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STUDY ON COMPUTER-AIDED SIMULATION PROCEDURE FOR MULTICOMPONENT SEPARATING CASCADE

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STUDY ON COMPUTER-AIDED SIMULATION PROCEDURE FOR MULTICOMPONENT SEPARATING CASCADE

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The present report reviews the author's study on the computer-aided simulation procedure for a multicomponent separating cascade. As a conclusion, two very powerful simulation procedures have been developed for cascades composed of separating elements whose separation factors are very large. They are applicable in cases where interstage flow rates are input variables for the calculation and stage separation factors are given either as constants or as functions of compositions of the up and down streams.

As an application of the new procedure, a computer-aided simulation study has been performed for hydrogen isotope separating cascades by porous membrane method. A cascade system configuration is developed and pertinent design specifications are determined in an example case of the feed conditions and separation requirements.

KEYWORDS : Multicomponent Separation, Cascade, Separation Factors, Interstage Flow Rates, Isotope Separation, Hydrogen Isotopes, Porous Membrane Method

多成分分離カスケードのコンピューターシミュレーションに関する研究

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（１９８２年１１月１５日受理）

本報は，多成分分離カスケードのコンピューターシミュレーションに関する著者の現在までの研究成果を系統的に整理したものである。１つの結論として，分離係数の大きい場合にでも適用できる非常に強力なシミュレーション手法が開発されている。その手法は，段間流量及び段分離係数（上昇流と下降流の組成の関数であってもよい）が計算の入力となっている場合に有効である。

シミュレーション手法の適用例として，多孔質隔膜法による水素同位体分離カスケードシステムの定常シミュレーションが行われている。フィードの条件及び希望出力条件を例として与え，システムのシミュレーションを行い，システム構成及び設計・操作変数の値の決定がなされている。

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1. Introduction

The cascade theories had been being developed mainly for uranium enrichment. There are two great advantages inherent in uranium enrichment : only two components are considered, and the separation factors are very close to unity. Because of these advantages, a number of simplifying approximations were acceptable and the analytical methods for uranium enriching cascades have already been completed by several workers.[1] In some situations, consideration of three components is needed (e.g. $^{235}UF_6$, $^{236}UF_6$, and $^{238}UF_6$), but assumption of very small separation factors close to unity is still applicable. Theories of multicomponent separating cascades were first developed by de la Garza et al.[2][3] on this assumption.

In recent years, hydrogen isotope separation seems a major subject in isotope separation technology due to the progress of nuclear fusion research and development. In this case, multicomponents (i.e. the three isotopic elements or six molecular species) must be treated, and the separation factors are very large. Yamamoto et al.[4] developed an analytical method which allows us to calculate the interstage flow rates and concentration of each component as output information from heads and tails separation factors. His method is applicable to cases of large separation factors. However, if the cut of mixture of each stage is prescribed and required to be independent of concentration, his method cannot directly be used any longer.

The most significant purpose of the present study is to develop a computer-aided simulation procedure in cases where

the cut of mixture of each stage is prescribed and required to be independent of concentration and as a result the interstage flow rates are input variables for the calculation, and the stage separation factors are given and very large.

A simulation model is first developed, and then it is improved to decrease the number of the independent variables for the Newton-Raphson iterative method. If the separation factors are independent of concentrations of up and down streams, the model can further be improved by decreasing the number of the independent variables. A total of three models are described and discussed, and an interesting conclusion is drawn by numerical experiments.

In Section 3, a computer simulation study is carried out for a hydrogen isotope separation system by porous membrane method, by using the third model. No study on hydrogen isotope separation by porous membrane method has been reported yet, so no information is available concerning applicability of this method, system configuration, separation performance expected, and system scale. Hence, this study is expected to present much new information.

2. Computer-Aided Simulation Procedure for Multicomponent Separating Cascade

2.1 Simulation Model I [5]

The simulation procedure developed here is based on a linearization of the model equations. This idea is similar to that reported by Naphtali and Sandholm [6] for multicomponent distillation calculations though the model equations are different from those of cascade calculations of our interest in the present study.

The model cascade for computer simulation is shown in Fig. 1. It is assumed that all the interstage flows, L_j's, L'_j's and L''_j's are initially calculated and used as input variables. The model equations are derived from the requirements for conservation of material and for satisfaction of relationship between concentrations of up and down streams.

The component material balances are expressed by

$$L_j x_{i,j} = L'_j x'_{i,j} + L''_j x''_{i,j} \quad , \quad (i = 1, \ldots, m \; ; \; j = 1, \ldots, N) \quad , \tag{1}$$

$$\left.\begin{aligned} L_1 x_{i,1} &= L''_2 x''_{i,2} + r_W L''_1 x''_{i,1} \\ L_j x_{i,j} &= L''_{j+1} x''_{i,j+1} + L'_{j-1} x'_{i,j-1} + P_j z_{i,j} - U_j x_{i,j} \\ L_N x_{i,N} &= L'_{N-1} x'_{i,N-1} + r_P L'_N x'_{i,N} \\ & \quad (i = 1, \ldots, m \; ; \; j = 2, \ldots, N-1) \end{aligned}\right\} \quad . \tag{2}$$

The separation factors are defined with respect to an arbitrary key component —— here, the n-th component is chosen —— by

$$\alpha_{i,j} = (x'_{i,j}/x'_{n,j})/(x''_{i,j}/x''_{n,j}) \quad , \tag{3}$$

$$(i \neq n \ ; \ j = 1, \ \ldots, \ N) \ .$$

It is obvious that the following equations must be satisfied :

$$\sum_{i=1}^{m} x_{i,j} = \sum_{i=1}^{m} x'_{i,j} = \sum_{i=1}^{m} x''_{i,j} = 1 \quad , \tag{4}$$

$$(j = 1, \ \ldots, \ N) \ .$$

The simulation can be performed by finding out rigorous solutions of all the basic equations.

In order to calculate the composition profile from the input variables (the interstage flow rates, feed conditions, number of total stages, flow rates of sidestreams, and separation factors), the 3mN variables, $x_{i,j}$'s, $x'_{i,j}$'s, and $x''_{i,j}$'s, are chosen as the independent variables, and the following 3mN functions to be zeroed are defined :

$$f_{i,j} = x_{i,j} - L'_j x'_{i,j}/L_j - L''_j x''_{i,j}/L_j = 0 \quad , \tag{5}$$

$$(i = 1, \ \ldots, \ m \ ; \ j = 1, \ \ldots, \ N),$$

$$\left.\begin{aligned} g_{i,1} &= x_{i,1} - L''_2 x''_{i,2}/L_1 - r_W L''_1 x''_{i,1}/L_1 = 0 \\ g_{i,j} &= x_{i,j} - L''_{j+1} x''_{i,j+1}/L_j - L'_{j-1} x'_{i,j-1}/L_j \\ &\quad - F_j z_{i,j}/L_j + U_j x_{i,j}/L_j = 0 \\ g_{i,N} &= x_{i,N} - L'_{N-1} x'_{i,N-1}/L_N - r_P L'_N x'_{i,N}/L_N = 0 \quad , \\ &(i = 1, \ \ldots, \ m \ ; \ j = 2, \ \ldots, \ N-1) \end{aligned}\right\} \ , \tag{6}$$

$$h_{i,j} = \alpha_{i,j} x'_{n,j} x''_{i,j} - x'_{i,j} x''_{n,j} = 0 \quad ,$$

$$h_{n,j} = \sum_{k=1}^{m} x'_{k,j} - \sum_{k=1}^{m} x''_{k,j} = 0 \ , \ (i \neq n \ ; \ j = 1, \ \ldots, \ N) . \tag{7}$$

The following vectors of order 3m are then defined :

$$\vec{x}_j = \begin{bmatrix} x_{1,j} \\ \vdots \\ x_{m,j} \\ x'_{1,j} \\ \vdots \\ x'_{m,j} \\ x''_{1,j} \\ \vdots \\ x''_{m,j} \end{bmatrix} , \qquad \vec{f}_j = \begin{bmatrix} f_{1,j} \\ \vdots \\ f_{m,j} \\ g_{1,j} \\ \vdots \\ g_{m,j} \\ h_{1,j} \\ \vdots \\ h_{m,j} \end{bmatrix} ,$$

$$(j = 1, \ldots, N) . \qquad (8)$$

In the above difinition, $\vec{x}_j$ is the vector of variables on the j'th stage and $\vec{f}_j$ is the vector of functions on that stage.

The simulation can be performed by solving the following 3mN-variable nonlinear simultaneous equations by use of the Newton-Raphson iterative method :

$$\left.\begin{aligned} \vec{f}_1 (\vec{x}_1^{\,t}, \ldots, \vec{x}_N^{\,t}) &= \vec{0} \\ &\vdots \\ \vec{f}_N (\vec{x}_1^{\,t}, \ldots, \vec{x}_N^{\,t}) &= \vec{0} \end{aligned}\right\} . \qquad (9)$$

The Jacobian matrix, $\overline{G}$, is given by

$$\overline{G} = \begin{bmatrix} \overline{\partial \vec{f}_1/\partial \vec{x}_1} & \cdots & \overline{\partial \vec{f}_1/\partial \vec{x}_N} \\ \vdots & & \vdots \\ \overline{\partial \vec{f}_N/\partial \vec{x}_1} & \cdots & \overline{\partial \vec{f}_N/\partial \vec{x}_N} \end{bmatrix} , \tag{10}$$

where

$$\overline{\partial \vec{f}_j/\partial \vec{x}_k} = \begin{bmatrix} \partial f_{1,j}/\partial x_{1,k} & \cdots & \partial f_{1,j}/\partial x''_{m,k} \\ \vdots & & \vdots \\ \partial h_{m,j}/\partial x_{1,k} & \cdots & \partial h_{m,j}/\partial x''_{m,k} \end{bmatrix} \tag{11}$$

The functions for stage j involve only variables on stages j-1, j and j+1. Therefore, the Jacobian matrix has a specific form written by

$$\overline{G} = \begin{bmatrix} \overline{B}_1 & \overline{C}_1 & \overline{0} & \cdots & \overline{0} \\ \overline{A}_2 & \overline{B}_2 & \overline{C}_2 & \cdots & \overline{0} \\ & & \cdots & & \\ \overline{0} & \cdots & \overline{A}_{N-1} & \overline{B}_{N-1} & \overline{C}_{N-1} \\ \overline{0} & \cdots & \overline{0} & \overline{A}_N & \overline{B}_N \end{bmatrix} , \tag{12}$$

where $\bar{A}_j$'s, $\bar{B}_j$'s, $\bar{C}_j$'s and $\bar{0}$'s are all square matrices of order 3m and their elements are derived as given in Appendix 1. In the iterative calculation, the new values of the independent variables are calculated for the next iterative step from the following procedure :

$$\begin{bmatrix} \vec{x}_1 \\ \vdots \\ \vec{x}_N \end{bmatrix} := \begin{bmatrix} \vec{x}_1 \\ \vdots \\ \vec{x}_N \end{bmatrix} - \begin{bmatrix} \Delta\vec{x}_1 \\ \vdots \\ \Delta\vec{x}_N \end{bmatrix} , \tag{13}$$

where

$$\begin{bmatrix} \Delta\vec{x}_1 \\ \vdots \\ \Delta\vec{x}_N \end{bmatrix} = (\bar{G})^{-1} \cdot \begin{bmatrix} \vec{f}_1 \\ \vdots \\ \vec{f}_N \end{bmatrix} . \tag{14}$$

In Eq.(14), $(\bar{G})^{-1}$ denotes the inverse matrix of the Jacobian. However, calculation of this inverse matrix is not necessary because the Jacobian has the tridiagonal matrix form if all the matrices, $\bar{A}_j$'s, $\bar{B}_j$'s, $\bar{C}_j$'s and $\bar{0}$'s, are redarded as scalars : $\Delta\vec{x}_j$'s in Eq.(14) can be calculated by using only matrix inversions of matrices of order 3m.

After the values of the independent variables are modified at the Newton-Raphson iterative step, they must be normalized by the following procedure :

$$x_{i,j} := x_{i,j} / \sum_{i=1}^{m} x_{i,j} \quad , \quad x'_{i,j} := x'_{i,j} / \sum_{i=1}^{m} x'_{i,j} \quad ,$$

$$x''_{i,j} := x''_{i,j} / \sum_{i=1}^{m} x''_{i,j} \quad ,$$

$$(\ i = 1, \ldots, m \ ; \ j = 1, \ldots, N \ ) \ . \tag{15}$$

If $h_{n,j}$ in Eq.(7) is replaced by

$$h_{n,j} = \sum_{i=1}^{m} x'_{i,j} - 1 \ , \tag{16}$$

this replacement results in elimination of the need for the normalization procedure expressed by Procedure (15). However, this does not always present improvement as shown by numerical experiments in 2.4.

In this model, the number of the independent variables is 3mN. This can be decreased as shown in the proceeding sections.

In 2.4, Model I-1 referes to the case where Eq.(7) is in use, and Model I-2 refers to the case where Eq.(16) is used skipping the normalization of mole fractions.

2.2 Improved Model (Model II) —— stage separation factors are dependent on concentrations of up and down streams ——

By eliminating $x_{i,j}$'s from Eq.(5) and Eq.(6), the number of the independent variables is decreased to 2mN. The functions which must equal zero can be defined by

$$\left.\begin{aligned} f_{i,1} &= x'_{i,1} + (L''_1/L'_1)(1 - r_W)x''_{i,1} - (L''_2/L'_1)x''_{i,2} \\ f_{i,j} &= x'_{i,j} + (L''_j/L'_j)x''_{i,j} - (L''_{j+1}/L'_j/u_j)x''_{i,j+1} \\ &\quad - (L'_{j-1}/L'_j/u_j)x'_{i,j-1} - (F_j/L'_j/u_j)z_{i,j} \\ u_j &= 1 + U_j/L_j \quad , \quad (j = 2, \ldots, N-1) \\ f_{i,N} &= x'_{i,N} + (L''_N/L'_N/(1 - r_P))x''_{i,N} \\ &\quad -(L'_{N-1}/L'_N/(1 - r_P))x'_{i,N-1} \quad , (i = 1, \ldots, m) \end{aligned}\right\} \quad (17)$$

$$\left.\begin{aligned} h_{i,j} &= \alpha_{i,j}x'_{n,j}x''_{i,j} - x'_{i,j}x''_{n,j} \quad , \\ h_{n,j} &= \sum_{i=1}^{m} x''_{i,j} - 1 \quad , \quad (i \neq n \; ; \; j = 1, \ldots, N). \end{aligned}\right. \quad (18)$$

Defining the vectors of order 2m, $\vec{x}_j$'s and $\vec{f}_j$'s, by

$$\vec{x}_j = \begin{bmatrix} x'_{1,j} \\ \vdots \\ x'_{m,j} \\ x''_{1,j} \\ \vdots \\ x''_{m,j} \end{bmatrix} \quad , \qquad \vec{f}_j = \begin{bmatrix} f_{1,j} \\ \vdots \\ f_{m,j} \\ h_{1,j} \\ \vdots \\ h_{m,j} \end{bmatrix} \quad , \quad (19)$$

the nonlinear simultaneous equations written by Eq.(9) are solved by using the Newton-Raphson iterative method where $x'_{i,j}$'s and $x''_{i,j}$'s are chosen as the independent variables.

The Jacobian matrix has a specific form written by Eq.(12), where elements of $\overline{A}_j$'s, $\overline{B}_j$'s, and $\overline{C}_j$'s (square matrices of order 2m) are given in Appendix 2.

(7)

2.3 Improved Model (Model III) —— stage separation factors are independent of concentrations of up and down streams ——

If the stage separation factors are independent of concentrations of the up and down streams, the number of the independent variables in the Newton-Raphson calculation can be further decreased to (m+1)N. Since this section is the key part of the present note, the mathematical simulation procedure is described in detail.

From Eq.(3), $x'_{i,j}$'s are given by

$$x'_{i,j} = \alpha_{i,j} x'_{n,j} x''_{i,j} / x''_{n,j} \quad . \tag{20}$$

Substitution of Eq.(20) into Eq.(17) results in elimination of all the concentrations of the up and down streams except $x'_{n,j}$'s. Replacing $h_{n,j}$ by g_j in Eq.(18), the functions which must equal zero are expressed by

$$\left.\begin{aligned}
f_{i,1} &= \alpha_{i,1} x''_{i,1} x'_{n,1} / x''_{n,1} + (1 - r_W) b_1 x''_{i,1} \\
&\quad - c_1 x''_{i,2} \\
f_{i,j} &= \alpha_{i,j} x''_{i,j} x'_{n,j} / x''_{n,j} + b_j x''_{i,j} - (c_j/u_j) x''_{i,j+1} \\
&\quad - (a_j/u_j) \alpha_{i,j-1} x''_{i,j-1} x'_{n,j-1} / x''_{n,j-1} \\
&\quad - (F_j/L'_j/u_j) z_{i,j} \\
f_{i,N} &= \alpha_{i,N} x''_{i,N} x'_{n,N} / x''_{n,N} + (b_N/(1 - r_P)) x''_{i,N} \\
&\quad - (a_N/(1 - r_P)) \alpha_{i,N-1} x''_{i,N-1} x'_{n,N-1} / x''_{n,N-1} \\
&\quad (i \neq n \ ; \ j = 2, \ \ldots, \ N-1)
\end{aligned}\right\} \quad , \tag{21}$$

$$f_{n,j} = \sum_{i=1}^{m} \alpha_{i,j} x''_{i,j} x'_{n,j} / x''_{n,j} - 1 \quad , \tag{22}$$

$$g_j = \sum_{i=1}^{m} x''_{i,j} - 1 \quad , \quad (j = 1, \ldots, N) \quad , \tag{23}$$

where

$$\left.\begin{aligned} a_j &= L'_{j-1}/L'_j \quad , \quad (j = 2, \ldots, N) \\ b_j &= L''_j/L'_j \quad , \quad (j = 1, \ldots, N) \\ c_j &= L''_{j+1}/L'_j \quad , \quad (j = 1, \ldots, N-1) \end{aligned}\right\} \quad . \tag{24}$$

Equation (22) is based on the following equation :

$$\sum_{i=1}^{m} x'_{i,j} = 1 \quad . \tag{25}$$

In this model, the following vectors of order (m+1) are defined :

$$\vec{x}_j = \begin{bmatrix} x''_{1,j} \\ \vdots \\ x''_{m,j} \\ x'_{n,j} \end{bmatrix} \quad , \qquad \vec{f}_j = \begin{bmatrix} f_{1,j} \\ \vdots \\ f_{m,j} \\ g_j \end{bmatrix} \quad . \tag{26}$$

The nonlinear simultaneous equations written by Eq. (9) are solved by using the Newton-Raphson iterative method where $x''_{i,j}$'s ($i = 1, \ldots, m$; $j = 1, \ldots, N$) and $x'_{n,j}$'s ($j = 1, \ldots, N$) are chosen as the independent variables.

Equation (11) is expressed by

$$\overline{\partial \vec{f}_j / \partial \vec{x}_k} = \begin{bmatrix} \partial f_{1,j}/\partial x''_{1,k} & \cdots & \partial f_{1,j}/\partial x''_{m,k} & \partial f_{1,j}/\partial x'_{n,k} \\ \vdots & & \vdots & \vdots \\ \partial f_{m,j}/\partial x''_{1,k} & \cdots & \partial f_{m,j}/\partial x''_{m,k} & \partial f_{m,j}/\partial x'_{n,k} \\ \partial g_j/\partial x''_{1,k} & \cdots & \partial g_j/\partial x''_{m,k} & \partial g_j/\partial x'_{n,k} \end{bmatrix} . \qquad (27)$$

and the Jacobian matrix given by Eq.(10) has the same structure as those in the previous two models written by Eq.(12). A_j's, B_j's, and C_j's are all square matrices of order (m+1) whose elements are given in Appendix 3.

The order of the matrices ($\overline{A}_j$'s, $\overline{B}_j$'s, $\overline{C}_j$'s and $\overline{0}$'s) and vectors ($\vec{f}_j$'s) is (m+1) in this model, while it is 3m in Model I. For this reason, the computation time needed at each iterative step, t, is expected to be greatly shortened ; the following equation is approximately satisfied :

$$t_{III} = t_I (m + 1)^2/(9m^2) \quad . \qquad (28)$$

2.4 Numerical Experiments

The purpose of this section is to explore differences in convergence characteristics among Models I-1, I-2 and III. For these numerical experiments, a five component system of N_2-O_2-^{41}Ar-^{85}Kr-^{133}Xe processed by a cascade using porous membrane, is chosen. The flow rate and composition of the feed stream are arbitrarily assumed as provided in Table 1. The stage separation factors are postulated to be the ideal values given by

$$\alpha_{i,j} = \sqrt{M_n/M_i} \quad , \quad (\text{ M denotes the molecular weight }) \, , \tag{29}$$

and independent of concentrations of the up and down streams.

Calculations are made for several cases given in Table 1, by using the three models. The initial values of the independent variables are set at the values equal to the feed mole fractions :

$$x_{i,j} := z_{i,N_F} \, , \quad x'_{i,j} := z_{i,N_F} \, , \quad x''_{i,j} := z_{i,N_F} \, ,$$
$$(\ i = 1, \ldots, m \ ; \ j = 1, \ldots, N\ ) \text{ for Models I-1 and I-2,}$$
$$x'_{n,j} := z_{n,N_F} \, , \quad x''_{i,j} := z_{i,N_F} \, ,$$
$$(\ i = 1, \ldots, m \ ; \ j = 1, \ldots, N\ ) \text{ for Model III.} \tag{30}$$

The calculation is considered solved when the following convergence criterion is satisfied :

$$J = \sum_{j=1}^{N} \sum_{i=1}^{m} (|f_{i,j}| + |g_{i,j}| + |h_{i,j}|)/(3mN) < 1.0 \times 10^{-7}$$
$$(\text{ Models I-1 and I-2 }) \, , \tag{31}$$

$$J = \sum_{j=1}^{N} (\sum_{i=1}^{m} |f_{i,j}| + |g_j|)/((m+1)N) < 1.0 \times 10^{-7}$$
$$(\text{ Model III }) \, .$$

The computer used is FACOM M-200 SYSTEM at Japan Atomic Energy Research Institute. If the successive iteration method was used for solving a set of nonlinear equations, the double precision would be needed for achievement of convergence. Even if the Newton-Raphson iterative method which is inherently more efficient is used, the single precision could be impermissible unless the Jacobian matrix is analytically calculated. However, in this section, it is expected that the efficiency in achievement of convergence is not significantly deteriorated by adoption of the single precision, because none of the above two reasons for the need for the double precision is found in the simulation models. For this reason, all the calculations are made in the single precision.

The top and bottom compositions calculated by using the three models are compared in Tables 2 and 3. The results by one of the models are in close agreement with those by the other two models, while minor differences are found in mole fractions of the heavy key component, Xe. Model III predominates over the other two models in accuracy, and results by Model I-2 are the least accurate among those obtained by the three models. The incorporation of the normalization of mole fractions in Model I-1 presents improvement in accuracy of results.

Their convergence characteristics are compared in Table 4. The number of total iterations needed in Model III is much smaller than those in the other two models ; it is over two orders of magnitude smaller in Case 5. The result in Case 5 indicates that Model I-2 does not always present less iterations in comparison to Model I-1. If Model III is used, the computation time needed at

each iterative step is roughly one order of magnitude shorter for a five component system (Eq.(28)), with the result that the total CPU time is approximately two orders of magnitude shorter.
The great decrease in the number of total iterations presented by Model III can be also appreciated in Fig. 2 where Case 1 is selected as a representative. The significant result observed is that Models I-1 and I-2 take on the characteristics of the successive iteration method in which the iterative calculation is greatly decelerated as the solution is approached. This indicates that if the number of the independent variables is excessively large, the Newton-Raphson method loses its efficiency and takes on the characteristics of the successive itaration method. This is a very interesting result which points out importance of decreasing the number of the independent variables at the expense of simplisity of the basic equations, to present less iterations as well as shorter computation time needed at each iteration. Another significant information learned from Table 4 is that the higher column performance results in greater difficulty in achievement of convergence in Models I-1 and I-2. On the other hand, the number of the total iterations needed is almost independent of the calculational condition in Model III. It is concluded that Model III is predominant both in rapidity of achievement of convergence and in stability, and it presents remarkable improvements of the other two models.

If the stage separation factors are given as functions of concentrations of the up and down streams, Model II must be used instead of Model III. The computation time needed at each iterative step in Model II is approximately nine-fourths of the time in Model I.

Additionally, the number of total iterations is expected to decrease, although the improvement will not be as remarkable as that in cases where the stage separation factors are independent of concentrations of the up and down streams. The two models (Models II and III) has thus been developed as highly efficient simulation models, and Model I should be set aside.

3. Computer Simulation Study for Hydrogen Isotope Separating Cascade by Porous Membrane Method

3.1 Cascade System by Porous Membrane Method for Hydrogen Isotope Separation

There are a number of methods other than cryogenic distillation and water/hydrogen exchange which could be used for hydrogen isotope separation. For example, the thermal diffusion method, porous membrane, Pd-alloy membrane, uranium-hydride, laser, and many other physical or chemical methods, could be interesting candidates.

Among these methods, the author is interested in the porous membrane method, because its technology has already been established by uranium enrichment. However, no study on this method has not been reported, so no information is available concerning the applicability of this method to hydrogen isotope separation, system configuration, and system scale.

In the present study, a computer simulation work is made by using Model III dealing with a hydrogen isotope separation system by porous membrane method in the mainstream fuel circulation system for fusion reactors.

Figure 3 shows the system configuration developed in the present study including input conditions and output requirements assumed. It should be noted that the separation requirements are more relaxed than those assumed elsewhere[8] : the purity of D_2 for use as the neutral beam required is 99 atom%, and the pure T_2 stream is not required. The system is composed of two cascades

and two catalytic equilibrators which promote the isotopic exchange reaction, $HT + D_2 = HD + DT$. The equilibrators are necessary because HT and D_2 cannot be separated by porous membrane diffusers alone on account of equality of their molecular weights. Each cascade has a sidestream which is recycled to the feed after being passed through the equilibrator. In the present work, the reflux ratio defined by

$$R = L'_j/P \ , \quad (j = 1, \ldots, N-1)$$

is given as one of the input data, and r_P and r_W are postulated to be zero.

In the actual operation, the isotopic exchange reactions, $H_2 + D_2 = 2HD$, $H_2 + T_2 = 2HT$, and $D_2 + T_2 = 2DT$, are expected to occur to some extent because of presence of tritium. The room temperature may be adequately high to promote these reactions being catalyzed by beta particles. However, occurence of these exchange reactions leads to enhancement of separation of the three isotopic elements. As an extreme case, if the gas streams leaving any stage were equilibrated, the catalytic equilibrators in the system could be eliminated. This fact is rather in favor of neglection of these exchange reactions within the cascade in determination of design specifications.

3.2 Parametric Surveys and Determination of Design Specifications

In order to find out pertinent design specifications which meet the separation requirements, brief parametric surveys are separately made for each cascade. All the calculations are made by using Model III, and the two-variable Newton-Raphson method developed in a previous work.[9] Since the partial derivatives needed in the two-variable Newton-Raphson method are not analytically calculated, all the calculations are made in the double precision. The stage separation factors are assumed to have ideal values given by Eq.(29). Parameters to be studied are the number of the total stages, reflux ratio, feed location, sidestream flow rate, sidestream location, and top product flow rate. In the present work, several cases are assumed and the design specifications are determined from the results of the calculations for each cascade. The calculational conditions and the results are summarized in Tables 5 and 6. Parametric surveys for Cascade 2 are made after design conditions of Cascade 1 are determined.

In Cascade 1, a lower percentage of H in the bottom product and a greatly low tritium concentration in the top product are both desired, and Case 12 is chosen in the present study. For Cascade 2, Case 6 is chosen by considering the desirability of a low percentage of H in the bottom product and a high-purity D_2 stream of the top product.

The specifications of the three output streams produced by the cascade system are given in Table 7. According to Table 7, the separation requirements described before are certainly met. In comparison to the cascade system for uranium enrichment, both the number of the total stages (approximately 300) and the interstage flow rates are far smaller (the order of magnitude of the feed flow rate is 100 g-mol/h for the commercial fusion reactor system) in this case. Therefore, the dimensions of the diffusers are never unacceptably large.

The conclusion is that the porous membrane method is worth while to investigate in further experimental studies as a possible method for hydrogen isotope separation.

4. Conclusion

(1) New computer-aided simulation models have been developed for multicomponent separating cascades. They are applicable and highly effective in cases where the cut of mixture is prescribed and required to be independent of concentrations and as a result the interstage flow rates and the stage separation factors are input variables for the calculation. One of the models have a feature that the stage separation factors are allowed to be given as functions of concentrations of the up and down streams. The stage separation factors can be very large in both of the two models.

(2) Yamamoto's analytical method is applicable in cases where the interstage flow rates and concentrations are calculated as output information from the heads and tails separation factors. Therefore, his method and the present simulation procedures allow us to mathematically simulate various types of cascades under a variety of conditions.

(3) Some numerical experiments indicate that if the number of the independent variables is excessively large, the Newton-Raphson method takes on the characteristics of the successive iteration method. The decrease in the number of the independent variables at the expense of the simplicity results in less iterations as well as a shorter computation time needed at each iterative step.

(4) A computer simulation study has been carried out for a hydrogen isotope separating cascade system by the porous membrane method, which is assumed to be a unit process in the fuel circulation system for fusion reactors. A system configuration is developed and design specifications are estimated. The results show that the porous membrane method is worth while to investigate in further experimental studies as a possible method for hydrogen isotope separation.

NOMENCLATURE

F_j : Flow rate of feed stream supplied to j-th stage

L_j : Flow rate of stream entering j-th stage

L'_j : Flow rate of stream leaving j-th stage upward

L''_j : Flow rate of stream leaving j-th stage downward

m : Total number of components

N : Number of total stages

r_p : Reflux ratio from top product

r_W : Reflux ratio from bottom product

U_j : Flow rate of sidestream from j-th stage

$x_{i,j}$: Mole fraction of i-th component in stream entering j-th stage

$x'_{i,j}$: Mole fraction of i-th component in stream leaving j-th stage upward

$x''_{i,j}$: Mole fraction of i-th component in stream leaving j-th stage downward

$z_{i,j}$: Mole fraction of i-th component in feed stream supplied to j-th stage

For instance, x, $\vec{f}$ and $\overline{G}$ denote a scalar, a vector and a matrix, respectively. $\vec{x}^t$ denotes the transposed vector of $\vec{x}$. $(\overline{G})^{-1}$ denotes the inverse matrix of $\overline{G}$.

X := Y means the procedure that the value of Y is regarded as the new value of X.

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Appendix

1. Elements of Matrices for Model I

$\bar{A}_j$ ($j = 2, \ldots, N$)

$$\partial f_{i,j}/\partial x_{k,j-1} = 0$$

$$\partial f_{i,j}/\partial x'_{k,j-1} = 0$$

$$\partial f_{i,j}/\partial x''_{k,j-1} = 0$$

$$\partial g_{i,j}/\partial x_{k,j-1} = 0$$

$$\partial g_{i,j}/\partial x'_{k,j-1} = \delta_{i,k}(- L'_{j-1}/L_j)$$

$$\partial g_{i,j}/\partial x''_{k,j-1} = 0$$

$$\partial h_{i,j}/\partial x_{k,j-1} = 0$$

$$\partial h_{i,j}/\partial x'_{k,j-1} = 0$$

$$\partial h_{i,j}/\partial x''_{k,j-1} = 0$$

$\bar{B}_j$ ($j = 1, \ldots, N$)

$$\partial f_{i,j}/\partial x_{k,j} = \delta_{i,k}$$

$$\partial f_{i,j}/\partial x'_{k,j} = - L'_j \delta_{i,k}/L_j$$

$$\partial f_{i,j}/\partial x''_{k,j} = - L''_j \delta_{i,k}/L_j$$

$$\partial g_{i,j}/\partial x_{k,j} = \delta_{i,k} \quad (j = 1, N)$$

$$= \delta_{i,k}(1 + U_j/L_j) \quad (j \neq 1, N)$$

$$\partial g_{i,j}/\partial x'_{k,j} = 0 \quad (j \neq N)$$

$$= - \delta_{i,k} r_P L'_N/L_N \quad (j = N)$$

$$\partial g_{i,j}/\partial x''_{k,j} = -\delta_{i,k} r_W L''_1/L_1 \quad (j = 1)$$

$$= 0 \quad (j \neq 1)$$

$$\partial h_{i,j}/\partial x_{k,j} = 0$$

$$\partial h_{i,j}/\partial x'_{k,j} = (\partial \alpha_{i,j}/\partial x'_{k,j}) x'_{n,j} x''_{i,j} + \alpha_{i,j} x''_{i,j} \delta_{k,n} - x''_{n,j} \delta_{i,k} \quad (i \neq n)$$

$$= 1.0$$

$$\partial h_{i,j}/\partial x''_{k,j} = (\partial \alpha_{i,j}/\partial x''_{k,j}) x'_{n,j} x''_{i,j} + \alpha_{i,j} x'_{n,j} \delta_{i,k} - x'_{i,j} \delta_{k,n} \quad (i \neq n)$$

$$= -1.0 \quad (i = n)$$

$\bar{C}_j$ (j = 1, ..., N-1)

$$\partial f_{i,j}/\partial x_{k,j+1} = 0$$

$$\partial f_{i,j}/\partial x'_{k,j+1} = 0$$

$$\partial f_{i,j}/\partial x''_{k,j+1} = 0$$

$$\partial g_{i,j}/\partial x_{k,j+1} = 0$$

$$\partial g_{i,j}/\partial x'_{k,j+1} = 0$$

$$\partial g_{i,j}/\partial x''_{k,j+1} = \delta_{i,k}(-L''_{j+1}/L_j)$$

$$\partial h_{i,j}/\partial x_{k,j+1} = 0$$

$$\partial h_{i,j}/\partial x'_{k,j+1} = 0$$

$$\partial h_{i,j}/\partial x''_{k,j+1} = 0$$

2. Elements of Matrices for Model II

$\overline{A}_j$ ($j = 2, \ldots, N$)

$$\partial f_{i,j}/\partial x'_{k,j-1} = -(L'_{j-1}/L'_j/u_j)\delta_{i,k} \quad (j \neq N)$$

$$= -(L'_{N-1}/L'_N/(1 - r_P))\delta_{i,k} \quad (j = N)$$

$$\partial f_{i,j}/\partial x''_{k,j-1} = 0$$

$$\partial h_{i,j}/\partial x'_{k,j-1} = 0$$

$$\partial h_{i,j}/\partial x''_{k,j-1} = 0$$

$\overline{B}_j$ ($j = 1, \ldots, N$)

$$\partial f_{i,j}/\partial x'_{k,j} = 1$$

$$\partial f_{i,j}/\partial x''_{k,j} = (L''_1/L'_1)(1 - r_W)\delta_{i,k} \quad (j = 1)$$

$$= (L''_j/L'_j)\delta_{i,k} \quad (j = 2, \ldots, N-1)$$

$$= (L''_N/L'_N/(1 - r_P))\delta_{i,k} \quad (j = N)$$

$$\partial h_{i,j}/\partial x'_{k,j} = (\partial \alpha_{i,j}/\partial x'_{k,j})x'_{n,j}x''_{i,j} + \alpha_{i,j}x''_{i,j}\delta_{k,n} - x''_{n,j}\delta_{i,k} \quad (i \neq n)$$

$$= 0 \quad (i = n)$$

$$\partial h_{i,j}/\partial x''_{k,j} = (\partial \alpha_{i,j}/\partial x''_{k,j}) x'_{n,j} x''_{i,j} + \alpha_{i,j} x'_{n,j} \delta_{i,k} - x'_{i,j} \delta_{k,n} \quad (i \neq n)$$

$$= 1 \quad (i = n)$$

$\overline{C}_j$ ($j = 1, \ldots, N-1$)

$$\partial f_{i,j}/\partial x'_{k,j+1} = 0$$

$$\partial f_{i,j}/\partial x''_{k,j+1} = - (L''_2/L'_1)\delta_{i,k} \quad (j = 1)$$

$$= - (L''_{j+1}/L'_j/u_j)\delta_{i,k} \quad (j \neq 1)$$

$$\partial h_{i,j}/\partial x'_{k,j+1} = 0$$

$$\partial h_{i,j}/\partial x''_{k,j+1} = 0$$

3. Elements of Matrices for Model III

$\overline{A}_j$ ($j = 2, \ldots, N$)

(i) $i \neq n$

$$\partial f_{i,j}/\partial x''_{k,j-1} = -(a_j/u_j)\alpha_{i,j-1}x'_{n,j-1}\delta_{i,k}/x''_{n,j-1} \quad (k \neq n)$$

$$= (a_j/u_j)\alpha_{i,j-1}x''_{i,j-1}x'_{n,j-1}/x''^{2}_{n,j-1} \quad (k = n)$$

$(j \neq N)$

$$\partial f_{i,N}/\partial x''_{k,N-1} = -(a_N/(1 - r_P))\alpha_{i,N-1}x'_{n,N-1}\delta_{i,k}/x''_{n,N-1}$$

$(k \neq n)$

$$= (a_N/(1 - r_P))\alpha_{i,N-1}x''_{i,N-1}x'_{n,N-1}/x''^{2}_{n,N-1}$$

$(k = n)$

$$\partial f_{i,j}/\partial x'_{n,j-1} = -(a_j/u_j)\alpha_{i,j-1}x''_{i,j-1}/x''_{n,j-1}$$

$$\partial g_j/\partial x''_{k,j-1} = 0$$

$$\partial g_j/\partial x'_{n,j-1} = 0$$

(ii) $i = n$

$$\partial f_{n,j}/\partial x''_{k,j-1} = 0$$

$$\partial f_{n,j}/\partial x'_{n,j-1} = 0$$

$\bar{B}_j$ ($j = 1, \ldots, N$)

(i) $i \neq n$

$$\partial f_{i,1}/\partial x''_{k,1} = \alpha_{i,1} x'_{n,1} \delta_{i,k}/x''_{n,1} + b_1(1 - r_W)\delta_{i,k} \quad (k \neq n)$$

$$\partial f_{i,j}/\partial x''_{k,j} = (\alpha_{i,j} x'_{n,j}/x''_{n,j} + b_j)\delta_{i,k} \quad (k \neq n)$$

$$(j = 2, \ldots, N-1)$$

$$\partial f_{i,N}/\partial x''_{k,N} = \alpha_{i,N} x'_{n,N} \delta_{i,k}/x''_{n,N} + b_N \delta_{i,k}/(1 - r_P) \quad (k \neq n)$$

$$\partial f_{i,j}/\partial x''_{k,j} = -\alpha_{i,j} x''_{i,j} x'_{n,j}/x''^2_{n,j} \quad (k = n)$$

$$\partial f_{i,j}/\partial x'_{n,j} = \alpha_{i,j} x''_{i,j}/x''_{n,j}$$

$$\partial g_j/\partial x''_{k,j} = 1$$

$$\partial g_j/\partial x'_{n,j} = 0$$

(ii) $i = n$

$$\partial f_{n,j}/\partial x''_{k,j} = \alpha_{k,j} x'_{n,j}/x''_{n,j} \quad (k \neq n)$$

$$\partial f_{n,j}/\partial x''_{k,j} = \sum_{\substack{q=1 \\ q \neq n}}^{m} \alpha_{q,j} x''_{q,j} x'_{n,j}/(-x''^2_{n,j}) \quad (k = n)$$

$$\partial f_{n,j}/\partial x'_{n,j} = \sum_{q=1}^{m} \alpha_{q,j} x''_{q,j}/x''_{n,j}$$

$\bar{C}_j$ ($j = 1, \ldots, N-1$)

(i) $i \neq n$

$$\partial f_{i,1}/\partial x''_{k,2} = -c_1\delta_{i,k} \quad (k \neq n)$$

$$= 0 \quad (k = n)$$

$$\partial f_{i,j}/\partial x''_{k,j+1} = -(c_j/u_j)\delta_{i,k} \quad (k \neq n)$$

$$= 0 \quad (k = n)$$

$$(j \neq 1)$$

$$\partial f_{i,j}/\partial x'_{n,j+1} = 0$$

$$\partial g_j/\partial x''_{k,j+1} = 0$$

$$\partial g_j/\partial x'_{n,j+1} = 0$$

(ii) $i = n$

$$\partial f_{n,j}/\partial x''_{k,j+1} = 0$$

$$\partial f_{n,j}/\partial x'_{n,j+1} = 0$$

In the equations listed above, $\delta_{i,k}$ denotes the Kronecker's delta defined by

$$\delta_{i,k} = \begin{cases} 1 & (i = k) \\ 0 & (i \neq k) \end{cases}.$$

Table 1 Calculational conditions for numerical experiments

Case	P	N	N_F	R
1	9.0	10	5	2.5
2	9.0	20	10	2.5
3	9.5	10	5	2.0
4	9.0	15	7	3.5
5	9.9	20	10	3.5

P : Flow rate of top product (g-mol/h)

N : Number of total stages

N_F : Feed stage number

R : Reflux ratio defined by $R = L'_j/P$ ($j = 1, \ldots, N-1$)

(1) Feed flow rate = 10 g-mol/h ,

Feed composition : N_2 = 50 %, O_2 = 49.2 %, Ar = 0.64 %,

Kr = 0.01 %, Xe = 0.15 % .

(2) $r_P = r_W = 0$.

(3) The cascade has only a single feed, top product and bottom product.

Table 2 Compositions of top products calculated by use of three models

Case	Model	N_2	O_2	Ar	Kr	Xe
1	I-1	0.511	0.484	0.556×10^{-2}	0.283×10^{-4}	0.120×10^{-3}
	I-2	0.511	0.484	0.556×10^{-2}	0.283×10^{-4}	0.118×10^{-3}
	III	0.511	0.484	0.556×10^{-2}	0.283×10^{-4}	0.120×10^{-3}
2	I-1	0.517	0.478	0.488×10^{-2}	0.108×10^{-4}	0.231×10^{-4}
	I-2	0.517	0.478	0.488×10^{-2}	0.107×10^{-4}	0.253×10^{-4}
	III	0.517	0.478	0.488×10^{-2}	0.108×10^{-4}	0.228×10^{-4}
3	I-1	0.505	0.488	0.599×10^{-2}	0.489×10^{-4}	0.271×10^{-3}
	I-2	0.505	0.488	0.599×10^{-2}	0.489×10^{-4}	0.269×10^{-3}
	III	0.505	0.488	0.599×10^{-2}	0.489×10^{-4}	0.273×10^{-3}
4	I-1	0.515	0.480	0.497×10^{-2}	0.673×10^{-5}	0.119×10^{-4}
	I-2	0.515	0.480	0.497×10^{-2}	0.673×10^{-5}	0.142×10^{-4}
	III	0.515	0.480	0.497×10^{-2}	0.673×10^{-5}	0.118×10^{-4}
5	I-1	0.503	0.491	0.611×10^{-2}	0.766×10^{-5}	0.555×10^{-5}
	I-2	0.503	0.491	0.612×10^{-2}	0.767×10^{-5}	0.548×10^{-5}
	III	0.503	0.491	0.612×10^{-2}	0.767×10^{-5}	0.559×10^{-5}

Table 3 Compositions of bottom products calculated by use of three models

Case	Model	N_2	O_2	Ar	Kr	Xe
1	I-1	0.403	0.569	0.140×10^{-1}	0.745×10^{-3}	0.138×10^{-1}
	I-2	0.403	0.569	0.140×10^{-1}	0.745×10^{-3}	0.135×10^{-1}
	III	0.403	0.569	0.140×10^{-1}	0.745×10^{-3}	0.139×10^{-1}
2	I-1	0.346	0.618	0.201×10^{-1}	0.903×10^{-3}	0.151×10^{-1}
	I-2	0.346	0.618	0.201×10^{-1}	0.903×10^{-3}	0.157×10^{-1}
	III	0.346	0.618	0.201×10^{-1}	0.903×10^{-3}	0.148×10^{-1}
3	I-1	0.397	0.563	0.142×10^{-1}	0.107×10^{-2}	0.246×10^{-1}
	I-2	0.397	0.563	0.142×10^{-1}	0.107×10^{-2}	0.242×10^{-1}
	III	0.397	0.563	0.142×10^{-1}	0.107×10^{-2}	0.248×10^{-1}
4	I-1	0.362	0.603	0.193×10^{-1}	0.939×10^{-3}	0.152×10^{-1}
	I-2	0.362	0.603	0.193×10^{-1}	0.939×10^{-3}	0.160×10^{-1}
	III	0.362	0.603	0.193×10^{-1}	0.939×10^{-3}	0.149×10^{-1}
5	I-1	0.251	0.558	0.347×10^{-1}	0.924×10^{-2}	0.146
	I-2	0.250	0.556	0.346×10^{-1}	0.924×10^{-2}	0.137
	III	0.250	0.556	0.346×10^{-1}	0.924×10^{-2}	0.149

Table 4 Convergence characteristics of three models

Case	Model	n	t
1	I-1	74	10.3
	I-2	60	8.3
	III	4	0.12
2	I-1	90	25.6
	I-2	63	17.5
	III	5	0.22
3	I-1	134	18.6
	I-2	116	15.9
	III	4	0.12
4	I-1	85	18.1
	I-2	40	8.2
	III	5	0.19
5	I-1	648	184.5
	I-2	854	239.0
	III	6	0.26

n : Number of total iterations needed

t : Total CPU time (sec)

Table 5 Parametric Surveys for Cascade 1

Case	P (g-mol/h)	R (-)	N (-)	N_F (-)	N_{SC} (-)	U_{SC} (g-mol/h)	$X''_{1,H}$ (atom%)	$C_{N,T}$ (Ci/h)
1	1.5	583.33	100	40	20	100	0.2471	4.53
2	1.7	514.71	100	40	20	100	0.2045	50.7
3	1.75	500	100	40	20	100	0.2032	70.5
4	2.0	437.5	100	40	20	100	0.2006	173
5	1.7	700	100	40	20	100	0.1755	23.1
6	1.7	700	100	30	15	100	0.1907	35.0
7	1.7	700	100	50	30	100	0.1728	23.9
8	1.7	700	100	40	60	100	0.1562	34.0
9	1.7	700	120	50	30	100	0.1603	10.9
10	1.7	700	150	60	30	100	0.1555	7.23
11	1.7	900	150	60	30	100	0.1447	0.0949
12	1.7	900	150	60	30	200	0.1345	0.0152
13	1.7	900	130	50	30	300	0.1251	0.0920

P : Flow rate of top product N : Number of total stages N_F : Feed stage number

N_{SC} : Sidestream stage number U_{SC} : Flow rate of sidestream

$X''_{1,H}$: Atom percentage of protium in bottom product

$C_{N,T}$: Tritium flow rate in top product

The feed flow rate is 100 g-mol/h and the reflux ratio R is defined by $R = L_j'/P$ (j=1, ..., N-1).

Table 6 Parametric Surveys for Cascade 2

Case	P (g-mol/h)	R (-)	N (-)	N_F (-)	N_{SC} (-)	U_{SC} (g-mol/h)	$X'_{N,D}$ (atom%)	$X''_{1,H}$ (atom%)
1	27.8	30	120	50	30	200	98.89	0.0118
2	27.8	50	100	45	25	200	99.11	0.00984
3	27.8	40	120	50	70	200	98.95	0.00486
4	27.8	40	120	45	25	200	99.29	0.0111
5	27.8	40	120	50	30	200	99.25	0.00917
6	27.8	50	130	50	30	200	99.37	0.00780

$X'_{N,D}$: Atom percentage of deuterium in top product

Table 7 Specifications of Three Output Streams

	Flow rate (g-mol/h)	Composition
Stream (1)	1.7	H_2 = 0.2094 X 10^{-1} HD = 0.9790 HT = 0.3052 X 10^{-6} D_2 = 0.3104 X 10^{-4} DT = 0.5200 X 10^{-9} T_2 = 0.2645 X 10^{-13}
Stream (2)	27.8	H_2 = 0.4053 X 10^{-5} HD = 0.6179 X 10^{-2} HT = 0.2929 X 10^{-2} D_2 = 0.9903 DT = 0.5607 X 10^{-3} T_2 = 0.8508 X 10^{-7}
Stream (3)	70.5	H_2 = 0.8048 X 10^{-14} HD = 0.2656 X 10^{-6} HT = 0.1557 X 10^{-3} D_2 = 0.5439 X 10^{-1} DT = 0.6300 T_2 = 0.3154

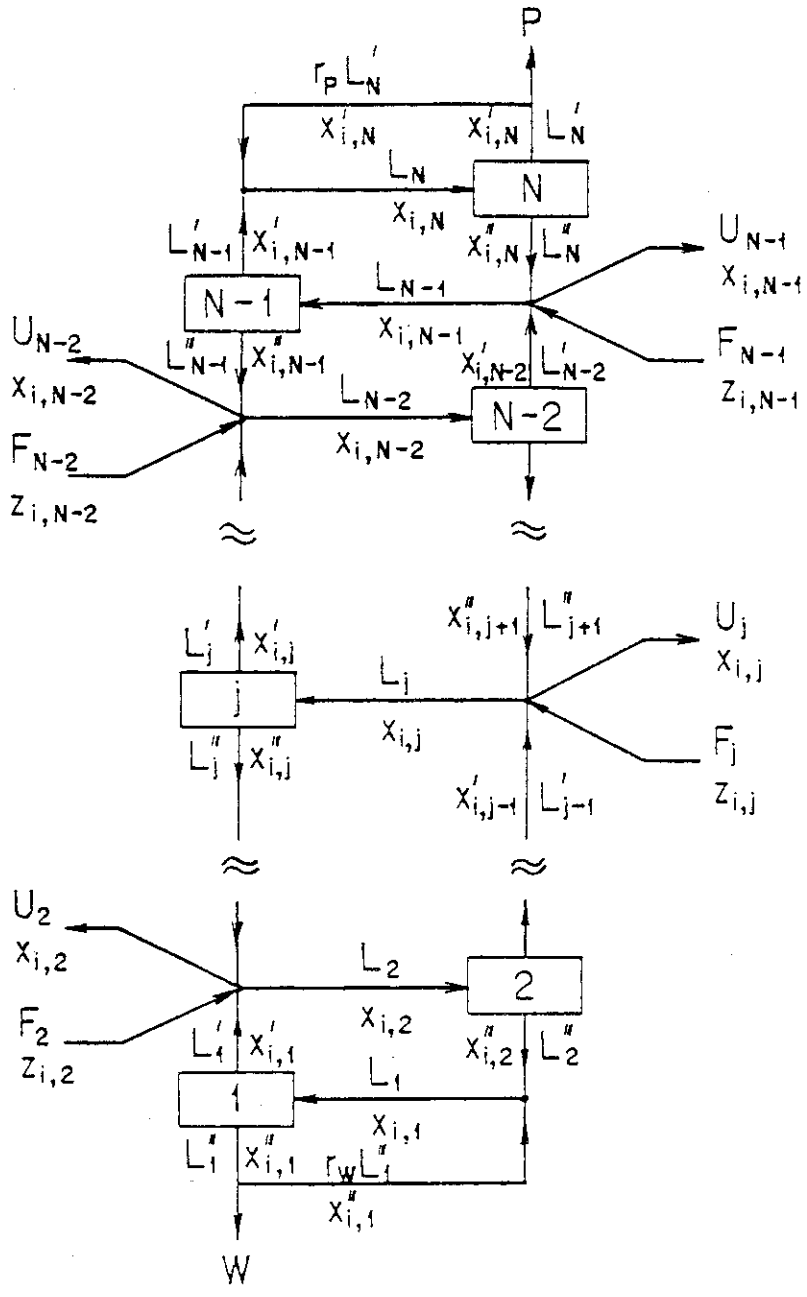

Fig. 1 Model Cascade for Computer-Aided Simulation

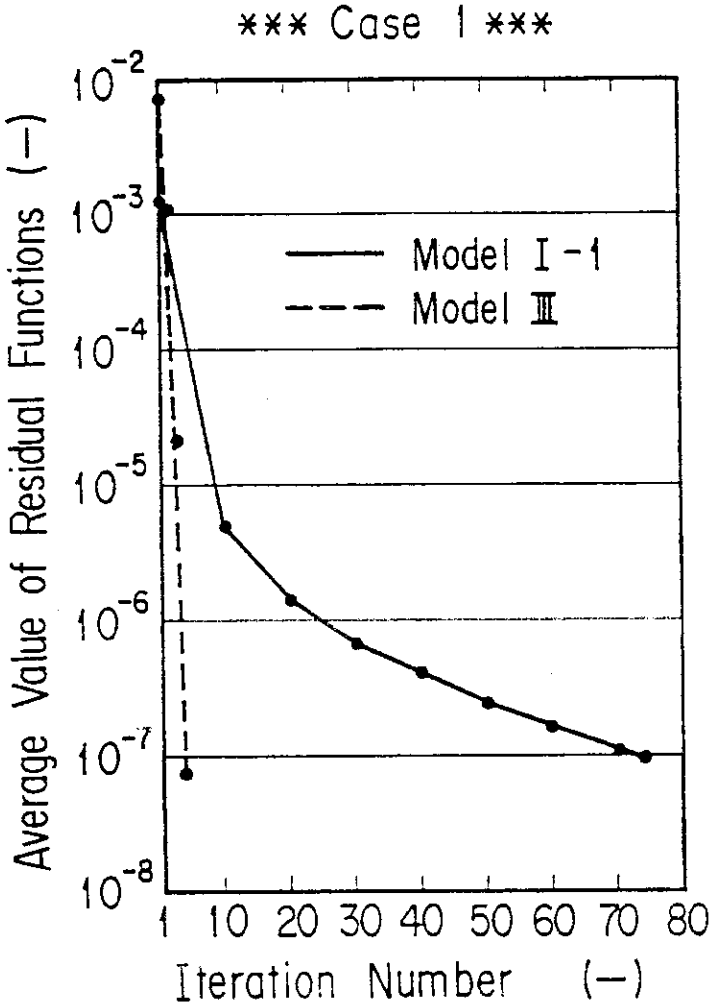

Fig. 2 Comparison between Model I-1 and Model III in Rapidity of Achievement of Convergence

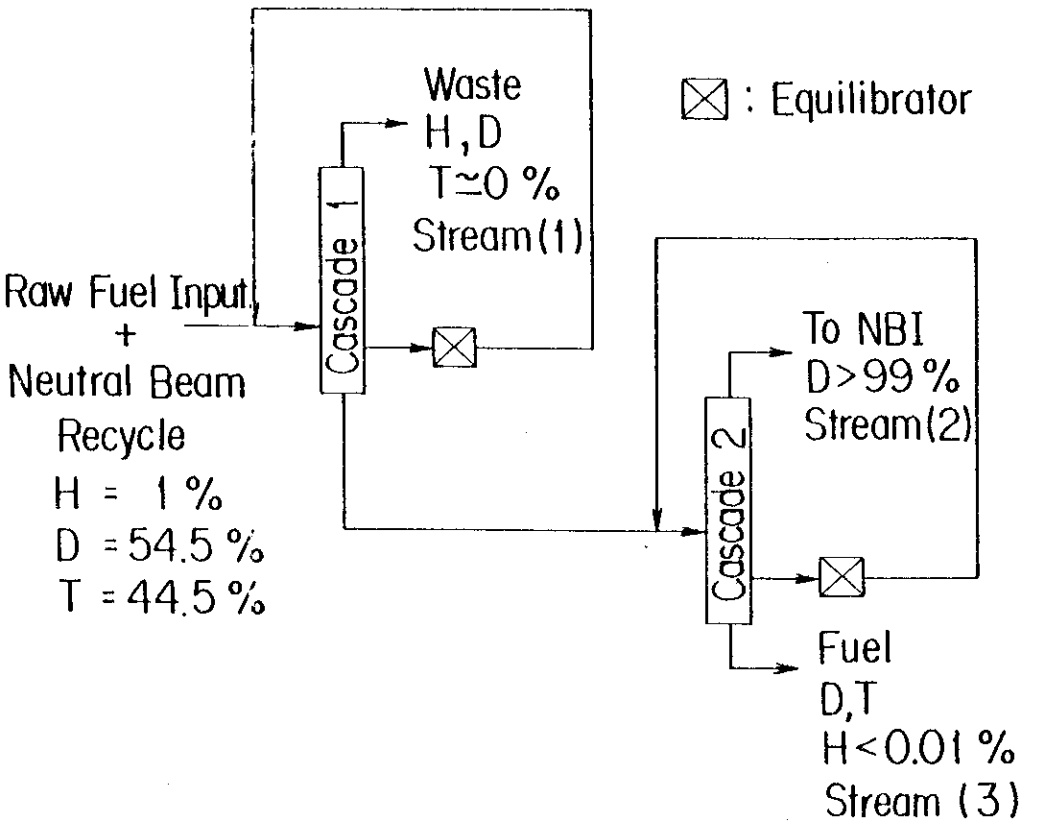

Fig. 3 System Configuration and Input and Output Specifications