6)) * 1.0D02
      APHF(2) = (XF2(1) + 0.5 * XF2(2) + 0.5 * XF2(3)) * 1.0D02
      APDF(2) = (0.5 * XF2(2) + XF2(4) + 0.5 * XF2(5)) * 1.0D02
      APTF(2) = (0.5 * XF2(3) + 0.5 * XF2(5) + XF2(6)) * 1.0D02
      APHF(3) = (XF3(1) + 0.5 * XF3(2) + 0.5 * XF3(3)) * 1.0D02
      APDF(3) = (0.5 * XF3(2) + XF3(4) + 0.5 * XF3(5)) * 1.0D02
      APTF(3) = (0.5 * XF3(3) + 0.5 * XF3(5) + XF3(6)) * 1.0D02
      PRINT 4500
      PRINT 4600, PR, ITR, NR
      PRINT 4700, NP, BFX
      PRINT 4800, NF1, NF2, NF3
      PRINT 4900, F1, F2, F3, D1, W
      PRINT 5000
      IF ( F1 .NE. 0.0D00 ) PRINT 2050, ( XF1(I), I = 1, NC ), APHF(1),
1APDF(1), APTF(1)
      IF ( F2 .NE. 0.0D00 ) PRINT 2050, ( XF2(I), I = 1, NC ), APHF(2),
1APDF(2), APTF(2)
      IF ( F3 .NE. 0.0D00 ) PRINT 2050, ( XF3(I), I = 1, NC ), APHF(3),
1APDF(3), APTF(3)

```

```

PRINT 5100
PRINT 2000, ( PHITP(J), J = 1, NP )
PRINT 2600
NP10 = NP - 10
IF ( NP .LE. 30 ) GO TO 510
PRINT 2000, ( T(J), J = 1, 15 )
PRINT 2000, ( T(J), J = NP10, NP )
GO TO 515
510 PRINT 2000, ( T(J), J = 1, NP )
515 CONTINUE
PRINT 5200
PRINT 5300, NFO, ( Y(NFO,I), I = 1, NC ), APHY, APDY, APTY
IF ( NP .LE. 30 ) GO TO 550
DO 520 J = 2, 15
520 PRINT 5300, J, ( XC(J,I), I = 1, NC ), APH(J), APD(J), APT(J)
DO 530 J = NP10, NP
530 PRINT 5300, J, ( XC(J,I), I = 1, NC ), APH(J), APD(J), APT(J)
GO TO 765
550 CONTINUE
DO 760 J = 2, NP
760 PRINT 5300, J, ( XC(J,I), I = 1, NC ), APH(J), APD(J), APT(J)
765 CONTINUE
GO TO ( 770, 800, 830, 860, 890 ), NR
770 DO 780 J = 1, NP
DO 780 I = 1, NC
780 XC1(J,I) = XC(J,I)
DO 790 J = 1, NP
790 TC1(J) = T(J)
DO 795 I = 1, NC
795 Y1(1,I) = Y(1,I)
GO TO 110
800 DO 810 J = 1, NP
DO 810 I = 1, NC
810 XC2(J,I) = XC(J,I)
DO 820 J = 1, NP
820 TC2(J) = T(J)
DO 825 I = 1, NC
825 Y2(1,I) = Y(1,I)
GO TO 110
830 DO 840 J = 1, NP
DO 840 I = 1, NC
840 XC3(J,I) = XC(J,I)
DO 850 J = 1, NP
850 TC3(J) = T(J)
DO 855 I = 1, NC
855 Y3(1,I) = Y(1,I)
GO TO 110
860 DO 870 J = 1, NP
DO 870 I = 1, NC
870 XC4(J,I) = XC(J,I)
DO 880 J = 1, NP
880 TC4(J) = T(J)
DO 885 I = 1, NC
885 Y4(1,I) = Y(1,I)
GO TO 110
890 DO 900 J = 1, NP
DO 900 I = 1, NC
900 XC5(J,I) = XC(J,I)
DO 910 J = 1, NP
910 TC5(J) = T(J)
DO 915 I = 1, NC
915 Y5(1,I) = Y(1,I)

```

```

      GO TO 110
1100 STOP
1200 FORMAT ( 9A8 )
1300 FORMAT ( '1', 9A8 )
1500 FORMAT ( 11I6 )
1700 FORMAT ( 6D12.6 )
1750 FORMAT ( 1P1D15.3, 1P6D15.6 )
1775 FORMAT ( 1P1D15.3, 1P5D15.6 )
1950 FORMAT ( '0', ' OPERATING PARAMETERS FOR COLUMN NO.=', 1I3 )
2000 FORMAT ( 1P6D15.6 )
2025 FORMAT ( '1', T35, ' TEMPERATURE/VAPOR PRESSURE DATA' )
2050 FORMAT ( 1P6D15.6, 1P3D12.3 )
2100 FORMAT ( '0', ' FEED COMPOSITION' )
2200 FORMAT ( '1', ' FITTING COEFFICIENTS FOR COLUMN NO.=', 1I3, ' FOR
1 PR=', 1P1D12.3, 'TORR' )
2300 FORMAT ( 1P5D15.6 )
2325 FORMAT ( '1', ' LIQUID COMPOSITIONS AND EQUILIBRIUM CONSTANTS FROM
1EQLBTH' )
2350 FORMAT ( '0', ' EQUILIBRATION AT TE=', 1P1D11.2, ' DEG KELVIN',
1' XD2=', 1P1D12.3, ' MOLES' )
2360 FORMAT ( '0', ' EQUILIBRIUM CONSTANTS FROM SUBROUTINE POLYPT' )
2370 FORMAT ( '0', T10, 'PT', T23, 'CX1', T38, 'CX2', T53, 'CX3', T68,
1' CX4', T83, 'CX5' )
2600 FORMAT ( '0', ' EQUILIBRIUM STAGE TEMPERATURES, DEG.K..(FROM L TO
1R IN ASCENDING ORDER OF PLATE NUMBER ) ' )
4500 FORMAT ( '1', ' CRYOGENIC DISTILLATION OF HYDROGEN ISOTOPES FOR DFM
1E/ISTA,....B. MISRA....., JUNE 1977 ' )
4600 FORMAT ( '0', ' ANALYTICAL RESULTS AT PT=', 1P1D12.3, ' TORR', '
1AFTER', 1I3, ' ITERATIONS', ' FOR COLUMN NO:', 1I3 )
4700 FORMAT ( ' NUMBER OF THEORETICAL STAGES:', 1I3, ' REFLUX RATIO
1L/D1=', 1P1D12.3 )
4800 FORMAT ( ' FIRST FEED PLATE LOCATION:', 1I3, ' 2ND FP LOCATION:',
1I3, ' 3RD FP LOCATION=', 1I3 )
4900 FORMAT ( ' FEED RATES:', 1P3D11.2, ' DISTILLATE:', 1P1D11.2, ' B
1OTTOMS:', 1P1D10.2 )
5000 FORMAT ( '0', ' FEED COMP.N-H2', T24, 'HD', T40, 'HT', T53, 'N-D2', T68, 'D
1T', T83, 'N-T2', T95, 'APH', T107, 'APD', T119, 'APT' )
5100 FORMAT ( '0', ' SUMMATION OF LIQUID MOLE FRACTIONS.....(FROM L TO
1R IN ASCENDING ORDER OF PLATE NUMBER ) ' )
5200 FORMAT ( '0', ' PLATE NO.', T15, 'N-H2', T29, 'HD', T44, 'HT', T59, 'N-D2',
1T75, 'DT', T89, 'N-T2', T102, 'APH', T114, 'APD', T126, 'APT' )
5300 FORMAT ( 1I6, 1P6D15.6, 1P3D12.3 )
      END
C SUBROUTINE MISRA FOR SIMULATION OF MULTICOMPONENT DISTILLATION
SUBROUTINE MISRA
  IMPLICIT REAL*8 (A-H,O-Z)
  DIMENSION A(100,100), B(100,6), APH(100), APD(100), APT(100),
1APHF(3), APDF(3), APTF(3), C1(6), C2(6), C3(6), C4(6), C5(6),
2DPHTP(100), PHITP(100), T(100), TP(100), V(100), XF1(6), XF2(6),
3XF3(6), X(100,6), XC(100,6), XK(100,6), Y(1,6)
  DIMENSION RK(6), KE(6), XF0(6), RK0(6)
  COMMON/MISRA2/D1, D2, F1, F2, BFX, TB, TD, VO, W, NP, N, INPUT,
1 NF1, NF2, NF3, NC, NS, NTRL, NR, IC2, ITR2
  COMMON/MISRA1/F3, XD2, XF3, KE, RK, XF0, RK0, NJ, IPRNT
  COMMON/MISRA3/APH, APD, APT, C1, C2, C3, C4, C5, APHY, APDY, APTY,
1PHITP, T, XF1, XF2, XC, Y, TOL
  COMMON /F402/PIVOT(100), INDEX(100)
  EQUIVALENCE ( E(1,1), X(1,1) )
  ITR1 = 0
  LO = NS - 1
  NFO = 1
  L1 = NS + 1

```

```

L2 = NF1 - 1
L3 = NF1 + 1
L4 = NF2 - 1
L5 = NF2 + 1
L6 = NF3 - 1
L7 = NF3 + 1
L8 = NP - 1
DO 50 J = 1, NP
50 V ( J ) = VO
IF ( IC2 .GT. 0 ) GO TO 60
DO 55 J = 1, NP
XJ = J
XNJ = NP
DT = ( TB - TD ) / XNJ
55 T(J) = TD + DT * XJ
60 CONTINUE
80 CONTINUE
ITB1 = ITR1 + 1
DO 90 J = 1, NP
DO 90 I = 1, NC
XK(J,I) = C1(I) + C2(I) * T(J) + C3(I) * T(J) ** (2.0D00) +
1C4(I) * T(J) ** (3.0D00) + C5(I) * T(J) ** (4.0D00)
90 CONTINUE
DO 400 I = 1, NC
DO 110 J = 1, NP
DO 110 K = 1, NP
110 A(J,K) = 0.0D00
DO 120 K = 1, M
DO 120 J = 1, NP
120 B(J,K) = 0.0D00
DO 130 J = 1, L8
K = J
130 A(J,K+1) = V(J+1) * XK(J+1,I)
DO 140 J = 1, NFO
K = J
140 A(J,K) = - ( V(J+1) + ( XK(J,I) - 1.0D00 ) * D1 )
DO 150 J = 2, L0
K = J
A(J,K-1) = V(J) - D1
150 A(J,K) = - ( V(J) * XK(J,I) + V(J+1) - D1 )
DO 155 J = NS, NS
K = J
A(J,K-1) = V(J) - D1
155 A(J,K) = - ( V(J) * XK(J,I) + V(J+1) - D1 - D2 )
DO 160 J = L1, L2
K = J
A(J,K-1) = V(J) - D1 - D2
160 A(J,K) = - ( V(J+1) - D1 - D2 + V(J) * XK(J,I) )
DO 170 J = NF1, NF1
K = J
A(J,K-1) = V(J) - D1 - D2
170 A(J,K) = - ( V(J+1) - D1 - D2 + F1 + V(J) * XK(J,I) )
DO 180 J = L3, L4
K = J
A(J,K-1) = V(J-1) - D1 - D2 + F1
180 A(J,K) = - ( V(J+1) - D1 - D2 + F1 + V(J) * XK(J,I) )
DO 190 J = NF2, NF2
K = J
A(J,K-1) = V(J) - D1 - D2 + F1
190 A(J,K) = - ( V(J+1) - D1 - D2 + F1 + F2 + V(J) * XK(J,I) )
DO 200 J = L5, L6
K = J

```

```

      A(J,K-1) = V(J) - D1 - D2 + F1 + F2
200 A(J,K) = - ( V(J+1) - D1 - D2 + F1 + F2 + V(J) * XK(J,I) )
      DO 210 J = NF3, NF3
      K = J
      A(J,K-1) = V(J) - D1 - D2 + F1 + F2
210 A(J,K) = - ( V(J) * XK(J,I) + V(J+1) + W )
      DO 220 J = L7, L8
      K = J
      A(J,K-1) = V(J) + W
220 A(J,K) = - ( V(J) * XK(J,I) + V(J+1) + W )
      DO 230 J = NP, NP
      K = J
      A(J,K) = - ( W + V(J) * XK(J,I) )
230 A(J,K-1) = W + V(J)
      DO 240 K = 1, M
      B(NF1,K) = - F1 * XF1(I)
      B(NF2,K) = - F2 * XF2(I)
      B(NF3,K) = - F3 * XF3(I)
240 CONTINUE
      CALL MATINV(A,NP,F,M,DETERM,100)
      DO 300 J = 1, NP
      DO 300 K = 1, M
300 XC(J,I) = X(J,K)
400 CONTINUE
      DO 420 J = 1, NP
420 TP(J) = T(J)
      DO 500 J = 1, NP
      SUM = 0.0D00
      SUMX = 0.0D00
      SUMXC = 0.0D00
      DO 430 I = 1, NC
      IF ( XC(J,I) .GT. 0.0D00 ) GO TO 430
      XC(J,I) = 1.0D-10
      IX = 1
430 SUMXC = SUMXC + XC(J,I)
      DO 440 I = 1, NC
440 XC(J,I) = XC(J,I) / SUMXC
      DO 460 I = 1, NC
      SUMX = SUMX + XF(I) * XC(J,I)
460 PHITP(J) = SUMX
      IF ( IX .GE. 1 ) GO TO 470
      IF ( DABS(PHITP(J) - 1.0D00) .LE. TOL ) GO TO 490
470 CONTINUE
      DO 480 I = 1, NC
      SUM = SUM + XC(J,I) * ( C2(I) + 2.0D00 * C3(I) * TP(J) + 3.0D00 *
1C4(I) * TP(J) ** (2.0D00) + 4.0D00 * C5(I) * TP(J) ** (3.0D00) )
      DPHITP(J) = SUM
      T(J) = TP(J) + ( 1.0D00 - PHITP(J) ) / DPHITP(J)
      IF ( T(J) .LT. 20.0D00 ) T(J) = 20.0D00
      IF ( T(J) .GT. 30.0D00 ) T(J) = 30.0D00
480 CONTINUE
      IX = 0
490 CONTINUE
      APH(J) = ( XC(J,1) + XC(J,2) * 0.50 + XC(J,3) * 0.50 ) / PHITP(J) *
11.0D02
      APD(J) = ( XC(J,2) * 0.50 + XC(J,4) + XC(J,5) * 0.50 ) / PHITP(J) *
11.0D02
      APT(J) = ( XC(J,3) * 0.50 + XC(J,5) * 0.50 + XC(J,6) ) / PHITP(J) *
11.0D02
500 CONTINUE
      IF ( ITR1 .LT. ITR2 ) GO TO 80
      DO 510 I = 1, NC

```



```

      Y(NF0,I) = XC(NF0,I) * XK(NF0,I)
      XC(NF0,I) = Y(NF0,I)
510  CONTINUE
      APHY = (Y(NF0,1) + 0.50D00 * Y(NF0,2) + 0.50D00 * Y(NF0,3)) * 100.0
      APDY = (0.50D00 * Y(NF0,2) + Y(NF0,4) + 0.50D00 * Y(NF0,5)) * 100.0
      APTY = (0.50D00 * Y(NF0,3) + 0.50D00 * Y(NF0,5) + Y(NF0,6)) * 100.0
600  RETURN
      END
C    SUBROUTINE POLYFT DETERMINES EQUILIBRIUM CONSTANTS BASED ON L.SQ
      SUBROUTINE POLYFT
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A1(20,6), B1(20,1), CX1(5,6), CX2(5,6), CX3(5,6),
      1CX4(5,6), CX5(5,6), DC(20,6), PT(5), RV1(5), VT(20), VP(20,6),
      2W1(5), XK(20,6), XKC(20,6), X1(5,1)
      COMMON/MISRA4/CX1, CX2, CX3, CX4, CX5, PT, VT, VP, NM1, N1, N1,
      1NP1, IP, NC1, NR1
      THRESH = 1.0D-10
      DO 180 L = 1, NR1
      DO 180 K = 1, NC1
      DO 20 I = 1, NP1
      DO 20 J = 1, IP
      XK(I,J) = VP(I,K) / PT(L)
      B1(I,J) = XK(I,J)
20  CONTINUE
      DO 25 I = 1, NP1
      DO 25 J = 1, IP
      DC(I,K) = XK(I,J)
25  CONTINUE
      DO 30 I = 1, N1
      DO 30 J = 1, N1
      XJ = J
      A1(I,J) = VT(I) ** ( XJ - 1.0D00 )
30  CONTINUE
      CALL MINFIT(NM1, N1, N1, A1, W1, IP, B1, IERR, RV1)
      DO 110 J = 1, IP
      DO 110 I = 1, N1
110  X1(I,J) = 0.0D00
      DO 130 K1 = 1, N1
      IF ( W1(K1) .LT. THRESH ) GO TO 130
      DO 120 I = 1, N1
      DO 120 J = 1, IP
120  X1(I,J) = X1(I,J) + A1(I,K1) * B1(K1,J) / W1(K1)
130  CONTINUE
      CX1(L,K) = X1(1,1)
      CX2(L,K) = X1(2,1)
      CX3(L,K) = X1(3,1)
      CX4(L,K) = X1(4,1)
      CX5(L,K) = X1(5,1)
180  CONTINUE
      RETURN
      END
C    SUBROUTINE EQLETB CALCULATES EQLEB. MOLE FRACTIONS
      SUBROUTINE EQLETB
      IMPLICIT REAL*8 (A-H,O-Z)
      EXTERNAL AUX
      DIMENSION RK(6), XF3(6), YE(6), XFO(6), I(3), WA(14), RK0(6)
      COMMON/MISRA1/F3, XD2, XF3, YE, RK, XFO, RK0, NJ,IPRNT
      N = 3
      ITHAX = 100
      NSIG = 6
      EPS = 1.0D-06
      KERR = 0

```

```

      ITR = 0
      DO 400 J = 1, NJ
      XJ = J
      H2 = XF3(1) * F3
      HD = XF3(2) * F3
      HT = XF3(3) * F3
      D2 = XF3(4) * F3 + XD2
      DT = XF3(5) * F3
      T2 = XF3(6) * F3
      SUMO = H2 + HD + HT + D2 + DT + T2
      IF ( ITR .GE. 1 ) GO TO 30
      X(1) = 0.50D00 * HT
      X(2) = 0.50D00 * HD
      X(3) = 0.50D00 * DT
30    CONTINUE
      ITR = 1
      CALL ZSYSTEM(AUX, EPS, NSIG, N, X, ITMAX, WA, PAR, IER)
      ECH2 = H2 + 0.50D00 * (HT + HD) - X(1) - X(2)
      ECD2 = D2 + 0.50D00 * (HD + DT) - X(2) - X(3)
      ECT2 = T2 + 0.50D00 * (HT + DT) - X(1) - X(3)
      ECHT = 2.0D00 * X(1)
      ECHD = 2.0D00 * X(2)
      ECDT = 2.0D00 * X(3)
      SUME = ECH2 + ECD2 + ECT2 + ECHD + ECHT + ECDT
      XE(1) = ECH2 / SUME
      XE(2) = ECHD / SUME
      XE(3) = ECHT / SUME
      XE(4) = ECD2 / SUME
      XE(5) = ECDT / SUME
      XE(6) = ECT2 / SUME
      RK0(1) = ECHT**2 / ECH2 / ECT2
      RK0(2) = ECHD**2 / ECD2 / ECH2
      RK0(3) = ECDT**2 / ECD2 / ECT2
      RK0(4) = ECHT * ECDT / ECT2 / ECHD
      RK0(5) = ECHD * ECHT / ECH2 / ECDT
      RK0(6) = ECHD * ECDT / ECD2 / ECHT
      DO 50 I = 1, 3
50    IF ( X(I) .LT. 0.0D00 ) KER = 1
      IF ( KER .EQ. 1 ) GO TO 210
      DO 100 I = 1, 6
100   XF3(I) = XE(I)
      F3 = F3 + XD2
400   CONTINUE
210   RETURN
      END
C    FUNCTION AUX IS AN AUXILIARY FUNCTION USED IN EQLBTR
      FUNCTION AUX(X, K, PAR)
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION X(1)
      DIMENSION RK(6), XF3(6), XE(6), XF0(6)
      COMMON/MISRA1/F3, XD2, XF3, XE, RK, XF0, NJ, IPRNT
      H2 = XF3(1) * F3
      HD = XF3(2) * F3
      HT = XF3(3) * F3
      D2 = XF3(4) * F3 + XD2
      DT = XF3(5) * F3
      T2 = XF3(6) * F3
      ECH2 = H2 + 0.50D00 * (HT + HD) - X(1) - X(2)
      ECD2 = D2 + 0.50D00 * (HD + DT) - X(2) - X(3)
      ECT2 = T2 + 0.50D00 * (HT + DT) - X(1) - X(3)
      ECHT = 2.0D00 * X(1)
      ECHD = 2.0D00 * X(2)

```

```

      ECDT = 2.0D00 * X(3)
      GO TO ( 10, 20, 30 ), K
10    AUX = (2.0D00 * X(1) )**2 - BK(1) * ( (FCH2) * (ECT2) )
      RETURN
20    AUX = (2.0D00 * X(2) )**2 - BK(2) * ( (FCH2) * (ECD2) )
      RETURN
30    AUX = (2.0D00 * X(3) )**2 - BK(3) * ( (ECD2) * (ECT2) )
      RETURN
      END

```

Distribution for ANL-78-96Internal:

M. Abdou	V. A. Maroni	D. L. Smith
C. C. Baker	W. E. Massey	H. C. Stevens
L. Burris	A. Melton	D. Webster
F. A. Cafasso	B. Misra (50)	A. B. Krisciunas
R. G. Clemmer	E. G. Pewitt	ANL Contract Copy
P. A. Finn	P. R. Raptis	ANL Libraries (5)
G. M. Kesser		TIS Files (6)

External:

DOE-TIC, for distribution per UC-20d (138)
 Manager, Chicago Operations and Regional Office, DOE
 Chief, Office of Patent Counsel, DOE-CORO
 President, Argonne Universities Association
 Chemical Engineering Division Review Committee:

- C. B. Alcock, U. Toronto
- R. C. Axtmann, Princeton U.
- J. T. Banchemo, U. Notre Dame
- T. Cole, Ford Motor Co.
- P. W. Gilles, U. Kansas
- R. J. Newman, Warren, N. J.
- H. Perry, Resources for the Future, Washington
- G. M. Rosenblatt, Pennsylvania State U.
- W. L. Worrell, U. Pennsylvania
- J. L. Anderson, Los Alamos Scientific Lab.
- F. E. Coffman, Office of Fusion Energy, USDOE
- J. F. Davis, Northwestern U.
- E. J. Hennelly, Savannah River Lab.
- R. G. Hickman, Lawrence Livermore Lab.
- E. F. Johnson, Princeton U.
- J. Powell, Brookhaven National Lab.
- D. Steiner, Oak Ridge National Lab.
- W. F. Vogelsang, U. Wisconsin, Madison
- J. S. Watson, Oak Ridge National Lab.
- L. J. Wittenberg, Mound Lab.