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TRANSIENT PROCESS IN GAS CENTRIFUGE CASCADES FOR SEPARATION OF MULTICOMPONENT ISOTOPE MIXTURES

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ABSTRACT

The transient process is studied in gas centrifuge cascades for separation of multicomponent isotope mixtures. Two important practical factors, the holdups in connecting pipes among separation stages and material losses, are taken into account in the partial differential-difference equations that describe the concentration distribution of components. The equations are solved at each time step through the *q*-iteration method. The effects on transient processes are investigated in terms of the total holdup in cascades, the cascade cut, the separation factor, and material losses and may be very significant.

Key Words: Multicomponent isotope separation; Transient process; Gas centrifuge cascade

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INTRODUCTION

Study of transient processes in separation cascades provides the knowledge for analyzing and optimizing separation processes. Also nontraditional, new separation approaches, such as the nonsteady state separation (1) are worth exploring. Methods for studying transient processes have been developed for an explicit method (2) and for an implicit method (3) of separation. Investigations into transient processes (3) has shown that to reflect the situations realistically, the holdups in gas centrifuges and other practical factors must be considered, including the holdups in the pipes connecting stages and material losses.

The holdups in the connecting pipes may have significant influence on the transient process, for instance, by affecting the transient time from one state to another. The holdup in a gas centrifuge is determined through the consideration of several factors, such as the saturated vapor pressure of the process gas, optimization of separation performance, and centrifuge operation safety. Therefore, the holdups in the centrifuges of a stage vary from case to case, depending on the process gas to be separated and the centrifuge parameters (i.e., the geometry and operating conditions), as do the holdups in the connecting pipes. If H, H', H'' represent the holdups in the centrifuges, in the upstream pipes, and in downstream pipes, respectively, of a stage, then 3 time parameters, H/G, H'/L', and H''/L'', can be introduced, with G, L', and L'' respectively being the entering flow, upstream flow, and downstream flow rates of the stage. These parameters have physical meaning. For example, H/G can be viewed as the time used to replace the gas in the centrifuges completely at the rate of G, or it can be understood as the time taken for a gas molecule to travel through a centrifuge at the corresponding stage. The transient process is influenced by the 3 time parameters. In some cases, the holdups in the connecting pipes are comparable to the holdups in the centrifuges, which may lead to $H/G < H'/L'$ or/and $H/G < H''/L''$. Neglecting the holdups in the connecting pipes means neglecting the times that gas travels in the pipes, which is clearly not appropriate. Therefore, the effects of H' and H'' on transient processes should be taken into account.

Material losses mainly result from the reduction of process gas amounts caused by chemical reactions of the process gas with contacting materials and may also have large influences on transient processes. The rate of losses may be small, but the accumulative effects can be significant. As shown in (4), when losses are considered for a matched abundance ratio cascade at the steady state, the total number of centrifuges must be increased by 24.5% to maintain the product rate, concentration, and recovery. Therefore, one can expect that transient processes with and without material losses can be quite different, and it is necessary to develop a method to investigate the effects of material losses not only for a matched abundance ratio cascade but also for a general cascade.

Apart from the holdups in the connecting pipes and material losses, other factors can also be important influential sources, but only 2 of them are studied

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here: the cascade cut and the separation factor. This study shows that certain factors may lead to unexpected results.

The implicit method (3) was chosen for further development because the effects of the holdups in connecting pipes and material losses could be included in our model. The implicit model has more advantages than does the explicit method (2) in 3 aspects: First, time discretization has an accuracy of a order higher; second, it is unconditionally stable; and third, it is faster in terms of computational time. Analytical methods were not used because they are not suitable for dealing with the complicated situations we studied.

In this paper, we describe the implicit method that was further developed to include the holdups in the connecting pipes and the material losses. Then we present the numerical experiments that were carried out to investigate the transient processes in several different cases in which the effects of the total holdup, the cascade cut, the separation factor, and material loss were mainly studied. The conclusions of the study close the presentation.

THE PARTIAL DIFFERENTIAL-DIFFERENCE EQUATIONS

The Equations

Assume that N_c components are found in an isotope mixture. For the ease of reference, the components are numbered sequentially from the lightest to the heaviest, starting with the numeral 1. A rather general cascade for separating the mixture is illustrated schematically in Fig. 1. A general cascade must be understood if complicated cascades, such as those with intermediate withdrawals, are to

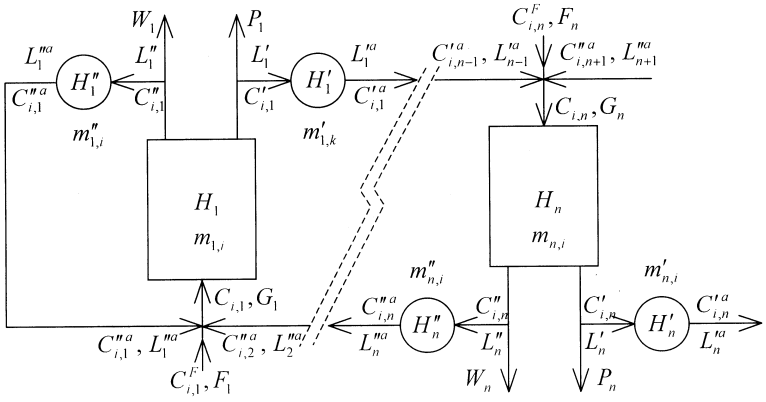

Figure 1. A schematic illustration of a cascade.

be investigated. In the figure, at the nth stage, H_n, H'_n and H''_n, represent the holdups in the gas centrifuges, the upstream pipes, and the downstream pipes. The rates of material losses for the ith component in the centrifuges and the pipes are $m_{n,i}$, $m'_{n,i}$ and $m''_{n,i}$, respectively. L'_n and L'^a_n are the upstream flows of the nth stage before and after passing through the pipe connecting stages n and $n+1$; L''_n and L''^a_n are the downstream flows before and after passing through the pipe connecting stages n and $n-1$. G_n is the entering flow at stage n. To effectively analyze the transient process of concentrations, one can assume that the flows inside the cascade are steady. With this assumption, one will easily find that L''^a_n satisfies following:

$$L''^a_n = L'^a_{n-1} - \sum_{l=1}^{n-1}\left[F_l - P_l - W_l - \sum_i (m_{l,i} + m'_{l,i} + m''_{l,i})\right] \tag{1}$$

or

$$L''^a_n = L'^a_{n-1} + \sum_{l=n}^{N}\left[F_l - P_l - W_l - \sum_i (m_{l,i} + m'_{l,i} + m''_{l,i})\right] \tag{2}$$

$C'_{i,n}$ and $C''_{i,n}$ are respectively the concentrations of the ith component in the head and tail flows immediately leaving the centrifuges, and $C'^a_{i,n}$ and $C''^a_{i,n}$ are the concentrations in the head and tail flows immediately before the mixing points. F_n, P_n, and W_n are the feed, product, and waste at stage n. At the 2 ends of the cascade, the following relationships hold:

$$L'^a_0 = L''^a_1, \qquad C'^a_{i,0} = C''^a_{i,1} \tag{3}$$

$$L''^a_{N+1} = L'^a_N, \qquad C''^a_{i,N+1} = C'^a_{i,N} \tag{4}$$

with N the total number of stages. Considering mass conservation of the ith component in the centrifuges at the nth stage, one obtains

$$\frac{\partial H_n \hat{C}_{i,n}}{\partial t} = L'^a_{n-1}C'^a_{i,n-1} + L''^a_{n+1}C''^a_{i,n+1} + F_n C^F_{i,n} - (L'_n + P_n)C'_{i,n} - (L''_n + W_n)C''_{i,n} - m_{n,i} \tag{5}$$

Here $\hat{C}_{i,n}$ is an averaged concentration of the ith component and is evaluated inside the gas centrifuge. The exact evaluation should be carried out through the separation analysis for a single gas centrifuge at the corresponding stage, i.e., by first solving the flow field and then the transport equations to obtain the concentration distribution C_i inside the centrifuge. Then $C_{i,n}$ can be calculated by

$$\hat{C}_{i,n} = \frac{\int C_i \rho dv}{\int \rho dv}$$

with ρ being the density of the process gas. The integrations are carried out over the whole domain in which the flow field is solved. This complicated evaluation

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is approximated by

$$\hat{C}_{i,n} = \frac{(L'_n + P_n)C'_{i,n} + (L''_n + W_n)C''_{i,n}}{L'_n + P_n + L''_n + W_n} \tag{6}$$

The following similar equations are obtained for the pipes:

$$\frac{\partial H'_n \hat{C}'_{i,n}}{\partial t} = L'_n C'_{i,n} - L'^a_n C'^a_{i,n} - m'_{n,i} \tag{7}$$

$$\frac{\partial H''_n \hat{C}''_{i,n}}{\partial t} = L''_n C''_{i,n} - L''^a_n C''^a_{i,n} - m''_{n,i} \tag{8}$$

Here $\hat{C}'_{i,n}$ and $\hat{C}''_{i,n}$ are averaged concentrations of the ith component in the upstream and downstream pipes respectively of stage n and should be evaluated in a way similar to that for $\hat{C}_{i,n}$. Without involving the complexity of solving the flow fields and pipe transport equations, $\hat{C}'_{i,n}$ must be associated with $C'_{i,n}$ and $C'^a_{i,n}$, and $\hat{C}''_{i,n}$ must be associated with $C''_{i,n}$ and $C''^a_{i,n}$. The simplest approximations for the associations are the following:

$$\hat{C}'_{i,n} \approx C'^a_{i,n}, \qquad \hat{C}''_{i,n} \approx C''^a_{i,n} \tag{9}$$

For gas centrifuges, a well-known empirical relation can be used (5)

$$\frac{C'_{i,n}/C''_{i,n}}{C'_{j,n}/C''_{j,n}} = \gamma_0^{M_j - M_i} \tag{10}$$

with γ_0 being the unit separation factor, and M_i and M_j the molar weights of the ith and jth components respectively. γ_0 is considered a constant as long as the centrifuges are working at flow states (e.g., the entering flow rate, the cut) that are close to the flow state at which γ_0 is measured. Equations (5,7,8, and 10) constitute the equation system, and together with the following condition, describe the transient behavior of concentration in a cascade:

$$\sum_{i=1}^{N_c} C'_{i,n} = \sum_{i=1}^{N_c} C''_{i,n} = \sum_{i=1}^{N_c} C'^a_{i,n} = \sum_{i=1}^{N_c} C''^a_{i,n} = 1 \tag{11}$$

Discretization

Based on (3), the discretization of Eqs. (5,7, and 8) can be accomplished through the Crank-Nicolson scheme; that is, for the equation $\partial f/\partial t = g$,

$$\frac{f^{m+1} - f^m}{\Delta t} = \frac{1}{2}(g^{m+1} + g^m) \tag{12}$$

where the superscripts indicate the time levels. One obtains, after some arrangements,

$$\begin{aligned}
&\frac{L'^{a}_{n-1}}{2}\,C'^{a(m+1)}_{i,n-1}+\left(\frac{H_n}{\Delta t}\,\frac{L'_n+P_n}{L'_n+P_n+L''_n+W_n}+\frac{L'_n+P_n}{2}\right)C'^{(m+1)}_{i,n}\\
&\quad+\left(\frac{H_n}{\Delta t}\,\frac{L''_n+W_n}{L'_n+P_n+L''_n+W_n}+\frac{L''_n+W_n}{2}\right)C''^{(m+1)}_{i,n}-\frac{L''^{a}_{n+1}}{2}C''^{a(m+1)}_{i,n+1}\\
&\quad=\frac{L'^{a}_{n-1}}{2}\,C'^{a(m)}_{i,n-1}+\left(\frac{H_n}{\Delta t}\,\frac{L'_n+P_n}{L'_n+P_n+L''_n+W_n}-\frac{L'_n+P_n}{2}\right)C'^{(m)}_{i,n}\\
&\quad+\left(\frac{H_n}{\Delta t}\,\frac{L''_n+W_n}{L'_n+P_n+L''_n+W_n}-\frac{L''_n+W_n}{2}\right)C''^{(m)}_{i,n}\\
&\quad+\frac{L''^{a}_{n+1}}{2}\,C''^{a(m)}_{i,n+1}+F_nC^F_{i,n}-m_{n,i}
\end{aligned}\tag{13}$$

$$\begin{aligned}
&\left(\frac{H'_n}{\Delta t}+\frac{L'^{a}_{n}}{2}\right)C'^{a(m+1)}_{i,n}-\frac{L'_n}{2}\,C'^{(m+1)}_{i,n}\\
&\qquad=\left(\frac{H'_n}{\Delta t}-\frac{L'^{a}_{n}}{2}\right)C'^{a(m)}_{i,n}+\frac{L'_n}{2}\,C'^{(m)}_{i,n}-m'_{n,i}
\end{aligned}\tag{14}$$

$$\begin{aligned}
&\left(\frac{H''_n}{\Delta t}+\frac{L''^{a}_{n}}{2}\right)C''^{a(m+1)}_{i,n}-\frac{L''_n}{2}\,C''^{(m+1)}_{i,n}\\
&\qquad=\left(\frac{H''_n}{\Delta t}-\frac{L''_n}{2}\right)C''^{a(m)}_{i,n}+\frac{L''_n}{2}\,C''^{(m)}_{i,n}-m''_{n,i}
\end{aligned}\tag{15}$$

Equations (14 and 15) can be used to eliminate the quantities with superscript "a" at time level $m+1$ in Eq. (13) and yields

$$\begin{aligned}
&-\frac{L'_{n-1}L'^{a}_{n-1}}{4}\left(\frac{H'_{n-1}}{\Delta t}+\frac{L'^{a}_{n-1}}{2}\right)^{-1}C'^{(m+1)}_{i,n-1}\\
&+\left(\frac{H_n}{\Delta t}\,\frac{L'_n+P_n}{L'_n+P_n+L''_n+W_n}+\frac{L'_n+P_n}{2}\right)C'^{(m+1)}_{i,n}\\
&+\left(\frac{H_n}{\Delta t}\,\frac{L''_n+W_n}{L'_n+P_n+L''_n+W_n}+\frac{L''_n+W_n}{2}\right)C''^{(m+1)}_{i,n}\\
&-\frac{L''_{n+1}L''^{a}_{n+1}}{4}\left(\frac{H''_{n+1}}{\Delta t}+\frac{L''^{a}_{n+1}}{2}\right)^{-1}C''^{(m+1)}_{i,n+1}\\
&=\frac{L'^{a}_{n-1}}{2}\left(\frac{H'_{n-1}}{\Delta t}+\frac{L'^{a}_{n-1}}{2}\right)^{-1}\left[\frac{L'_{n-1}}{2}\,C'^{(m)}_{i,n-1}+\left(\frac{H'_{n-1}}{\Delta t}-\frac{L'^{a}_{n-1}}{2}\right)C'^{a(m)}_{i,n-1}\right]\\
&+\left(\frac{H_n}{\Delta t}\,\frac{L'_n+P_n}{L'_n+P_n+L''_n+W_n}-\frac{L'_n+P_n}{2}\right)C'^{(m)}_{i,n}
\end{aligned}\tag{16}$$

$$+\left(\frac{H_n}{\Delta t}\frac{L''_n+W_n}{L'_n+P_n+L''_n+W_n}-\frac{L''_n+W_n}{2}\right)C''^{(m)}_{i,n}$$
$$+\frac{L''^a_{n+1}}{2}\left(\frac{H''_{n+1}}{\Delta t}+\frac{L''^a_{n+1}}{2}\right)^{-1}\left[\frac{L''_{n+1}}{2}C''^{(m)}_{i,n+1}+\left(\frac{H''_{n+1}}{\Delta t}-\frac{L''^a_{n+1}}{2}\right)C''^{a(m)}_{i,n+1}\right]$$
$$+F_nC^F_{i,n}-m_{n,i}-\frac{L'^a_{n-1}}{2}\left(\frac{H'_{n-1}}{\Delta t}+\frac{L'^a_{n-1}}{2}\right)^{-1}m'_{n-1,i}$$
$$-\frac{L''^a_{n+1}}{2}\left(\frac{H''_{n+1}}{\Delta t}+\frac{L''^a_{n+1}}{2}\right)^{-1}m''_{n+1,i}$$

Note that for the 2 special cases $n = 1$ and $n = N$, Eqs. (3 and 4) should be taken into account, and $m'_{0,i} = m''_{1,i}$, $m''_{N+1,i} = m'_{N,i}$. Also note that $m_{n,i}$, $m'_{n,i}$, and $m''_{n,i}$ are treated as constants in the discretization.

Determination of the Cascade Hydraulic Status

According to Eq. (16), the concentration distribution in a cascade can be determined only when the hydraulic status of the cascade is known. Because the flows in the cascade are assumed to be steady, the hydraulic status is time independent. The hydraulic status describes how the process gas flow is established and is described by F_n, P_n, and W_n, which are referred to as the external hydraulic parameters, as well as L'_n and L''_n, which are the internal hydraulic parameters. The other 2 internal hydraulic parameters, stage cut θ_n and the stage entering flow rate G_n, are more often used than L''_n and are given by

$$\theta_n = \frac{(L'_n + P_n)}{(L'_n + P_n + L''_n + W_n)} \tag{17}$$

$$G_n = L'_n + P_n + L''_n + W_n + \sum_i m_{n,i} \tag{18}$$

If no material was lost and the external hydraulic parameters F_n, P_n, and W_n are specified,

$$\sum_n (F_n - P_n - W_n) = 0 \tag{19}$$

The hydraulic status of a cascade is fully determined by specifying other $N + 1$ internal hydraulic parameters, which can be classified in the following 4 cases:

all upstream flow rates L'_n, $n = 0,1, \ldots, N$;
all stage cuts θ_n, $n = 1, \ldots, N$, plus either L' or G at any stage;
all entering flow rates G_n, $n = 1, \ldots, N$, plus either L' or θ at any stage;
and one of the 3 parameters was specified at L', θ, and G at any $N - 1$ stages, and 2 were specified at the remaining stage.

In each case, any other hydraulic parameters that are not specified can be easily calculated by means of mass conservation consideration. The number of parameters specified depends on cascade performance optimization or practical considerations; they are assumed to have been already specified so that for cascades without material losses the hydraulic status was determined.

When material losses exist, determining the hydraulic status is a little more complicated. The first case is an example that will not lose applicability for use in a general way. In practice L'_n is a quantity easy to measure and control. Without material losses, the internal hydraulic parameters are readily specified because the external parameters F, P, and W can be given independently of the internal ones.[1] With material losses, the total mass conservation in a cascade requires that

$$\sum_n \left(F_n - P_n - W_n - \sum_i (m_{n,i} + m'_{n,i} + m''_{n,i}) \right) = 0 \tag{20}$$

be satisfied instead of Eq. (19). Because the material losses $m_{n,i}$, $m'_{n,i}$, and $m''_{n,i}$ may be functions of the corresponding flow rates G_n, L'_n, and L''_n, the external parameters F, P, or W are associated with the internal hydraulic parameters and cannot be chosen independently. Suppose that the internal and external hydraulic parameters have already been obtained for a cascade, but material losses were not considered in the calculations. Terms related to material losses must be added back into the equations and some changes to the obtained hydraulic parameters must be made to satisfy the demands of mass conservation. Usually the material loss in a pipe is proportional to the flow rate. So it is assumed that

$$m_{n,i} = aC_{n,i}G_n, \quad m'_{n,i} = a'C'_{n,i}L'_n, \quad m''_{n,i} = a''C''_{n,i}L''_n \tag{21}$$

where a, a' and a'' are the experimentally derived proportion constants. Hence from Eq. (18),

$$G_n = \frac{(L'_n + P_n + L''_n + W_n)}{1 - a} \tag{22}$$

For mass conservation to be satisfied, F, P, or W, or all 3 should be modified. We chose to modify P and W. For the situation where no material was lost, we denote P and W as $\tilde{P}$ and $\tilde{W}$ and define $d'_n \geq 0$ and $d''_n \geq 0$, $n = 1, \ldots, N$, for $\sum_n (d'_n + d''_n) = 1$, and we obtain

$$\begin{aligned} P_n &= \tilde{P}_n - bd'_n \sum_l (m_{l,i} + m'_{l,i} + m''_{l,i}) \\ W_n &= \tilde{W}_n - bd''_n \sum_l (m_{l,i} + m'_{l,i} + m''_{l,i}) \end{aligned} \tag{23}$$

[1]Strictly speaking, the specification of F, P, and W is not completely independent of L', because , L'' may be less than zero (Eqs. 1 or 2), and so θ is greater than 1 or a negative value if somewhere F, P, or W is too large in relation to L'. This rarely happens in practice because L' is usually a few times larger than F, P, and W.

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The parameter b (> 0) was chosen such that Eq. (20) is satisfied. The quantities d'_n and d''_n determine how the effect of the total material losses are distributed to P and W and should be chosen according to practical considerations. For example, for an ordinary simple cascade with only $W_1 \neq 0$ and $P_N \neq 0$, and if the product rate P_N is to be maintained as equal to $\tilde{P}_N$, then $d'_N = 0$ and $d''_1 = 1$ are the appropriate choices.

Solution of the Equations

At each time step, the system of nonlinear equations defined by Eqs. (10 and 16) can be solved efficiently through the use of the q-iteration method proposed by Zeng and Ying; for details of the method, readers are referred to (3,6). The tail concentration C'' is the quantity obtained at each stage after calculating the solution, and thus C' is computed from Eq. (10). Other quantities, such as C'^a and C''^a, if needed, can be easily computed through Eqs. (14 and 15). On convergence, the condition identified in Eq. (11) is automatically satisfied, and the criterion for convergence is

$$\max\left(\left|\sum_n C_{i,n} - 1\right|, \quad \left|\sum_n C'_{i,n} - 1\right|, \quad \left|\sum_n C''_{i,n} - 1\right|\right) \leq \varepsilon_1 \tag{24}$$

with ε_1 a small number and fixed at 10^{-6} in the following numerical experiments.

The steady state is thought to be reached if the total mass conservation is satisfied at a given accuracy:

$$err = \left(\sum_n \sum_i (F_n C^F_{i,n} - P_n C'_{i,n} - W_n C''_{i,n} - m_{n,i} - m'_{n,i} - m''_{n,i})^2\right)^{1/2} \leq \varepsilon_2 \tag{25}$$

where ε_2 is also a small number and is fixed at 10^{-6}.

NUMERICAL EXPERIMENTS

In exploring some of the factors that affect the transient process we restricted our interests to the following few questions: How is the transient process influenced by the holdups? Does the cascade cut have any impact? How much can the separation factor affect the transient process? What is the effect of material losses? Though thoroughly revealing the effects of these factors is difficult, the analyses serve as examples and show that useful information can be gained by using this method about transient processes. The main facts used in our analyses are the time history of mass conservation (i.e., the value of the left-hand side of Eq. (25) as a function of the number of time steps) and the time T_s spent to reach steady state (the transient time).

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Table 1. Natural Abundance of Xe Stable Isotopes

^{124}Xe	^{126}Xe	^{128}Xe	^{129}Xe	^{130}Xe	^{131}Xe	^{132}Xe	^{134}Xe	^{136}Xe
9.3 $\times 10^{-4}$	9.0 $\times 10^{-4}$	1.917 $\times 10^{-2}$	2.644 $\times 10^{-1}$	4.08 $\times 10^{-2}$	2.118 $\times 10^{-1}$	2.689 $\times 10^{-1}$	1.044 $\times 10^{-1}$	8.87 $\times 10^{-2}$

The cascade in the numerical experiments is chosen to be a typical square cascade with constant upstream flow rates and with 1 feed at stage N_F and 2 withdrawals at stages $n = 1$ and $n = N$, i.e., $F_{N_F} \neq 0$, $W_1 \neq 0$, and $P_N \neq 0$. All flow rates and holdups are scaled with respect to F, and the dimension of Δt depends on that of F_{N_F}. For example, if the dimension of F_{N_F} is kg/hr, $L'_n = 5$ and $H_n = 0.1$ means that $L'_n/F_{N_F} = 5$ and $H_n/F_{N_F} = 0.1$ (hour), and the dimension of Δt is hour. To obtain sufficient accuracy for time marching but not consume too much computer time, the time step Δt is chosen through the use of numerical experiments. The process gas is Xe, and the feed in most experiments has natural abundance as given in Table 1.

Note that in any numerical experiment only 1 parameter is changed and all other parameters are kept unchanged. This is sometimes very hard or even impossible in practice. For example, to just alter the holdups inside centrifuges without affecting the separation factor is impossible. Also note that some parameter values may be unrealistic (such as a zero holdup, $N_F = 1$, or $N_F = N$). In such cases, our aim was 2-fold: first, we wanted to see the tendency of parameter change, and second we wanted to see the sensitivity of the change. The initial concentration distribution is such that at each stage the concentration of a component is equal to that in the feed.

Choice of the Time Step Δt

To obtain an appropriate value of Δt, the following experiments were carried out on a cascade with $N = 61$; $N_F = 31$; $P_N = 0.2$; $H_n = 0.1$; $H'_n = H''_n = 0.05$; $L'_n = 10$; and $\gamma_0 = 1.4$. The transient times are given in Table 2.

If the transient process is accurately resolved, the transient times should be identical regardless of Δt; in other words, the smaller Δt is, the more time steps are proportionally needed. If the time step Δt is no larger than 0.5, the transient times are approximately equal. Because a Δt value equal to 0.5 gives an inaccurate re-

Table 2. Transient Time T_s Used to Reach Steady State for Different Values of Δt

Δt	0.001	0.01	0.1	0.5	1
T_s	143.862	143.58	143.8	168.0	576

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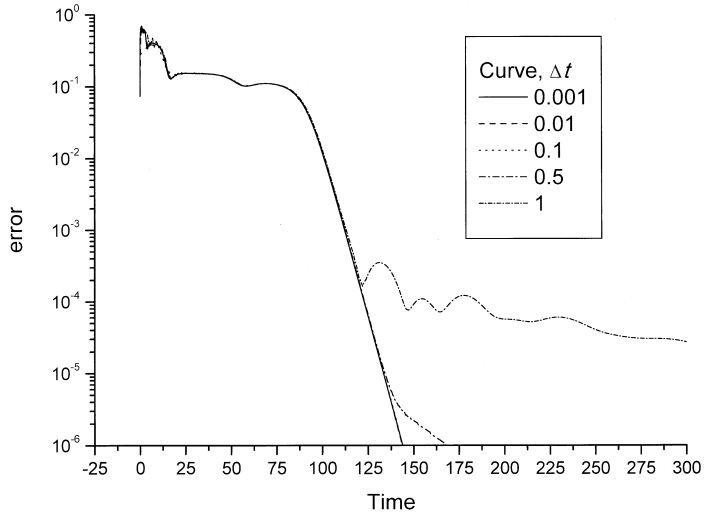

Figure 2. The time histories of transient process error for different values of the time step Δt.

sult, which is demonstrated in the time history shown in Fig. 2, only 0.001, 0.01, and 0.1 values of Δt are small enough to provide accurate calculations. Because $\Delta t = 0.001$ may be too small and leads to too many time steps and $\Delta t = 0.1$ is close to the value that gives inaccurate results, $\Delta t = 0.01$ was adopted, unless otherwise explicitly stated. The separation factor γ_0 was also fixed, except for the case in which its influence on the transient process was investigated.

The basic cascade described above is used in the following numerical experiments. Some of the parameters were changed for different investigations, and these parameter changes are indicated.

Effects of Holdups

Based on Eq. (16), as long as the ratios $H/\Delta t$, $H'/\Delta t$ and $H''/\Delta t$ at each stage are not changed, we find that the time histories for these ratios are identical. This result implies that the transient time is proportional to the total holdup. The transient times are measured for various cases (Table 3). Case nos. 4–7 have a nonzero holdup only at the 50th stage. These cases are not realistic but serve as tests to show how the transient time changes with the total holdup. The transient times against the total holdups are plotted in Fig. 3, which shows that the data give a very good proportional relation. This situation is very easily understandable. If the

Table 3. Cascade Parameters for Investigating the Effects of Holdups

Case	H_n	H'_n, H''_n	n
1	0.01	0	For all n
2	1	0	For all n
3*	0.005	0.0025	For all n
4	0.061	0	50
5	0.61	0	50
6	6.1	0	50
7	61	0	50
8**	0.1	0.05	For all n
9	0.25	0.125	For all n
10	0	0.4	For all n

* $\Delta t = 0.0001$; ** $\Delta t = 0.001$.

whole cascade is in a container filled with an amount of gas equal to the total holdup, the gas inside the cascade is refreshed at a rate F_{N_F}. Then the time taken to refresh the whole gas can be estimated by the total holdup divided by F_{N_F}. Therefore, for a specific F_{N_F}, the transient time is proportional to the total holdup, and of course, the holdups in connecting pipes should not be ignored.

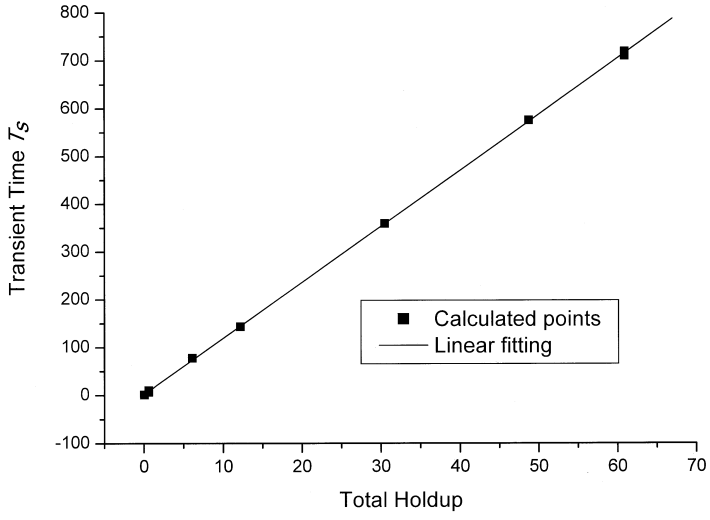

Figure 3. The transient time T_s versus the total holdup in a cascade.

Effects of Cascade Cut

Although the concentration distributions are very different for different cascade cuts, change of the cascade cut causes little changes to the internal hydraulic status when the upstream flow rate is relatively large compared with the feed as it was in our case. One can see hardly any obvious dependence of the transient process on the cascade cut, but the results are somewhat surprising. Figure 4 presents the transient time T_s against the cascade cut P_N/F_{N_F}, which is obtained for 4 cascades with different lengths, $N = 11$, 21, 41, and 61, with plotting intervals of 0.025. The feed locations are all at the centers of the cascades, and $L_n' = 10$. To obtain a clear plot (to avoid generating many curves), we assumed that the feed contains only 6 components, ^{124}Xe, ^{126}Xe, ^{128}Xe, ^{129}Xe, ^{130}Xe, and ^{131}Xe, with concentrations 0.1, 0.2, 0.2, 0.2, 0.2, and 0.1. The peaks occurred at 0.1, 0.3, 0.5, 0.7, and 0.9. (The 2 exceptions, $N = 11$ and 61 when $P_N/F_{N_F} = 0.5$ will be subsequently addressed.) These 5 values of the cascade cut are just the concentration sums in the feed of the first 1, 2, 3, 4, and 5 components, respectively. That is

$$\frac{P_N}{F_{N_F}} = \sum_{i=1}^{N_c'} C_{i,N_F}^F$$

with $Nc' = 1$, 2, 3, 4, and 5, respectively. This phenomenon can hardly be thought of as a coincidence. An isotope mixture with N_c components can be split into

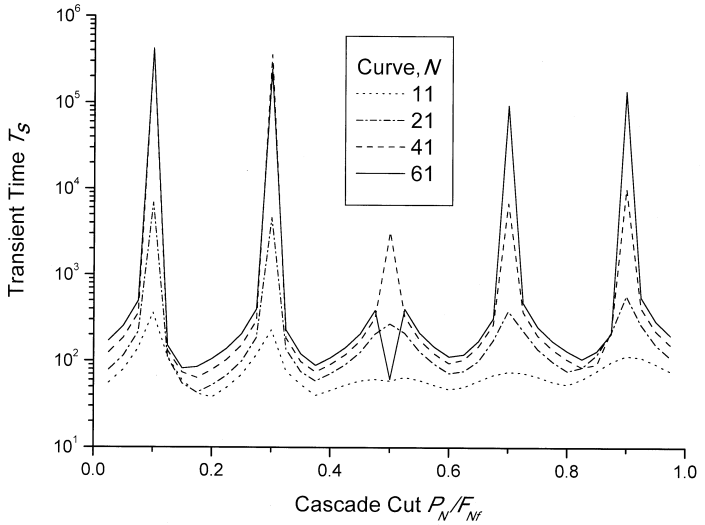

Figure 4. Dependence of the transient time T_s on the cascade cut for 4 cascades of length $N = 11$, 21, 41, and 61. The feed location of each cascade is at the center of the cascade.

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2 groups of components, called a light group and a heavy group, such that the molecular weight of any component in the light group is smaller than that of any component in the heavy group. There are $N_c - 1$ ways of splitting, yielding $N_c - 1$ light groups containing 1, 2, . . . and $N_c - 1$ components, respectively. Zeng and Ying (7) showed that for a sufficiently long cascade, if the cascade cut

$$\frac{P_N}{F_{N_F}} = \sum_{i=1}^{N_c'} C_{i,N_F}^F$$

components 1, . . ., N_c' in the light group appeared only in the product, and components $N_c' + 1$, . . ., N_c in the heavy group appeared only in the waste. That is,

$$\frac{P_N}{F_{N_F}} = \sum_{i=1}^{N_c'} C_{i,N_F}^F$$

resulted in a complete separation of the 2 groups. Therefore, the results here suggest that the more completely the 2 groups are separated, the greater the transient process time. For the 2 exceptions, the steady states were quickly reached. This phenomenon is somehow related to the feed location. In Fig. 5, the values of T_s corresponding to $P_N/F_{N_F} = 0.1, 0.3, 0.5, 0.7$, and 0.9 are plotted for the cascade of length $N = 61$. Indeed, some feed locations showed very short transient times. However, some feed locations, around $N_F = 50$, led to extremely long transient times for $P_N/F_{N_F} = 0.1$ and 0.3. Steady states were not reached within 200 000 000 time steps.

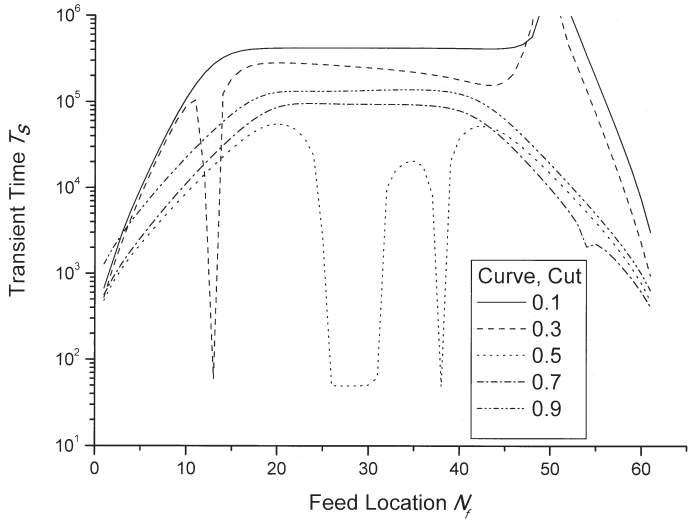

Figure 5. Dependence of the transient time T_s on the feed location for 5 cascade cuts, $P_N/F_{N_F} = 0.1, 0.3, 0.5, 0.7$, and 0.9. The cascade length $N = 61$, and the feed location is at center of the cascade.

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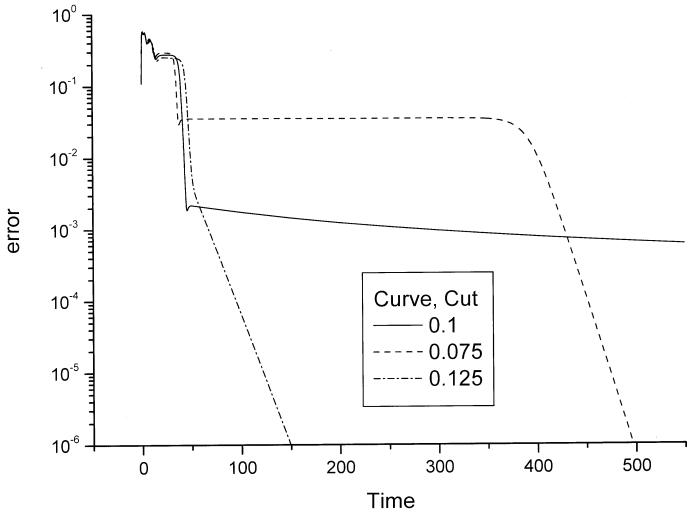

Figure 6. The time histories of error for 3 transient processes corresponding to 3 cascade cuts, $P_N/F_{N_F} = 0.075$, 0.1, and 0.125. The cascade length $N = 61$, and the feed lcoation is at the center of the cascade.

Often the lightest or the heaviest component is to be separated. Therefore, we studied further the separation of these 2 components. We considered only the lightest component. Figure 6 compares the time history of a transient process (curve 1) corresponding to $P_N/F_{N_F} = C_1^F = 0.1$ with those of another 2 transient processes (curves 2 and 3) corresponding to $P_N/F_{N_F} = 0.075$ and 0.125. When the cascade cut was equal to the concentration sum in the feed of the light group components (which consists only of the first component ^{124}Xe), the error reduced slowly. This is the phenomenon previously observed. For both $P_N/F_{N_F} = 0.075$ and 0.1, the theoretical concentration of ^{124}Xe in the product is very close to 1. Does a longer transient time mean that the concentration of ^{124}Xe in the product also needs longer time to reach 1? To answer this question the times were measured 5 times when the concentration of ^{124}Xe in the product was 0.9–0.99999; the results are given in Table 4. For a more specific measurement to be obtained, in

Table 4. Times Spent to Obtain Specific Measurements of the Product Concentration of ^{124}Xe

Cascade Cut	$C_{N,1}$				
	9.0×10^{-1}	9.9×10^{-1}	9.99×10^{-1}	9.999×10^{-1}	9.9999×10^{-1}
0.075	0.62	8.29	35.66	62.88	89.22
0.1	0.63	155.66	2 827.25	29 499.93	296 799.58

which one more 9 is shown in the concentration for $P_N/F_{N_F} = 0.1$, time must be increased by a factor of 10, while for $P_N/F_{N_F} = 0.075$ the time increase is small. Theoretically the lightest component can be enriched to a very high concentration as long as the cascade cut is no larger than its concentration in the feed (7). However, the above observation suggests that if one wants to enrich the lightest component to a very high purity, the cascade cut should take a slightly smaller value than $P_N/F_{N_F} = C_1^F$.

Effects of the Separation Factor γ_0

The separation factor affects concentration distribution in cascades, but whether and how it affects the transient process is unclear. Figure 7 presents the transient processes for different values of γ_0. The steady state was reached most slowly when $\gamma_0 = 1.07$. When γ_0 is larger than a certain value, here about 1.4, the transient processes do not appear to be very different. But the larger γ_0 is, the more suddenly the steady state is approached. Therefore, to determine whether or not the steady state has been reached after some time of a separation run, one must take samples more frequently for a cascade with a large γ_0 than for a cascade with a small γ_0.

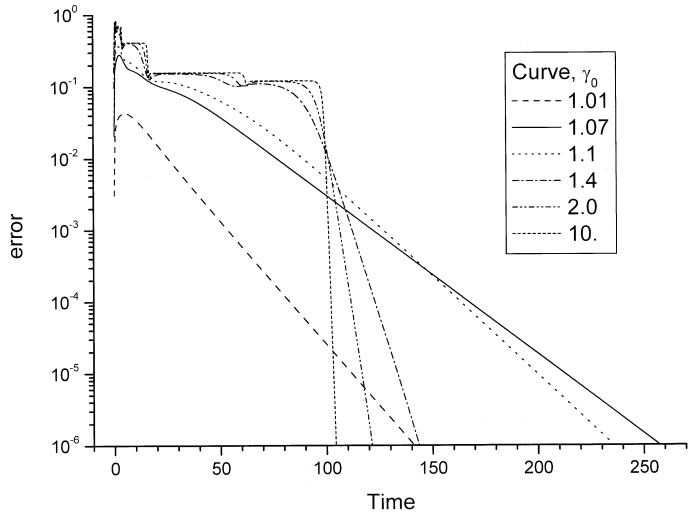

Figure 7. Dependence of the transient process on γ_0. The cascade length $N = 61$, and the feed lcoation is at the center of the cascade.

Table 5. The Withdrawals for Different Values of a

a	0	10^{-6}	10^{-5}	10^{-4}	10^{-3}
W_1	0.800 000	0.797 771	0.777 718	0.578 132	−1.325 27
P_N	0.200 000	0.199 752	0.197 524	0.175 348	−0.036 141

Effects of Material Losses

When $d_1'' = 0.9$ and $d_N' = 0.1$, 90% of the effects resulting from material losses is contributed to the waste and 10% to the product. For simplicity, the loss proportion constants were assumed to be equal, $a = a' = a''$, and 3 values were considered, namely, $a = 10^{-4}$, 10^{-5}, and 10^{-6}. The constant a can take a value larger than 10^{-4}; however, not much margin was allowed for it in this example because when $a = 10^{-3}$ the losses were too great to allow any withdrawals, as W_1 and P_N became negative to satisfy mass conservation. Table 5 lists the amount of withdrawals for different amounts of material losses. Figure 8 shows the distributions of G_n and θ_n corresponding to the above 3 cases of material losses as well as those of G_n and θ_n without material losses. Both G_n and θ_n were changed slightly due to the losses. This is expected because L_n' was fixed.

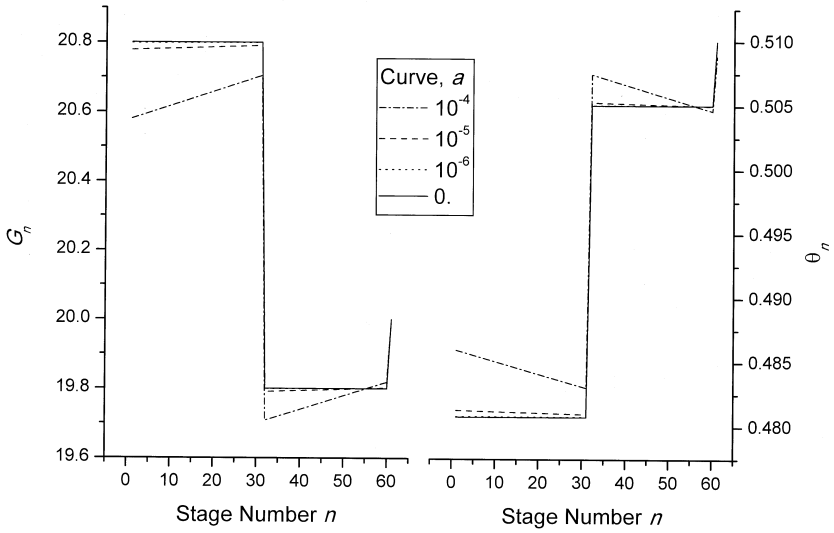

Figure 8. Distributions of the entering flow rate G_n and the stage cut θ_n along a cascade for 4 values of the material loss proportion constant $a = 0$, 10^{-6}, 10^{-5}, and 10^{-4}.

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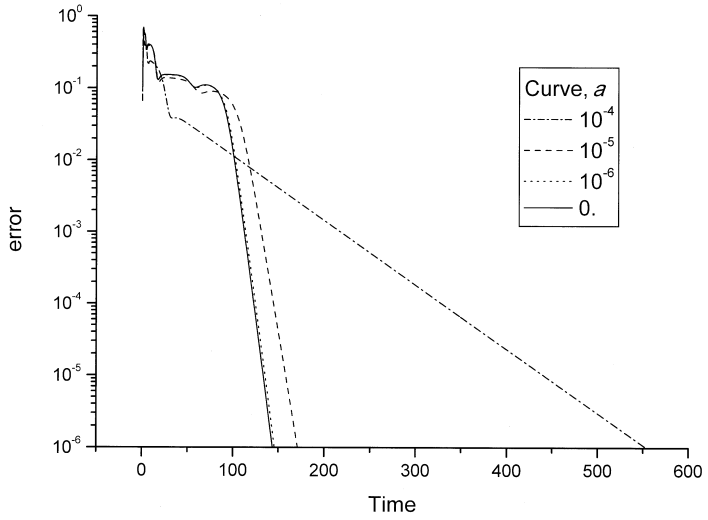

Figure 9. The time histories of error of 4 transient processes corresponding to 4 values of the material-loss proportion constant $a = 0$, 10^{-6}, 10^{-5}, and 10^{-4}.

The transient processes are illustrated in Fig. 9. The material losses may result in significant differences in transient processes and prolong the transient time.

CONCLUSIONS

We investigated numerically the effects of 4 practical factors, the holdups inside cascades, the cascade cut, the separation factor, and material losses on the transient processes in cascades for separating multicomponent isotope mixtures. The investigation was carried out through solutions to a set of nonlinear differential-difference equations governing mass conservation in cascades. To describe situations as closely as possible to real conditions, the equations were designed to take the holdups in connecting pipes among separation stages and material losses into account during the analysis. The Crank-Nicolson scheme was used to discretize the temporal terms, and the resulting system of nonlinear algebraic equations at each time step were solved by the q-iteration method.

The results demonstrate that all 4 factors have significant effects on transient processes. The transient time is proportional to the total holdup in a cascade. An interesting phenomenon is found for the effects of the cascade cut. For a sufficiently long cascade, when the cascade cut shows special values, which are the concentration sums in the feed of the components in the light groups, the transient times are extremely long. However, change of feed location may sometimes shorten the transient processes. As for the separation factor, small values give gentle changes whereas

large values cause sudden transitions. The longest transient time was observed at a relatively small value. The more material losses, the longer is the transient process.

Only the phenomena that are observed during the numerical experiments are presented. Understanding some of the phenomena might be a subject of future research, but making use of the phenomena (or ridding a system of them) is of practical interest. For this purpose, the current method will be of help because it can be easily modified to investigate more factors of practical interests, such as the propagation of light impurities.

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REFERENCES

1. Yu Sosnin, L.; Tcheltsov, A.N. Centrifugal Extraction of Highly Enriched ^{123}Te for the Production of ^{123}I at a Cyclotron. Nucl. Instr. and Meth. **1999,** *A,* 438, 14–19.
2. Wu, H.; Ying, C.; Liu, G. Calculational Methods for Determining the Distribution of Components in a Separation Cascade for Multicomponent Mixture. Sep. Sci. Technol. **1998,** *33* (6), 887–898.
3. Zeng, S.; Ying, C. A Second-Order Time-Accurate Method for Determination of Concentration Distribution of Multicomponent Mixtures in Separation Cascades. Sep. Sci. Technol. **2000,** *35* (5), 729–741.
4. Kholpanov, L.P.; Sulaberidze, G.A.; Patapov, D.V.; Chuzhinov, V.A. Multicomponent Isotope Separating Cascade with Losses. Chem. Eng. and Proc. **1997,** *36* (3), 189–193.
5. Ying, C.; Guo, Z.; Wood, H.G. Solution of the Diffusion Equations in a Gas Centrifuge for Separation of Multicomponent Mixtures. Sep. Sci. Technol. **1996,** *31* (18), 2455–2471.
6. Zeng, S.; Ying, C. A Robust and Efficient Calculation Procedure for Determining Concentration Distribution of Multicomponent Mixture. Sep. Sci. Technol. **2000,** *35* (4), 613–622.
7. Zeng, S; Ying, C. A Method of Separating a Middle Component in Multicomponent Isotope Mixtures by Gas Centrifuge Cascades. Sep. Sci. Technol. **2000,** *35* (14), 2173–2188.

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