Simulation of separation time of Neon stable isotopes using a transient square cascade

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Abstract
In this study, the separation of Neon stable isotopes in a transient square cascade has been simulated. The transient state equations for the square cascade were derived and discretized using the Crank–Nicolson solution method. The simulations showed that isotopes have an optimum value in the product flow at a specific time (optimum separation time), which is effective in the cost of isotope separation. The results indicated that by increasing the isotope mole fraction of Neon-20 in the feed from 0.05 to 0.7, the time to reach the maximum concentration of this isotope in the product (optimum time) increases by 2.7 times. In the case of heavy isotope (Neon-22), the concentration trend is the opposite of the Neon-20. Also, results showed that as the unit separation factor increases, the optimum times at low concentrations of light isotope (and high concentrations of heavy isotope) decreases.
Keywords: Isotopic separation, Stable isotope, Square cascade, Transient time, Neon

Introduction
The separation of stable isotopes is vital due to their widespread application in medicine, industry, and agriculture. Recently, various methods have been proposed for the separation of stable isotopes. Among the isotopic separation methods, the thermal diffusion method has great importance due to features such as high separation coefficient and convenience in the process and operation[1]. Roger and Rutherford (1973) designed a cascade to separate Krypton-85 using a thermal diffusion column [2]. Zieger et al. (1982) optimized the intermediate isotope enrichment in multi-component systems [3]. Vasaru and Gheorghe (2003) studied the separation of carbon-13 in a 7-stage cascade using 19 thermal diffusion columns [1]. Liangjun et al. (2004) compared the design parameters of a thermal diffusion column with experimental and theoretical results for Neon-22 separation[4]. The use of conventional cascades for multi-component separation with high purity requires the cost of constructing several cascades and providing feed for these cascades. Due to these problems and costs, in 2002, unusual transient cascades were introduced. A comparison between conventional and transient cascades was made by Yanfeng et al. (2004)[5, 6].
In this study, the separation time of Neon stable isotopes in a 17-stage transient square cascade of thermal diffusion columns was investigated.

Modeling and solution method
the schematic of the square cascade is presented in Fig. 1.

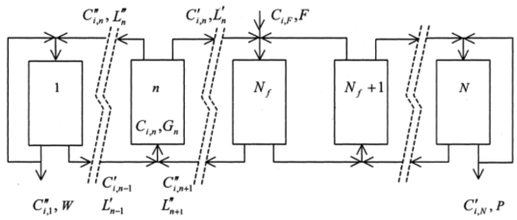

Figure 1. Schematic of the utilized square cascade

In this figure Ci,n , C'i,n and C"i,n are isotope concentrations of i-th component in the input, light output, and heavy output streams, respectively, for n-th stage. F, P, and W are Feed, Product, and Waste of the cascade. Gn denotes input of n-th stage. L'n and L"n are the upstream and downstream flow rates. Hn specifies the hold-up of each stage.
The mass balance of the i-th isotope around n-th stage is given by

$$\frac{\partial\left(H_n \hat{C}_{i,n}\right)}{\partial t} = L'_{n-1}C'_{i,n-1} + L''_{n+1}C''_{i,n+1} - L'_n C'_{i,n} - L''_n C''_{i,n} + C \qquad (1)$$

Where parameter C is defined as follows.

$$C = \begin{cases} FC_{i,F} & n = N_F \\ 0 & n \neq N_F \end{cases} \qquad (2)$$

$\hat{C}_{i,n}$ is the average concentration of i-th isotope in n-th stage, which is calculated as follows.

$$\hat{C}_{i,n}(L'_n + L''_n) = C'_{i,n}L'_n + C''_{i,n}L'' \qquad (3)$$

The q-iteration method was used to solve a set of equations.

$$q_{i,n} = q_{k,n}\gamma_0^{M_k - M_i} \qquad (4)$$

Where γ_0 is the unit separation factor.

The value of q for the i-th isotope was specified by initial guessing the value of q for the isotope k in all stages. For a time step, the set of eq. (1) is solved, and the convergence condition (5) is checked. Otherwise, the values of q are corrected.

$$\sum_i C_{i,n} = \sum_i C'_{i,n} = \sum_i C''_{i,n} = 1 \qquad (5)$$

Results and discussion

The characteristics of the examined square cascade are given in Table 1.

Table 1. Specifications of the simulated square cascade

Stage hold-up (cm^3)	Cascade Feed (sccm)	Cascade cut	Number of columns in each stage	Stage Feed (sccm)	Feed stage	Number of stages
3750	50	0.9075	6	250	16	17

In Fig. 2, the Neon stable isotope concentration diagrams are plotted in terms of time in the product stream. The unit separation factor of the thermal diffusion column, in this case, is assumed to be 1.15.

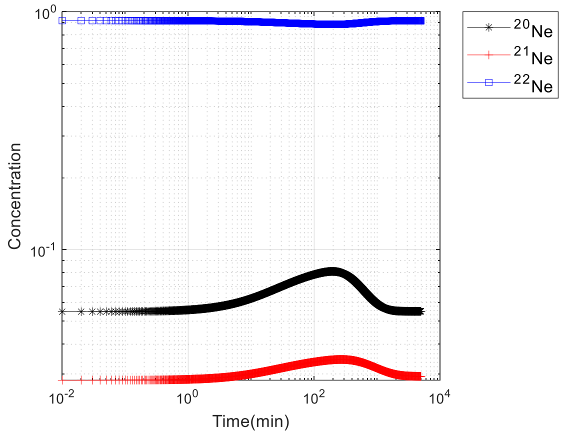

Figure 2. The concentration of Neon isotopes in the cascade product stream in the case 1.

As shown in Fig. 2, the Neon isotopes 20, 21, and 22 reach their optimum concentrations in 182, 253, and 182 seconds, respectively. We named these times the optimum separation time. The graph trend is similar for light (Ne-20) and middle (Ne-21) isotope, while the graph has the reverse trend for heavy isotope (Ne-22).

Different simulation tests are performed to investigate the effect of feed concentration and the unit separation factor on the optimum separation time, as detailed in Table 3. According to Table 3, it is observed that by increasing the isotope concentration of Ne-20 in the feed from 0.05 to 0.7, the time to reach the maximum amount of this isotope in the product increases. At a high concentration of Ne-20 isotope in feed, the optimum time is almost constant. As the unit separation factor increases, the amount of optimum separation times at low concentrations of light isotope (and high concentrations of heavy isotope) decreases.

Table 3. Different simulation cases

Case No.	Concentrations of Ne-20 in the feed (mole fraction)	Unit separation factor	Optimum time in the product Ne-20 (min)
1	0.05	1.15	182
2	0.2	1.15	201
3	0.5	1.15	311
4	0.7	1.15	495
5	0.9	1.15	450
6	0.95	1.15	500
7	0.05	1.4	118
8	0.2	1.4	116
9	0.5	1.4	276
10	0.7	1.4	556
11	0.9	1.4	450
12	0.95	1.4	500

It should be noted that the natural abundances of Neon stable isotopes are 90.48%, 0.27%, and 9.25% for Neon-20, Neon-21, and Neon-22, respectively.

Conclusions

In this study, the transient equations of the square cascade were solved. due to the high cost of product loss in achieving a certain purity, it is possible to reduce separation costs by changing the parameters such as unit separation factor and feed concentration. The results showed that by increasing the isotope concentration of Ne-20 in the feed from 0.05 to 0.7, the time to reach the maximum concentration of this isotope in the product (optimum separation time) increases. At high concentrations of light isotope, the optimum separation time value does not change with a change in the unit separation factor.

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