Analysis and Improvement of the Q-iteration Method

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Abstract. The $q$-iteration method is simple, efficient and robust in determining the concentration distribution in an isotope separation cascade with a known hydraulic state. The expression of the quantity $q$ and the value of the relaxation factor of the $q$-iteration method have a significant influence on the convergence rate of iteration. Through analyzing the convergence of the $q$-iteration method, an improved method for updating $q$ is proposed, and the value range of the relaxation factor is obtained. Numerical analysis shows that the improved method can significantly speed up the convergence. By selecting an appropriate value of the relaxation factor, the convergence can be further improved.

1. Introduction
Isotopes have been widely used and have played an important role in many fields such as medicine, physics, material science, environmental science, and geography. Different separation methods, such as rectification method, electromagnetic method, thermal diffusion method, gas diffusion method, gas centrifugation method and laser method, can be used for different isotopes [1]. Among them, gas centrifugation is the largest and most advanced uranium isotope separation method at present [2], and is also widely used for the separation of many other isotopes. Usually, it is necessary to form separation cascades since the separation capacity of a single machine does not meet the requirements of product concentration and yield in normal conditions [3].

To analyze and optimize the separation performance of centrifugal cascade, it is necessary to determine the concentration distribution of mixture components in the cascade. In 2000, Zeng [4][5] proposed a new iterative method, called the “$q$-iteration method”, which combines robustness, efficiency, simplicity and ease of use. The $q$-iteration method can deal with complex practical situations, including the material loss in cascades, different separation coefficients and multiple material feeds and withdrawals, which is more practical than the previous relevant calculation methods [6].

However, in the practice of numerical calculation, through the analysis of the $q$-iteration method, it is found that the expression of the quantity $q$ is not unique. Meanwhile, the value of the relaxation factor has a significant influence on the convergence speed. So, what is the most reasonable formula? How should the relaxation factor take values? In this paper, these two problems are studied, and the convergence of the $q$-iteration method is analyzed through numerical calculation.

2. Fundamental equations
We consider the separation process of a multi-component mixture in a conventional two-piped separation cascade with $N$ stages, as illustrated in Figure 1. The mixture to be separated has $N_C$ components, which are numbered from 1 to $N_C$ according to the relative molar masses from small to large. $G_n$, $L'_n$ and $L''_n$ are the inflow, head flow and tail flow of the $n$th stage, $C_{i,n}$, $C'_{i,n}$ and $C''_{i,n}$
(i = 1, 2, ⋯ , N_C) are the corresponding concentrations in the flows. For the sake of analysis without loss of generality, we assume the cascade has only one feed F introduced at stage \( N_F \) and two withdrawals (the product \( P \) and the waste \( W \) at stage \( N \) and stage 1, namely \( P = L'_N \) and \( W = L''_1 \)).

\[
\begin{align*}
L''_n, C''_i, L'_n, C'_i, F, N_F, N-1, N
\end{align*}
\]

**Figure 1.** A typical two-piped cascade with one feed and two withdrawals.

Assuming that there are no mass losses, the mass conservation equation for a single stage is:

\[
C_{i,n}G_n = C'_{i,n}L'_n + C''_{i,n}L''_n
\]  

(1)

At the confluent points, the mass conservation equation is:

\[
C_{i,n}G_n = C'_{i,n-1}L'_{n-1} + C''_{i,n+1}L''_{n+1} + \delta(n, N_F)FC'_i
\]  

(2)

Here, \( \delta(x, y) \) is the Kronecker-\( \delta \) function. Since there is no re-circulating flow at both ends of the cascade, \( C'_{i,0}, L'_0, C''_{i,N+1} \) and \( L''_{N+1} \) should be discarded. Combining equation (2) and equation (1), we can get the mass conservation equation for the \( i \)th component:

\[
-C'_{i,n-1}L'_{n-1} + C'_{i,n}L'_n + C''_{i,n}L''_n - C''_{i,n+1}L''_{n+1} = \delta(n, N_F)FC'_i
\]  

(3)

Naturally, the concentrations should meet the constraint condition, that is, the sum of concentrations for each component in the mixture is equal to 1:

\[
\sum_{i=1}^{N_C} C_{i,n} = \sum_{i=1}^{N_C} C'_{i,n} = \sum_{i=1}^{N_C} C''_{i,n} = 1, \quad n = 1, 2, ⋯ , N
\]  

(4)

The separation performance for a single-stage is characterized by the separation factor \( \gamma_{ij} \) between the concentrations of any two components [8]:

\[
\gamma_{ij} = \frac{C'_{i,n}/C''_{i,n}}{C'_{j,n}/C''_{j,n}} = \gamma_{0}^{M_i, M_j}, \quad 1 \leq i, j \leq N_C
\]  

(5)

Here \( \gamma_0 \) is the total separation factor per unit mass and can be obtained either through experiment or by separation analysis [9][10]. With a known hydraulic state of the cascade, the concentration distribution of each component in the cascade can be determined by solving equations (3)-(5).

3. \( q \)-iteration method for solving equations

Due to the non-linearity in equation (5), an iterative method is usually adopted to solve the equations. Different from the commonly used methods which choose the concentrations themselves as the iteration variables, the \( q \)-iteration method takes place over the quantity \( q_{i,n} \equiv C'_{i,n}/C''_{i,n} \) (\( n = 1, 2, ⋯ , N \)), the ratio of head concentration to tail concentration of a certain component (denoted as the \( k \)th component). According to equation (5), the quantity \( q \) of the \( i \)th component at stage \( n \) is

\[
q_{i,n} = \frac{C'_i/n}{C''_i/n} = q_{k,n} \gamma_{ik}
\]  

(6)
Then we can have a relationship between the head concentration and the tail concentration as $C_{i,a} = C''_{i,a}q_{k,a}$. Therefore, the equation (3) can be linearized as

$$-q_{k,a}C_{i,a} + (q_{k,a} + L_{a}^{\prime})C_{i,a} - L_{a}^{\prime}C_{i,a+1}^{n} = \delta(n,N_{F})FC_{i}^{F}$$

(Eq. 7)

Evidently, with known $q_{k,a}$, the distribution of the tail concentration, $C_{i,a}$ can be easily obtained by solving equation (7), and then the distribution of the head concentration, $C''_{i,a}$ can also be obtained by using the above relationship between $C_{i,a}$ and $C_{i,a}$. However, since the assumed value of $q_{k,a}$ is unlikely to be the correct value and the concentrations obtained cannot meet constraint condition (4), it is necessary to modify $q_{k,a}$ and re-solve equation (7). Thus, the calculation process of the $q$-iteration method is as follows:

Step 1. Set the number of iteration steps $m = 0$, and the initial value of concentrations for each component $C_{i,a}^{(0)} = C_{i,a}^{(0)}(i = 1,2,\ldots,N_{C}, n = 1,2,\ldots,N_{n})$.

Step 2. Set the initial quantity $q_{k,a}^{(0)} = 1 (n = 1,2,\ldots,N_{n})$, go to Step 5.

Step 3. Calculate $q_{k,a}^{new}$ through

$$q_{k,a}^{new} = \sum_{i=1}^{N_{C}} C_{i,a}^{m-1} \left( \sum_{i=1}^{N_{C}} \gamma_{i}^{\prime} C_{i,a}^{m-1} \right)$$

(Eq. 8)

Step 4. Introduce relaxation to correct the quantity $q$:

$$q_{k,a}^{(m)} = (1 - \omega)q_{k,a}^{(m-1)} + \omega q_{k,a}^{new}, 0 < \omega \leq 1$$

(Eq. 9)

Step 5. Solve equation (7) and obtain the distribution of tail concentration $C_{i,a}^{(m)}$, and then calculate the distribution of $C_{i,a}^{(m)}$ and $C_{i,a}^{(m)}$.

Step 6. Determine whether the convergence criterion is satisfied. If

$$\max_{1 \leq n \leq N} \left\{ \left| \sum_{i=1}^{N_{C}} C_{i,a}^{(m)} - 1 \right|, \left| \sum_{i=1}^{N_{C}} C_{i,a}^{(m)} - 1 \right|, \left| \sum_{i=1}^{N_{C}} C_{i,a}^{(m)} - 1 \right| \right\} < \varepsilon_{0}$$

Stop the iteration and output the number of iterations $N_{iter}$ and the distribution of concentrations ($\varepsilon_{0}$ is a given small number, e.g., $\varepsilon_{0} = 10^{-6}$). Otherwise, go back to Step 3, $m := m + 1$.

4. Analysis of the formula of $q$ and the convergence of the $q$-iteration method

When the iteration converges, all the concentrations will meet constraint condition (4), that is,

$$\sum_{i=1}^{N_{C}} C_{i,a}^{(m)} = \sum_{i=1}^{N_{C}} q_{k,a}^{(m)} C_{i,a}^{(m)} = \sum_{i=1}^{N_{C}} C_{i,a}^{(m)} \Rightarrow q_{k,a}^{new} = \sum_{i=1}^{N_{C}} C_{i,a}^{new} / \sum_{i=1}^{N_{C}} \gamma_{i}^{\prime} C_{i,a}^{new}$$

However, other expressions of the quantity $q_{k,a}^{new}$ can also be derived through constraint conditions in condition (4), which also enable the $q$-iteration method to determine the distribution of concentrations. Different formulas have significant effects on the convergence speed of the iteration, but there is no relevant research to investigate the influence of these different formulas on the convergence.

In addition, what needs to be explained is that the purpose of introducing the relaxation is to ensure that the $q$-iteration method can still converge effectively under some extreme conditions (such as a very long cascade and small $P$). In general, we take the relaxation factor as $0 < \omega \leq 1$. But in fact, choosing such a range of relaxation factor may be incorrect, when $\omega > 1$ (the $q$-iteration method is over-relaxed), the convergence speed may be faster, which will be explained by numerical results later.

Therefore, in this section, the influence of the formula of $q_{k,a}^{new}$ on the convergence speed is analyzed, and the possibility of further optimizing the convergence of the $q$-iteration method is discussed.
4.1. The formula of q

We note that in equation (8), for the \( m \)th iteration, \( (1 - \theta_n) \) and \( (1 - \theta_n) \) are the concentrations obtained by solving the linear equation (7) in the previous iteration, and naturally satisfy the mass conservation equation (1):

\[
q^{(m-1)}(n_i, n_i) = \theta_n q^{(m-1)}(n_i, n_i) + (1 - \theta_n) q^{(m-1)}(n_i, n_i) + (1 - \theta_n) q^{(m-1)}(n_i, n_i)
\]

Here, \( \theta_n \) is the cut of the \( n \)th stage, defined as \( \theta_n = L_n^1 / G_n = 1 - L_n^1 / G_n \). According to equation (8), \( q_{\text{new}}^{(m)} \) can be written as the following weighted average with \( \theta_n \) as the weight:

\[
q_{\text{new}}^{(m)}(n_i, n_i) = \theta_n q^{(m-1)}(n_i, n_i) + (1 - \theta_n) \sum_{i=1}^{N_i} C^{(m-1)}(n_i, n_i) / \sum_{i=1}^{N_i} \gamma_{ik} C^{(m-1)}(n_i, n_i)
\]

(11)

where, the first term is the quantity \( q_{\text{new}}^{(m)}(n_i, n_i) \) used to solve the linear equations in the previous iteration, while the second term is the updated term after the iteration, which is defined as follows for the convenience of description:

\[
q_{\text{act}}^{(m)}(n_i, n_i) = \sum_{i=1}^{N_i} C^{(m-1)}(n_i, n_i) / \sum_{i=1}^{N_i} \gamma_{ik} C^{(m-1)}(n_i, n_i)
\]

(12)

Note that the difference between \( q_{\text{act}}^{(m)}(n_i, n_i) \) and the original one defined in equation (8).

Then we have \( q_{\text{new}}^{(m)} = q_{\text{act}}^{(m)} \) and we can also write the quantity \( q_{\text{act}}^{(m)} \) as the weighted average of \( q_{\text{act}}^{(m)} \) and \( q_{\text{act}}^{(m)} \) :

\[
q_{\text{act}}^{(m)} = [1 - \omega(1 - \theta_n)] q_{\text{act}}^{(m-1)} + \omega(1 - \theta_n) q_{\text{act}}^{(m)}
\]

(13)

Thus, the calculation process of \( q \)-iteration method is to gradually approach the real distribution of concentration by repeating the cycle of calculating \( q_{\text{act}}^{(m)} \) and solving the equation (7).

4.2. The convergence of the \( q \)-iteration method

To further analyze the convergence of the \( q \)-iteration method, we define \( \tilde{q}_{k,n} = q_{k,n} / q_{\text{act}}^{(m)} \) as the reduced \( q \). According to equation (13), there is

\[
\tilde{q}_{k,n}^{(m)} = q_{k,n} / q_{\text{act}}^{(m)} = (1 - \omega + \omega \theta_n) q_{k,n}^{(m-1)} + \omega(1 - \theta_n)
\]

(14)

According to constraint condition (4), as the iteration progresses, \( q_{k,n}^{(m)} \) and \( q_{\text{act}}^{(m)} \) will eventually approach the same value \( q_{\text{final}}^{(m)} \), defined as:

\[
q_{\text{final}}^{(m)} = \left( \sum_{i=1}^{N_i} \gamma_{ik} C^{(m-1)}(n_i, n_i) \right)^{-1}
\]

Correspondingly, \( \tilde{q}_{k,n}^{(m)} \) will gradually approach 1 as the number of iteration steps \( m \) increases. Therefore, a very direct and important basis for judging the convergence of the \( q \)-iteration method is how fast \( \tilde{q}_{k,n}^{(m)} \) is close to 1, in other words, how fast the error \( \varepsilon = \left| \tilde{q}_{k,n} - 1 \right| \) decreases. Based on this, we define the error amplification factor \( \rho^{(m)} = \varepsilon^{(m)} / \varepsilon^{(m-1)} \) to describe the change of \( \varepsilon \) and characterize the convergence. According to equation (14), we have

\[
\rho^{(m)} = \left| \tilde{q}_{k,n}^{(m)} - 1 \right| / \left| \tilde{q}_{k,n}^{(m-1)} - 1 \right| = \left| 1 - \omega + \omega \theta_n \right|
\]

The error \( \varepsilon \) will gradually decrease only when \( \rho^{(m)} = \left| 1 - \omega + \omega \theta_n \right| < 1 \), which, therefore, gives that the value range of \( \omega \) is

\[
0 < \omega < 2(1 - \theta_n)
\]

(15)
However, it needs to be specifically stated that equation (15) is only a necessary but insufficient condition for the iteration to be able to converge. For some special conditions, the $q$-iteration method may still not converge or converge very slowly, which will be explained in detail through numerical results later.

4.3. A new formula of calculating the quantity $q$

Note that in equation (15), the upper limit of the value range is related to the cut of each stage. In most cases, $\theta_n$ are not the same from stage to stage, so it is impossible to have an accurate value range of $\omega$. In order to deal with this problem, we choose to rewrite the calculation formula of $q_{k,n}^{\text{new}}$. Let $q_{k,n}^{\text{new}} = q_{k,n}^{\text{act}}$, then there is a new formula for calculating $q_{k,n}^{\text{new}}$:

$$
q_{k,n}^{\text{new}} = \sum_{i=1}^{N_c} C_{i,n}^m \frac{\sum_{i=1}^{N_c} \gamma_{ik} C_{i,k}^{m-1}}{\sum_{i=1}^{N_c} C_{i,n}^m} (16)
$$

Then the expressions of $q_{k,n}^{(m)}$ and $\rho^{(m)}$ are:

$$
q_{k,n}^{(m)} = (1-\omega)q_{k,n}^{(m-1)} + \omega \quad \text{and} \quad \rho^{(m)} = \|1 - \omega\|
$$

Similarly, when the iteration converges, $\rho^{(m)} = \|1 - \omega\| < 1$, and the value range that the relaxation factor should satisfy is

$$
0 < \omega < 2
$$

Comparing equations (15) and (17), it can be found that by using the new formula (16), the upper limit of $\omega$ becomes a constant so that an accurate value range of the relaxation factor can be obtained. However, as before, the value range in equation (17) is also a necessary but insufficient condition for the iteration to be able to converge. For very few special cases, the $q$-iteration method is no longer robust, and its convergence speed will be greatly reduced.

5. Numerical Calculation of the convergence of $q$-iteration method

5.1. Numerical verification of the improvement of the convergence

Besides obtaining an accurate upper limit of the relaxation factor $\omega$, using formula (16) to calculate the quantity $q_{k,n}^{\text{new}}$, the $q$-iteration method also becomes more efficient to some extent. The problem of a square cascade [4] is chosen to verify this.

The known parameters of the cascade are the number of stages $N = 20$, the feed position $N_F = 2$, the constant stage inflow rate $G_s / F = 10$, the cut of the cascade $\Theta = P / F = 0.2$ and the cut of the first stage $\theta = 0.5(1-W/G_i)$. Xenon is chosen as the process gas due to its large number of components ($N_c = 9$) and large separation factor ($\gamma_0 = 1.4$). The relative molecular mass and natural abundance of each component of Xe isotopes are given in Table 1. Choose the fifth component $^{130}\text{Xe}$ as the key component, set the relaxation factor $\omega = 0.8$ and the convergence criterion $\varepsilon = 10^{-6}$.

| Relative molecular mass | 124 | 126 | 128 | 129 | 130 | 131 | 132 | 134 | 136 |
|------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| Natural abundance (%)  | 0.093 | 0.09 | 1.917 | 26.44 | 4.08 | 21.18 | 26.89 | 10.44 | 8.87 |

Using formulas (8) and (16) to calculate the quantity $q_{k,n}^{\text{new}}$, respectively, the convergence is completed after 100 iterations and 45 iterations. Figure 2 presents the corresponding convergence histories of the $q$-iteration method. It can be found that using the new formula (16), the error $\varepsilon$ decreases faster, indicating that a significant improvement on convergence has been achieved.

For the two different calculation formulas of $q_{k,n}^{\text{new}}$, Figure 3 shows that variation of the number of iterations, $N_{\text{iter}}$, as the change of the relaxation factor $\omega$ from 0 to 2. Using formula (16), $N_{\text{iter}}$ decreases first and then increases sharply with the increase of $\omega$, which is consistent with the value
range in equation (17) and demonstrates that there is an optimal value of $\omega$. As a comparison, $N_{\text{iter}}$ decreases monotonically with the increase of $\omega$ using formula (8). Because the value range of $\omega$ is unknown for formula (8), it is difficult for us to further improve the convergence.

The numerical results also show that for the improved $q$-iteration method using formula (16), when the $q$-iteration method is over-relaxed ($\omega \approx 1.44$), the convergence speed reaches the fastest. This optimal value of $\omega$ is contrary to the judgment that the smaller $\rho^{(m)}$ is, the faster the convergence speed will be, and it also helps us to reconsider the value range $0 < \omega \leq 1$ we used before and further improve the convergence.

![Figure 2](image1.png)

**Figure 2.** Convergence histories of the $q$-iteration method using formula (8) and (16) to calculate $q_{k,n}^{\text{new}}$.

![Figure 3](image2.png)

**Figure 3.** The variations of the number of iterations $N_{\text{iter}}$ with the relaxation factor $\omega$ using different formulas of $q_{k,n}^{\text{new}}$.

5.2. The influence of relaxation factor on the convergence of $q$-iteration method

To better characterize the influence of the relaxation factor on the convergence of the $q$-iteration method, without loss of generality, we use a hypothetical process gas $X$, which has $N_c = 5$ components, with their relative molecular masses and natural abundances given in Table 2.

Keeping other parameters fixed, only changing the relaxation factor $\omega$ and the cut of the cascade $\Theta$,
the number of iterations $N_{\text{iter}}$ under different working conditions are presented in Figure 4. When the relaxation factor is close to 0 or 2 (the upper and lower sides of the contour map), $N_{\text{iter}}$ exceeds 1000, which is again in line with the value range $0 < \omega < 2$ in equation (17).

| Relative molecular mass | 134 | 135 | 137 | 138 | 140 |
|-------------------------|-----|-----|-----|-----|-----|
| Natural abundance (%)   | 0.1 | 0.2 | 0.2 | 0.2 | 0.3 |

Figure 4. Contour map of $N_{\text{iter}}$ under different conditions as $\Theta$ and $\omega$ varies.

A large shaded area appears in the upper right corner of the contour map, which indicates that when the cascade cut $\Theta$ is large, a large $\omega$ leads the iteration to diverge. Furthermore, when $\Theta$ takes some special values ($\Theta = 0.1, 0.3, 0.5, 0.7$), $N_{\text{iter}}$ increases greatly. This is the special situation that the $q$-iteration method may converge very slowly even if the relaxation factor takes its value within the value range, which we mentioned before. The values of $\Theta$ in these special conditions satisfy the following relationship [7]:

$$\Theta = P/F = \sum_{i=1}^{s} C_i^r, \ 1 \leq s < N_C$$

(18)

This means that for a mixture that contains $N_C$ components, the components numbered 1 to $s$ only appear in the product, while the remaining components only appear in the waste. This phenomenon shows that the $q$-iteration method still has its limitations in solving the distribution of concentrations in the cascade under such special conditions, and for a longer cascade and a larger separation factor $\gamma_0$, the difficulty of convergence of the $q$-iteration method will be more obvious [7].

To verify that using formula (16), the convergence of the $q$-iteration method is still improved when $\Theta$ takes these special values, with the fixed relaxation factor as $\omega = 0.8$, the change of $N_{\text{iter}}$ with the increase of $\Theta$ is shown in Figure 5. We can find that no matter which formula in calculating $q_{\text{new}}$ is used, the $q$-iteration method seems to have some difficulties when solving the special conditions described in equation (18). However, using formula (16) to improve the $q$-iteration method, the convergence is significantly speeded up, and $N_{\text{iter}}$ is approximately reduced by half.
6. Conclusion
In this paper, the q-iteration method for solving the distribution of concentration in the cascade is analyzed and the convergence of the q-iteration method is discussed. Mathematical deductions and analysis show that to obtain the final concentration results, the process of the q-iteration method is actually to repeat the cycle of solving the linear equations and calculating the quantity $q_{k,n}^{\text{act}}$.

A new formula of calculating $q_{k,n}^{\text{new}}$ is constructed to improve the performance of the q-iteration method. An accurate value range of the relaxation factor is obtained and is $0 < \omega < 2$. It is found that the convergence speed of the q-iteration method can be increased significantly.

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