A fast combined momentumed Newton-SSI solver for multicomponent phase equilibrium PT flash calculation

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Abstract. Solving multicomponent phase equilibrium PT flash calculation efficiently depends on the rapid solution of the Rachford-Rice equation. To improve the convergence rate of the classical Newton method for solving the Rachford-Rice equation, this paper proposes a momentumed Newton method that incorporates the momentum technique into the classical Newton method. By integrating the momentumed Newton method with successive substitution iterative method, a fast combined momentumed Newton-SSI solver is designed for multicomponent PT flash calculation. Numerical results demonstrate that the proposed combined momentum-enhanced Newton-SSI method outperforms the combined Newton-SSI method in terms of convergence efficiency, yielding faster convergence in practical numerical calculations.

Keywords: Flash calculation · Rachford-Rice equation · Newton method · Momentumed technique · Successive substitution iterative

1 Introduction

Flash calculation is mainly to determine the phase fraction, and composition of each phase of multi-component mixtures [1]. In practical engineering applications, the accuracy and efficiency of the flash calculation directly determine the reliability of subsequent process design and system optimization [2]. For example, it is widely used such as reservoir numerical simulation, wellbore multiphase flow calculation, and oil-gas separation device design, directly affecting the improvement of oil recovery and the control of development costs [3]. In the chemical industry, the design and optimization of core separation units rely on the phase equilibrium data provided by flash calculations [4]. For the energy storage and utilization, flash calculation also provides key support for the simulation of phase change processes of multicomponent working fluids [5].

The core difficulty of the flash calculation lies in solving the control equation that describes the phase splitting behavior of multicomponent mixtures [6]. Among them, the Rachford-Rice equation [7] is a widely used and representative nonlinear algebraic equation. The Rachford-Rice equation is based on the

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principles of material balance and phase equilibrium, it is the core basis for determining the vapor phase mole fraction and the phase composition of each component in the flash calculation [8]. The solution quality of this equation affects the computational efficiency of the flash calculation.

The classical Newton method [9] is one of the simple and effective algorithms for solving nonlinear algebraic equations. The Newton method is based on the idea of Taylor series expansion, approximating the original function by its tangent line at the current iteration point, thereby constructing the iterative scheme [10]. Due to its second order convergence characteristic, the Newton method has become a popular approach for solving the Rachford-Rice equation [11,12]. Scholars have carried out extensive research on the improvement of this type of method, forming a variety of optimization strategies and improved schemes.

With the rapid development of machine learning and the large-scale optimization, momentum-based accelerative techniques have garnered renewed widespread attention. In recent years, the application of momentum strategies in various numerical methods has achieved remarkable results. It has been verified that the minibatch heavy ball momentum method possesses optimal linear convergence in quadratic optimization [13]. The iterative Hessian sketch method with momentum has been proposed, whose convergence rate is independent of the condition number of the data matrix [14]. a dynamic momentum strategy has been developed to accelerate power iteration and inverse power iteration [15]. The momentum technique has been integrated into the iteratively preconditioned gradient-descent algorithm, with linear convergence achieved [16].

In this paper, to accelerate the convergence rate of the Newton method for solving the Rachford-Rice equation, we propose a momentum-accelerated Newton method. Based on the classical Newton method, this method takes advantage of the efficient convergence of momentum acceleration technology in optimization algorithms. Furthermore, by organically integrating the momentum-accelerated Newton method into the complete process of the flash calculation, we establish a new solution framework for the flash calculation. We present numerical examples to verify the effectiveness of the proposed algorithm in solving multi-component flash calculation problems, and it requires fewer iteration steps than the classical Newton method and the Newton method.

The structure of this paper is organized as follows. In Section 2, we introduce a concise summary of the PT flash calculation model, focusing on the Rachford-Rice equation. In Section 3, we present a momentum-accelerated Newton method for the Rachford-Rice equation, and further construct a combined momentumed Newton-SSI solver for the flash calculation. In Section 4, we provide a numerical example for multicomponent two phase flash calculation, and compare the combined momentumed Newton-SSI solver with the combined Newton-SSI solver to verify the efficiency and convergence of the proposed method. Finally, we draw conclusions and provide feasible directions for future work in Section 5.

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2 Mathematical model

In this subsection, we describe and analysis the mathematical model of the flash calculation. The equilibrium flash vaporization of multicomponent liquids can be visualized as a simple distillation process using a single equilibrium stage. It is significantly different and more complex compared to the flash vaporization of single component liquids. For multicomponent liquids, calculating the amounts of flashed vapor and residual liquid in equilibrium with each other at a given temperature and pressure requires an iterative trial-and-error solution. Such calculations are commonly referred to as PT equilibrium flash calculations.

Assume that a Peng-Robinson fluid mixture [17] of M components stays in the vapor-liquid equilibrium at the specified moles, pressure, and temperature. Thus, for a two-phase case, the Helmholtz free energy density $f(\mathbf{n})$ of this system [18] has the following form:

$$\begin{aligned} f(n) =& RT \sum_{i=1}^{M} n_i(\ln n_i - 1) - nRT \ln(1 - nb(n)) \\ &+ \frac{na(T,n)}{2\sqrt{2}b(n)} \ln \frac{1 + (1-\sqrt{2})nb(n)}{1 + (1+\sqrt{2})nb(n)}. \end{aligned}$$

Here, $n = \sum_{i=1}^{M} n_i$ is the overall molar density, R is the ideal gas constant, and T is the temperature. The Peng-Robinson parameters a and b are functions of the molar composition.

There are many ways to formulate two-phase splitting. A simple and direct approach is the equality of fugacities to provide the conditions for phase equilibrium

$$f_i^L(T, P, x_1, \ldots, x_M) = f_i^V(T, P, y_1, \ldots, y_M),$$

where x_i and y_i represent the mole fraction of component i in the liquid phase and in the vapor phase, respectively. The equilibrium condition is

$$Px_i\varphi_i^L(T, P, x_1, x_2, \ldots, x_M) = Py_i\varphi_i^V(T, p, y_1, y_2, \ldots, y_M), i = 1, 2, \ldots, M. \quad (1)$$

For further details on φ_i^L and φ_i^V, refer to [17]. Moreover, the equilibrium condition (1) is equivalent to

$$y_i = K_i x_i, i = 1, 2, \ldots, M, \quad (2)$$

which relates the vapor-liquid equilibrium ratio K_i to the ratio of fugacity coefficients. Here, $K_i = K_i(T, P, x_1, x_2, \ldots, x_M, y_1, y_2, \ldots, y_M)$. The fugacity coefficients can be obtained from the volumetric properties given by an equation of state, such as the Soave-Redlick-Kwong (SRK) [19] and the Peng-Robinson (PR) equation of state [20,21].

Consider a vapor-liquid system of F moles with overall composition z_i at known pressure P and temperature T. Let F, L and V denote the moles of feed phases, the number of moles of the liquid phase with composition x_i and the

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number of moles of the vapor phase with composition y_i, respectively. The total mass balance equation is given by

$$F = L + V, \tag{3}$$

and the component mass balance equation is given by

$$z_i F = x_i L + y_i V, \quad i = 1, 2, \ldots, M. \tag{4}$$

Combining the two equations (3) and (4), it yields that

$$z_i = y_i \beta + x_i (1 - \beta), \quad i = 1, 2, \ldots, M, \tag{5}$$

where z_i is the known mole fraction of component i and $\beta = \frac{V}{F}$ is called the vaporization rate or vapor fraction.

According to equations (2) and (5), two relationships for vapor and liquid compositions are obtained:

$$x_i = \frac{z_i}{1 + \beta(K_i - 1)}, \quad i = 1, 2, \ldots, M, \tag{6}$$

and

$$y_i = \frac{z_i K_i}{1 + \beta(K_i - 1)}, \quad i = 1, 2, \ldots, M. \tag{7}$$

Therefore, once β is solved from the Rachford-Rice equation, the compositions x_i and y_i can be calculated immediately.

Since the sum of mole fractions in either the liquid or vapor phase equals 1, that is

$$\sum_{i=1}^{M} x_i = 1, \quad \sum_{i=1}^{M} y_i = 1. \tag{8}$$

According to equations (8), (6) and (7), it yields that

$$\sum_{i=1}^{M} \frac{z_i}{1 + \beta(K_i - 1)} = 1, \tag{9}$$

and

$$\sum_{i=1}^{M} \frac{z_i K_i}{1 + \beta(K_i - 1)} = 1. \tag{10}$$

Subtracting the equations (9) and (10), we obtain

$$\sum_{i=1}^{M} \frac{z_i (K_i - 1)}{1 + \beta(K_i - 1)} = 0,$$

which is actually the Rachford-Rice equation. It can be expressed as a nonlinear equation of the variable β, that is

$$F(\beta) = \sum_{i=1}^{M} \frac{(K_i - 1) z_i}{1 + \beta(K_i - 1)} = 0. \tag{11}$$

The Newton method is commonly adopted for solving the Rachford-Rice equation (11), whose detailed implementation will be introduced in the section 3.

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3 A fast combined momentumed Newton-SSI solver

In this subsection, we first introduce the Newton method for solving the Rachford-Rice equation (11), then we propose a fast momentumed Newton method, finally combine the proposed momentumed Newton method with SSI method and establish a combined momentumed Newton-SSI solver for the flash calculation.

For the Rachford-Rice equation, since K_i and z_i are fixed, the general formula for the k-th iteration of the Newton method is obtained by

$$F(\beta_k) + F'(\beta_k)(\beta_{k+1} - \beta_k) = 0. \tag{12}$$

Here, $F'(\beta_k)$ is the first order derivative of $F_{n_c+1}(\beta)$ and is given by

$$F'(\beta) = \frac{dF(\beta)}{d\beta} = -\sum_{i=1}^{M} \frac{(K_i - 1)^2 z_i}{[1 + \beta(K_i - 1)]^2}.$$

Thus, the general iterative scheme for the calculation of the vapor fraction β can be derived as

$$\beta_{k+1} = \beta_k + \frac{\sum\limits_{i=1}^{M} \frac{z_i}{1+\beta_k(K_i-1)}}{\sum\limits_{i=1}^{M} \frac{z_i(K_i-1)^2}{(1+\beta_k(K_i-1))^2}}.$$

Because $F'(\beta)$ is negative, $F(\beta)$ is a monotonic decreasing function of β. This feature of the Rachford-Rice expression is important in solving Eq. (11).

Note that solving the equation (12) by the Newton method is feasible, but there is a risk of convergence to an incorrect value of β. It is crucial to initialize the solver with a reasonable initial value, such as $(\beta_{\max} + \beta_{\min})/2$.

The pesudocode of the Newton method for the Rachford-Rice equation is discribed as Algorithm 1.

Algorithm 1 Newton method for the Rachford-Rice equation

1: **Input:** Initial guess $\beta^{(0)}$, composition z_i $(i = 1, \ldots, M)$ and equilibrium ratios K_i.
2: **Output:** Vapor phase mole fraction $\beta^{(k+1)}$.
3: **for** $k = 0, 1, \cdots$ **do**
4: Compute $F(\beta^{(k)}) = \sum\limits_{i=1}^{M} \frac{(K_i-1)z_i}{1+\beta^{(k)}(K_i-1)}$
5: Compute $F'(\beta^{(k)}) = -\sum\limits_{i=1}^{M} \frac{(K_i-1)^2 z_i}{\left(1+\beta^{(k)}(K_i-1)\right)^2}$
6: Update $\beta^{(k+1)} = \beta^{(k)} - \frac{F(\beta^{(k)})}{F'(\beta^{(k)})}$
7: **end for**

In this paper, to accelerate the convergence speed of the classical Newton method for solving the Rachford-Rice equation, we propose a momentum-accelerated Newton method. Based on the classical Newton method, this method

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takes advantage of the efficient convergence of momentum acceleration technology in optimization algorithms.

The pesudocode of the momentumed Newton method for the Rachford-Rice equation is discribed as Algorithm 2.

Algorithm 2 Momentumed Newton method for the Rachford-Rice equation

1: **Input:** Initial guess $\beta^{(0)}$, composition z_i $(i = 1, \ldots, M)$, equilibrium ratios K_i, and momentumed parameter $m \in [0, 1)$.
2: **Output:** Vapor phase mole fraction $\beta^{(k+1)}$.
3: **for** $k = 0, 1, \cdots$ **do**
4: Compute $F(\beta^{(k)}) = \sum_{i=1}^{M} \frac{(K_i-1)z_i}{1+\beta^{(k)}(K_i-1)}$
5: Compute $F'(\beta^{(k)}) = -\sum_{i=1}^{M} \frac{(K_i-1)^2 z_i}{\left(1+\beta^{(k)}(K_i-1)\right)^2}$
6: Update $\beta^{(k+1)} = \beta^{(k)} - \frac{F(\beta^{(k)})}{F'(\beta^{(k)})} + m(\beta^{(k)} - \beta^{(k-1)})$
7: **end for**

The convergence of the momentumed Newton method for the Rachford-Rice equation is given in Theorem 1.

Theorem 1. Assume that there exists a solution $\beta^* \in \mathbb{R}$ such that $F(\beta^*) = 0$ and the function F satisfies the local tangential cone condition. There exists $\gamma \in (0, 1)$ and the momentum parameter $m \in [0, 1)$ satisfies $a_1 + a_2 < 1$, where $a_1 = 1 - \gamma + 3m + 2m^2, a_2 = m + 2m^2$. Let $\beta^{(1)} = \beta^{(0)}$, the sequence $\{\beta^{(k)}\}_{k=0}^{\infty}$ generated by Algorithm 2 satisfies

$$|\beta^{(k)} - \beta^*|^2 \leq q^k(1 + \delta)|\beta^{(0)} - \beta^*|^2,$$

where $q = \frac{a_1+\sqrt{a_1^2+4a_2}}{2} \in (0, 1)$ and $\delta = q - a_1$.

Proof. Define the error $e_k = \beta^{(k)} - \beta^*$. The iterative scheme in Algorithm 2 can be rewritten as

$$e_{k+1} = A_k + m(e_k - e_{k-1}),$$

where $A_k = \beta^{(k)} - \frac{F(\beta^{(k)})}{F'(\beta^{(k)})} - \beta^*$ is the error term of the classical Newton method.

Taking the square of both sides, it yields that

$$\begin{aligned} e_{k+1}^2 &= \big(A_k + m(e_k - e_{k-1})\big)^2 \\ &= A_k^2 + 2mA_k(e_k - e_{k-1}) + m^2(e_k - e_{k-1})^2. \end{aligned} \tag{13}$$

For the term A_k^2 in (13), by the local tangential cone condition [25], we directly have

$$A_k^2 \leq e_k^2 - \gamma e_k^2.$$

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For the term $2mA_k(e_k - e_{k-1})$ in (13), by splitting the term and discard the non-positive part (using the sign consistency of A_k with e_k, e_{k-1} in local convergence):

$$2mA_k(e_k - e_{k-1}) = 2mA_k e_k - 2mA_k e_{k-1} \leq 2mA_k e_k.$$

Further, since $|A_k| \leq |e_k|$, we obtain

$$2mA_k e_k \leq 2me_k^2.$$

For consistency with the recursive form, we use relaxed expansion:

$$2mA_k(e_k - e_{k-1}) \leq 3me_k^2 + me_{k-1}^2.$$

For the term $m^2(e_k - e_{k-1})^2$ in (13), by the triangle inequality $(e_k - e_{k-1})^2 \leq 2e_k^2 + 2e_{k-1}^2$, we get

$$m^2(e_k - e_{k-1})^2 \leq 2m^2e_k^2 + 2m^2e_{k-1}^2.$$

Substitute the three term estimations into the expansion of e_{k+1}^2, and let $E_k = e_k^2$. Thus, it holds that

$$\begin{aligned} E_{k+1} &\leq (1 - \gamma + 3m + 2m^2)E_k + (m + 2m^2)E_{k-1} \\ &= a_1E_k + a_2E_{k-1}, \end{aligned}$$

where $a_1 = 1 - \gamma + 3m + 2m^2$ and $a_2 = m + 2m^2$.

By the condition $a_1 + a_2 < 1$ and $a_1, a_2 \geq 0$, according to [24], for the non-negative sequence $\{E_k\}$ satisfying $E_{k+1} \leq a_1E_k + a_2E_{k-1}$, there exists $q \in (0, 1)$ and $\delta > 0$ such that

$$E_{k+1} \leq q^k(1 + \delta)E_0, \tag{14}$$

where

$$q = \frac{a_1 + \sqrt{a_1^2 + 4a_2}}{2}, \quad \delta = q - a_1,$$

and $a_1 + a_2 \leq q < 1$.

Substituting $E_k = e_k^2 = (\beta^{(k)} - \beta^*)^2$ into (14), it yields that

$$|\beta^{(k)} - \beta^*|^2 \leq q^k(1 + \delta)|\beta^{(0)} - \beta^*|^2.$$

Then the conclusion of Theorem 1 is proved.

The successive substitution iterative (SSI) method [22] is a fundamental algorithm in flash calculations [23], which is relatively simple to implement and yields robust results. Its iterative variable is chosen as the vapor-liquid equilibrium constant, denoted as K_i. Combining with the definition of the vapor-liquid equilibrium constant from (2), we obtain $K_i = \frac{\varphi(x_i)}{\varphi(y_i)}$.

Subsequently, at the $(s+1)$th iteration of the combined momentumed Newton-SSI solver, the K_i^{s+1} is computed by

$$K_i^{s+1} = \frac{f^s(x_i)/(x_i^sP)}{f^s(y_i)/(y_i^sP)} = \frac{y_i^s}{x_i^s} \cdot \left(\frac{f^s(x_i)}{f^s(y_i)}\right) = K_i^s \cdot \frac{f^s(x_i)}{f^s(y_i)}. \tag{15}$$

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For more details on the calculation of K_i, refer to [21].

Furthermore, to solve the phase equilibrium flash calculation model, by combining the fast momentumed Newton with the SSI method, we proposed a new momentumed Newton-SSI solver, which is described as Algorithm 3.

Algorithm 3 Combined momentumed Newton-SSI Solver for flash calcualtion

1: **Input:** Initial guess $\beta^{(0)}$, composition z_i, initial guess of equilibrium constant $K_i^{(0)}$, temperature T, pressure P.
2: **Output:** Vapor phase mole fraction $\beta^{(s+1)}$, liquid phase composition $x_i^{(s+1)}$, vapor phase composition $y_i^{(s+1)}$.
3: **for** $s = 0, 1, \cdots$ **do**
4: Solve the Rachford-Rice equation (11) by using the momentumed Newton method (Algorithm 2).
5: Update the vapor phase mole fraction $\beta^{(s+1)}$.
6: Update the vapor phase composition $x_i^{(s+1)}$ by the equation (6).
7: Update the liquid phase composition $y_i^{(s+1)}$ by the equation (7).
8: Update $K_i^{(s+1)}$ by the equation (15).
9: **end for**

4 Numerical experiments

In this section, we systematically investigate the robustness and computational efficiency of the fast momentumed Newton-SSI solver through several typical multicomponent phase equilibrium flash calculation cases. First, we focus on analyzing the influence of the momentum parameter on the convergence rate, stability, and numerical performance of the proposed algorithm, and identify the reasonable selection range and functional mechanism of this key parameter.

On this basis, we comprehensively compare the method developed in this work with the classical Newton-SSI method and the Newton-SSI method under identical conditions.The performance of each algorithm is quantitatively evaluated from multiple perspectives, including the number of iterations, computational time, and convergence reliability, so as to verify the effectiveness of the proposed fast momentumed relaxation strategy in accelerating convergence and improving robustness.

In our numerical experiments, the initial guess for the vapor fraction is set as $\beta^{(0)} = 0.5$, and the universal gas constant is taken as $R = 8.314$ J/(mol·K).

It is well known that the convergence performance of phase equilibrium calculations is highly sensitive to the initial guess of the equilibrium K-values. If the initial guess is close to the exact equilibrium solution, the iterative procedure can converge rapidly, otherwise, the algorithm may even fail to converge. To obtain a reliable and effective initial guess, the Wilson correlation is widely adopted in the literature and is also used in our work. The initial K-values are

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calculated as

$$K_i^{(0)} = K_i^{\text{Wilson}} = \frac{P_{c,i}}{P} \exp\left(5.37(1+\omega_i)\left(1-\frac{T_{c,i}}{T}\right)\right), \tag{16}$$

where $T_{c,i}$, $P_{c,i}$ and ω_i are called the critical temperature , the critical pressure and the acentric factor of the i-th component, respectively.

All iterations are terminated when the maximum relative error (denoted by 'MRerr') satisfies the predefined convergence criterion

$$\text{MRerr} = \max_{i=1,\cdots,M}\left(\left|\frac{K_i^{(s+1)} - K_i^{(s)}}{K_i^{(s+1)}}\right|\right) \leq 10^{-10}, \tag{17}$$

or when the number of iterations exceeds a prescribed maximum value, e.g., 200.

4.1 Six-components two phase flash calculation problem

In the numerical test, we focus on solving a six-components two-phase flash calculation problem, which is a typical and representative test case in the field of phase equilibrium flash calculations. This experiment is specifically designed to initially verify the convergence rate of the proposed fast combined momentumed Newton-SSI solver in handling multi-component flash systems under standard operating conditions.

Given the initial temperature $T = -67.78°\text{C}$ and pressure $P = 5.76$ Mpa. The fluid mixture involved in this flash calculation consists of six components. In Table 1, we presents the detailed molar composition of the mixture as well as the key thermophysical properties of each individual component, such as critical temperature (denoted as 'T_c'), critical pressure (denoted as 'P_c'), the acentric factor and the binary interaction parameters (denoted as 'BIP'). These parameters are of great significance as they serve as essential input data for the calculation of equilibrium constants (K_i) using the Wilson correlation and the subsequent solution of the Rachford-Rice equation, which are crucial steps in the flash calculation process. Additionally, the selection of this six-component system is to simulate practical industrial scenarios, ensuring the practicality and universality of the experimental results.

To illustrate the impact of the momentum parameter on the convergence performance of the fast momentumed Newton-SSI solver. In Fig. 1, we plot the curve of the number of iterations versus the momentum parameter for the fast momentumed Newton-SSI method. Here, the momentum parameter values ranging from 0 to 0.8.

From the Fig. 1, we observe that when the momentum parameter is around 0.3, the number of iterations reaches a minimum, indicating that the algorithm converges fastest within this interval, which is the optimal parameter choice for this test case. Moreover, The algorithm is highly sensitive to the value of the momentum parameter. Too small or too large a parameter will undermine the effect of momentumed acceleration, and even lead to a much slower convergence speed

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Table 1. Composition of the fluid and the properties of components.

Component	z_i	P_c(Mpa)	T_c(°C)	ω_i	BIP					
					N_2	C_1	C_2	C_3	nC_4	nC_5
N_2	0.0200	3.40	-146.77	0.040	0.0000	0.0180	0.0390	0.0460	0.0470	0.0480
C_1	0.8866	4.60	-82.41	0.008	0.0180	0.0000	0.0050	0.0100	0.0145	0.0182
C_2	0.0492	4.87	32.36	0.098	0.0390	0.0050	0.0000	0.0017	0.0032	0.0048
C_3	0.0246	4.24	96.88	0.152	0.0460	0.0100	0.0017	0.0000	0.0012	0.0024
nC_4	0.0098	3.79	152.19	0.193	0.0470	0.0145	0.0032	0.0012	0.0000	0.0008
nC_5	0.0098	3.37	196.74	0.251	0.0480	0.0182	0.0048	0.0024	0.0008	0.0000

than the standard Newton method. This shows that a reasonable choice of the momentum parameter is crucial to exerting the advantages of the momentumed strategy.

Fig. 1 intuitively verifies the significant influence of the momentum parameter on the convergence properties of the momentumed Newton method: there exists an optimal parameter interval that can maximize the convergence speed of the algorithm; deviating from this interval will lead to the deterioration of convergence performance. This provides clear guidance for the selection of the momentum parameter in subsequent algorithm applications, that is, parameter values around 0.3 should be preferentially selected to balance the convergence speed and numerical stability.

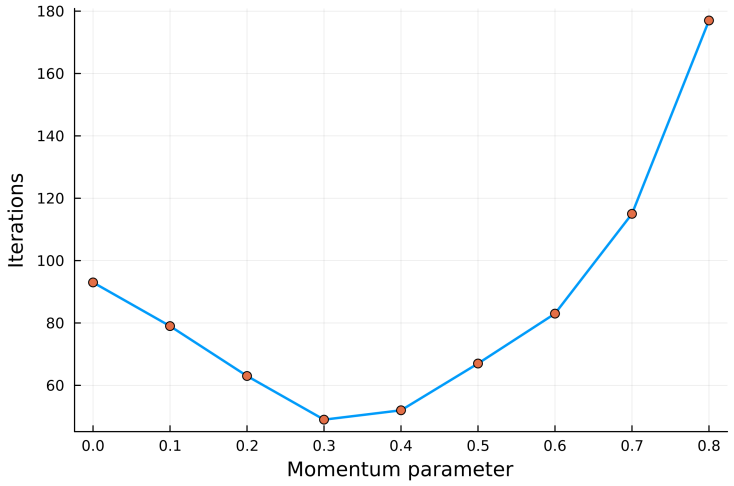

Fig. 1. Impact of the momentum parameter on the combined momentumed Newton-SSI method.

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Table 2. Numerical results of two solvers for the six-component two-phase flash calculation.

Numerical results of the combined Newton-SSI solver						
Results	N_2	C_1	C_2	C_3	nC_4	nC_5
x_i^{approx}	0.015054	0.858013	0.062689	0.034708	0.014566	0.014969
y_i^{approx}	0.028669	0.936708	0.025556	0.006882	0.001445	0.000739
K_i^{approx}	1.904442	1.091718	0.407665	0.198273	0.099221	0.049378
Numerical results of the combined momentumed Newton-SSI solver						
Results	N_2	C_1	C_2	C_3	nC_4	nC_5
x_i^{approx}	0.015054	0.858013	0.062689	0.034708	0.014566	0.014969
y_i^{approx}	0.028669	0.936708	0.025556	0.006882	0.001445	0.000739
K_i^{approx}	1.904442	1.091718	0.407665	0.198273	0.099221	0.049378

In Table 2, we presents the numerical results obtained from the combined Newton-SSI method and the combined momentumed Newton-SSI method ($m = 0.3$) for the six-component two-phase flash calculation. This table mainly lists the key output approximate results, including the liquid phase molar composition (x_i^{approx}), the vapor phase molar composition (y_i^{approx}), and the equilibrium constants (K_i^{approx}) for each component.

From Table 2, we observe that the values of x_i, y_i and K_i obtained by both methods are identical for all six components, up to six decimal places. This confirms that the introduction of the momentumed acceleration in the Newton-SSI method does not alter the final solution of the flash calculation problem. This validates the effectiveness of the combined momentumed Newton-SSI solver for the phase equilibrium flash calculation.

In Fig. 2 and Fig. 3, we depict the convergence curve of the maximum relative error defined in (17) versus the number of iteration for the combined Newton-SSI method and the combined momentumed Newton-SSI method, respectively.

From Fig. 2 and Fig. 3, we observe that both the combined Newton-SSI method and the combined momentumed Newton-SSI method can converge to the solution successfully. The combined momentumed Newton-SSI method converges much faster than the combined Newton-SSI method with nearly a 50% reduction in iterations.This indicates that the introduction of the momentumed strategy significantly accelerates the convergence rate, reducing the number of iterations by nearly half.

Fig. 2 and Fig. 3 clearly demonstrate that the combined momentumed Newton-SSI method, by incorporating the momentum parameter, effectively accelerates the convergence of the combined Newton-SSI iteration. It significantly reduces the number of iterations required for convergence while ensuring numerical stability. This validates the effectiveness of the momentumed strategy in flash cal-

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culations and provides a superior algorithmic choice for the efficient solution of multicomponent phase equilibrium problems.

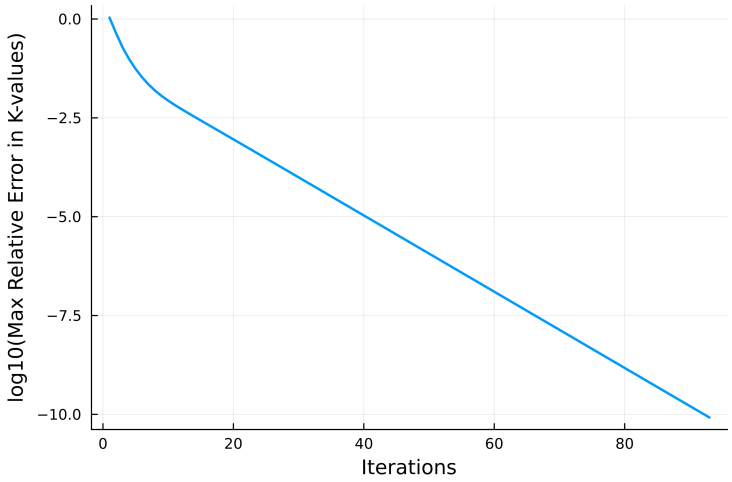

Fig. 2. The convergence curve of the combined Newton-SSI method.

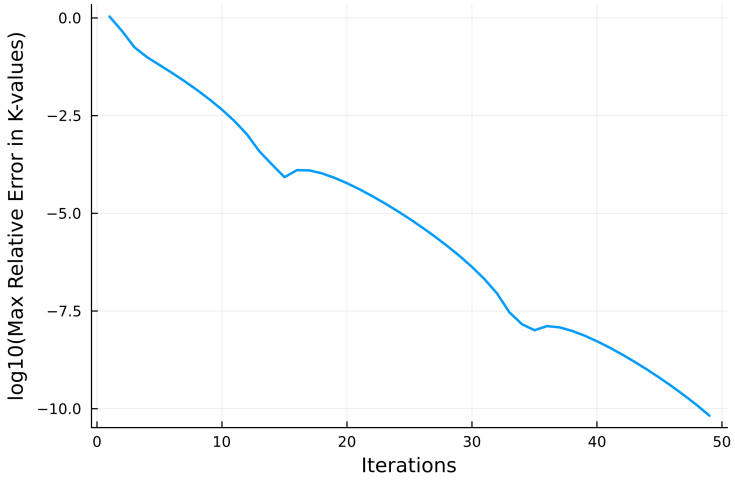

Fig. 3. The convergence curve of the combined momentumed Newton-SSI method.

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5 Conclusions

This paper presents a momentum-accelerated Newton method for solving the Rachford-Rice equation arising in multicomponent PT flash calculation. Furthermore, by combining the momentumed Newton method with the successive substitution iterative method, a unified combined momentumed Newton–SSI solver is constructed for efficient flash calculation. Numerical experiments verify that the proposed method exhibits better convergence property and requires fewer iteration steps than the combined Newton–SSI solver.

Future work will focus on the investigation of adaptive selection strategies for momentum parameters, so as to further improve the stability and robustness of the algorithm under various working conditions. Moreover, the proposed combined momentumed Newton-SSI solver will be integrated with the relevant reduction variable method for the BIP matrix, aiming to effectively promote the flash calculation with a large number of components.

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