

ERROR ANALYSIS OF STABILIZED CONVEX SPLITTING BDF k METHOD FOR THE MOLECULAR BEAM EPITAXIAL MODEL WITH SLOPE SELECTION*

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Abstract

The k -th ($k = 3, 4, 5$) order backward differential formula (BDF k) is applied to develop the high order energy stable schemes for the molecular beam epitaxial model with slope selection. The numerical schemes are established by combining the convex splitting technique with the k -th order accurate Douglas-Dupont stabilization term in the form of $S\tau^{k-1}\Delta_h(\phi^n - \phi^{n-1})$. With the help of the new constructed discrete gradient structure of the k -th order explicit extrapolation formula, the stabilized BDF k scheme is proved to preserve energy dissipation law at the discrete levels and unconditionally stable in the energy norm. By using the discrete orthogonal convolution kernels and the associated convolution embedding inequalities, the L^2 norm error estimate is established under a weak constraint of time-step size. Numerical simulations are presented to demonstrate the accuracy and efficiency of the proposed numerical schemes.

Mathematics subject classification: 65M06, 65M12.

Key words: The molecular beam epitaxial model, High order stabilized convex splitting BDF k scheme, Discrete gradient structure, Unconditional energy dissipation, L^2 norm convergence analysis.

1. Introduction

The molecular beam epitaxial technique can be used to obtain high-quality crystalline materials and form the structures with very high precision in the vertical direction [25]. In this paper, we consider the molecular beam epitaxial (MBE) model with slope selection [16], that is

$$\partial_t \Phi = -\kappa \mu, \quad \mu = \epsilon^2 \Delta^2 \Phi - \nabla \cdot [(|\nabla \Phi|^2 - 1) \nabla \Phi], \quad \mathbf{x} \in \Omega, \quad (1.1)$$

which can be regarded as the L^2 gradient flow of the energy functional

$$E[\Phi] = \int_{\Omega} \left[\frac{\epsilon^2}{2} |\Delta \Phi|^2 + \frac{1}{4} (|\nabla \Phi|^2 - 1)^2 \right] d\mathbf{x}. \quad (1.2)$$

The above mentioned Φ indicates the periodic scaled height function. The chemical potential μ can be seen as the variational derivative of the functional (1.2) and be calculated by $\mu = \delta E / \delta \Phi$

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formally. Parameters κ and ϵ^2 are the mobility coefficient and the dissipation coefficient respectively. The fourth order term and the nonlinear second order term model the surface diffusion and the Ehrlich-Schwoebel effect respectively [9,31]. Due to the slope selection in the dynamics evolution, the solution of the model (1.1) is featured by the shape of pyramids or pyramid-like structures.

We consider the model (1.1) with the periodic boundary conditions and the initial condition $\Phi(\mathbf{x}, 0) = \phi_0(\mathbf{x})$. It reveals that the MBE model with slope selection has the properties of the mass conservation and the energy dissipation. Given $(u, v) = \int_{\Omega} uv \, d\mathbf{x}$ is the inner product in $L^2(\Omega)$ and $\|u\|_{L^2(\Omega)} = \sqrt{(u, u)}$ is the corresponding norm. Simple calculation leads to the mass conservation law $(\Phi(t), 1) = (\phi_0, 1)$ and the energy dissipation law as follows:

$$\frac{d}{dt}E[\Phi] = -\kappa\|\partial_t\Phi\|_{L^2}^2 \leq 0. \quad (1.3)$$

Many efficient and stable numerical methods have been developed and analyzed for the MBE equation with or without slope selection. See the relevant references [1, 7, 8, 11, 19, 22, 27–30, 33, 35–39], etc. To the best of our knowledge, several effective strategies have been developed to design the unconditional energy stable numerical schemes, such as the stabilized method, the convex splitting method, the invariant energy quadratization (IEQ) method and the scalar auxiliary variable (SAV) method, etc. Among these methods, we focus on the convex splitting strategy in dealing with the temporal approximation. In [35], the convex splitting method was applied to develop the first order unconditionally stable scheme for the MBE model. The second order convex splitting schemes [33] were proposed for the same model. The MBE model with slope selection was solved by a fully discrete finite difference scheme combining the convex splitting strategy [29]. And, the convergence analysis was carried out carefully. The first and second order linear energy stable schemes [2, 4] based on the convex splitting method were devised for a thin film model without slope selection. A second order unconditionally energy stable finite difference scheme [11], which combines the second order backward differentiation formula (BDF) and convex splitting method, was presented and analyzed for the MBE model with slope selection.

The high order energy stable numerical methods are more desirable because of the long time coarsening process of the MBE model, such as that in [3, 13, 15, 17], etc. The third order linear BDF schemes were devised for the MBE model without slope selection in [13, 17], and the modified energy dissipation law and the convergence of the numerical schemes were proved rigorously. Especially, the Douglas-Dupont type stabilization term in the form of $S\tau^2\Delta_h\delta_1\phi^n$, was added to ensure the energy stability for any temporal steps [13]. Recently, the fully implicit BDF methods up to fifth order [15] were studied for the no-slope MBE equation. Under certain temporal step constraints, the modified energy dissipation law and L^2 norm error analysis of the numerical schemes were constructed by using the tools including the discrete gradient structure of k -th order BDF (BDF k) formula and the discrete orthogonal convolution (DOC) kernels. Based on this idea, we proposed the BDF3-5 schemes [18] for the MBE model with slope selection, and analyzed those schemes under the theoretical framework [24]. However, the above proposed BDF3-5 schemes were proved to be uniquely solvable and energy stable under the temporal step constraint $\tau \leq 2\epsilon^2 \min\{2\sigma_{Lk}, b_0^{(k)}\}/\kappa$.

In this work, the unconditionally energy stable high order accurate methods, which remove the temporal step constraint on the energy dissipation law, are concerned for solving MBE model with slope selection. We combine the high order BDF formulas and the convex splitting method to deal with the time approximation in the time evolution process. However, for the

convex splitting strategy, the explicit treatment of the concave term might lead to the energy stability loss. Therefore, an artificial stabilized term, which always has the same order as the numerical scheme, is considered to replenish the energy. For example, the Douglas-Dupont type regularization terms in the form of $S\tau^{k-1}\Delta_N^s\delta_1u^n$ ($s = 1$ or 2) for $k = 1, 2, 3$, were applied to devise the unconditional energy stable schemes for the MBE models in [4, 13, 37]. From this perspective, we note that a third order convex splitting BDF scheme [6] was designed for the Cahn-Hilliard equation, and the theoretical analysis was demonstrated rigorously. Our main purpose is to construct the high order convex splitting BDF schemes with a class of stabilized terms and analyze them in the aspect of the unconditional stability and L^2 norm convergence for the MBE model with slope selection subject to the periodic boundary conditions. The main contributions are listed as follows:

1. For $k=3, 4, 5$, the k -th order accurate Douglas-Dupont type stabilization term $S\tau^{k-1}\Delta_h\delta_1\phi^n$ is added to construct the stabilized convex splitting BDF k scheme.
2. The discrete gradient decomposition is presented for the explicit extrapolation formula combining the implicit cubic term. For the properly selected stabilization parameter S , the energy dissipation law at the discrete levels is demonstrated for the proposed numerical scheme with respect to any time step τ .
3. With the help of the new proposed convolution embedding inequality, the error estimate of the stabilized BDF k ($k = 3, 4, 5$) method is proved in the L^2 norm rigorously.

The rest of the paper is organized as follows. In the next section, the stabilized convex splitting BDF k scheme is proposed with the spatial approximation by Fourier pseudo-spectral method. In Section 3, we show the unique solvability of the proposed BDF k scheme. The energy dissipation law at the discrete levels is established in a modified version, which leads to the prior estimate of the numerical solution. The convergence analysis is demonstrated with the help of the DOC kernels and convolution embedding inequalities in Section 4. In Section 5, numerical experiments are given to test the accuracy and efficiency of the developed k -th order ($k = 3, 4, 5$) scheme. Finally, a brief conclusion is presented in Section 6.

2. Numerical Scheme

In this section, we present the high order stabilized fully discrete numerical scheme for the MBE model with slope selection based on the k -th ($k = 3, 4, 5$) order accurate BDF formula, convex splitting strategy and Fourier pseudo-spectral method.

As a preliminary, some notations and definitions are presented. One divides the time interval $[0, T]$ by the nodes $t_n = n\tau$ ($0 \leq n \leq N$) with time step $\tau = T/N$. Given an arbitrary real sequence $\{v^n \mid n = 0, 1, 2, \dots, N\}$, define the following difference operators:

$$\delta_1v^n = v^n - v^{n-1}, \quad \delta_{m+1}v^n = \delta_m(\delta_1v^n) = \delta_mv^n - \delta_mv^{n-1}, \quad m \geq 1.$$

Denote the k -th order explicit extrapolation formula as follows:

$$\hat{v}^{(n,k)} = v^n - \delta_kv^n, \quad k = 3, 4, 5.$$

For any index $k = 3, 4, 5$, the BDF k formula is written as the convolution summation, namely

$$D_kv^n = \frac{1}{\tau} \sum_{\ell=1}^n b_{n-\ell}^{(k)} \delta_1v^\ell, \quad n \geq k, \quad (2.1)$$

Table 2.1: The BDF k kernels $b_j^{(k)}$.

BDF k	$b_0^{(k)}$	$b_1^{(k)}$	$b_2^{(k)}$	$b_3^{(k)}$	$b_4^{(k)}$
$k=3$	11/6	-7/6	1/3		
$k=4$	25/12	-23/12	13/12	-1/4	
$k=5$	137/60	-163/60	137/60	-21/20	1/5

in which the coefficients $b_j^{(k)}$ with $0 \leq j \leq n$ ($b_j^{(k)} = 0$ if $j \geq k$) are the so-called BDF k kernels presented in Table 2.1. In [24], the DOC kernels $\theta_j^{(k)}$ corresponding to the discrete BDF k kernels were firstly proposed by

$$\theta_0^{(k)} = \frac{1}{b_0^{(k)}}, \quad \theta_{n-j}^{(k)} = -\frac{1}{b_0^{(k)}} \sum_{\ell=j+1}^n \theta_{n-\ell}^{(k)} b_{\ell-j}^{(k)}, \quad j = k, k+1, \dots, n-2, n-1,$$

which will play an important role in the subsequent analysis including the mass conservation and error estimate. One verifies that the DOC kernels satisfy the DOC identity, that is

$$\sum_{\ell=j}^n \theta_{n-\ell}^{(k)} b_{\ell-j}^{(k)} \equiv \delta_{nj},$$

where δ_{nj} is the Kronecker delta symbol. Furthermore, by using the DOC kernels, the BDF k formula $D_k \phi^n$ can be transformed into the following form:

$$\sum_{j=k}^n \theta_{n-j}^{(k)} D_k \phi^j = \frac{1}{\tau} \phi_1^{(k,n)} + \frac{1}{\tau} \delta_1 \phi^n, \tag{2.2}$$

in which $\phi_1^{(k,n)}$ only contains the values of former $k-1$ levels, namely

$$\phi_1^{(k,n)} = \sum_{\ell=1}^{k-1} \delta_1 \phi^\ell \sum_{j=k}^n \theta_{n-j}^{(k)} b_{j-\ell}^{(k)}, \quad n \geq k. \tag{2.3}$$

One divides the space domain $\Omega = (0, L)^2$ by using the uniform meshes

$$\Omega_h = \{\mathbf{x}_h = (ih, jh) \mid 1 \leq i, j \leq M\},$$

where M is an even integer, and $h = L/M$ is the spatial step. Define the space of grid functions

$$\mathbb{V}_h = \{v \mid v = (v_h) \text{ is } (L, L)\text{-period for } \mathbf{x}_h \in \bar{\Omega}_h = \Omega_h \cup \partial\Omega_h\}.$$

Denote the space \mathcal{F}_M , which contains all the trigonometric polynomials of degree up to $M/2$. Suppose $P_M : L^2(\Omega) \rightarrow \mathcal{F}_M$ and $I_M : L^2(\Omega) \rightarrow \mathcal{F}_M$ are the standard L^2 projection operator and the trigonometric interpolation operator, respectively [32],

$$(P_M v)(\mathbf{x}) = \sum_{\ell, m=-M/2}^{M/2-1} \hat{v}_{\ell, m} e_{\ell, m}(\mathbf{x}), \quad (I_M v)(\mathbf{x}) = \sum_{\ell, m=-M/2}^{M/2-1} \tilde{v}_{\ell, m} e_{\ell, m}(\mathbf{x}),$$

where

$$e_{\ell, m}(\mathbf{x}) = \exp \frac{2\pi i(\ell x + m y)}{L}.$$

The projection coefficients $\hat{v}_{\ell,m}$ are the standard Fourier coefficients of function $v(\mathbf{x})$, and the pseudo-spectral coefficients $\tilde{v}_{\ell,m}$ are determined by $(I_M v)(\mathbf{x}_h) = v_h$. In turn, the Fourier pseudo-spectral p -th order derivatives of v_h with respect to x and y , are separately defined by

$$\mathcal{D}_x^p v_h = \sum_{\ell,m=-M/2}^{M/2-1} \left(\frac{2\pi\ell i}{L} \right)^p \tilde{v}_{\ell,m} e_{\ell,m}(\mathbf{x}_h), \quad \mathcal{D}_y^p v_h = \sum_{\ell,m=-M/2}^{M/2-1} \left(\frac{2\pi m i}{L} \right)^p \tilde{v}_{\ell,m} e_{\ell,m}(\mathbf{x}_h).$$

Furthermore, the discrete gradient and Laplacian are represented by the following equation:

$$\nabla_h v_h = (\mathcal{D}_x^1 v_h, \mathcal{D}_y^1 v_h)^\top, \quad \Delta_h v_h = \nabla_h \cdot (\nabla_h v_h) = \mathcal{D}_x^2 v_h + \mathcal{D}_y^2 v_h.$$

For any grid functions $v, w \in \mathbb{V}_h$, define the discrete inner product and the related norms by

$$\begin{aligned} \langle v, w \rangle &= h^2 \sum_{\mathbf{x}_h \in \Omega_h} v_h w_h, & \|v\|_{l^2} &= \sqrt{\langle v, v \rangle}, \\ \|v\|_{l^q} &= \sqrt[q]{h^2 \sum_{\mathbf{x}_h \in \Omega_h} |v_h|^q}, & \|\nabla_h v\| &= \sqrt{h^2 \sum_{\mathbf{x}_h \in \Omega_h} |\nabla_h v_h|^2}. \end{aligned}$$

For arbitrary grid functions $v, w \in \mathbb{V}_h$, the discrete Green's formulas [32] hold

$$\langle -\Delta_h v, w \rangle = \langle \nabla_h v, \nabla_h w \rangle, \quad \langle \Delta_h^2 v, w \rangle = \langle \Delta_h v, \Delta_h w \rangle. \quad (2.4)$$

Now, we are ready to design the numerical schemes for the MBE model with the slope selection (1.1). The BDFk ($k = 3, 4, 5$) formula is used for approximation in time, the concave term is approximated by the k -th order accurate explicit extrapolation formula, and the spatial operators are approached by Fourier pseudo-spectral method. In addition, the k -th order Douglas-Dupont type stabilization term is added to ensure the unconditional stability. For the sake of presentation, we denote the exact solution by $\Phi_h^n = \Phi(\mathbf{x}_h, t_n)$ and its approximate value by $\phi_h^n \approx \Phi(\mathbf{x}_h, t_n)$. Furthermore, we present the fully discrete stabilized convex splitting BDFk scheme to simulate the MBE model (1.1). That is, finding $\phi^n \in \mathbb{V}_h$ such that

$$\begin{aligned} D_k \phi^n &= -\kappa \mu^n + S \tau^{k-1} \Delta_h \delta_1 \phi^n, \\ \mu^n &= \epsilon^2 \Delta_h^2 \phi^n - \nabla_h \cdot (|\nabla_h \phi^n|^2 \nabla_h \phi^n) + \Delta_h \hat{\phi}^{(n,k)}, \quad k \leq n \leq N, \end{aligned} \quad (2.5)$$

where $S \geq 0$ is called the stabilized parameter. From the above scheme, once the initial value is given, one needs to choose certain numerical method to compute the numerical solution of the former $k - 1$ time levels, and the selected method should ensure the accuracy of the proposed numerical schemes.

Remark 2.1. The BDF method is applied to get the high order time approximation in the proposed numerical scheme for simulating the MBE model with slope selection. From this perspective, other algorithms such as the ETD multi-step scheme [3] are also very efficient for solving gradient flows. For the proposed BDF-type scheme and the ETD-based scheme [3], they all require other methods, such as Runge-Kutta method, to provide starting values. The advantage of the ETD multi-step method is explicit, while it requires to design an iteration method to solve the BDF method. However, the calculation of a matrix exponential may be expensive, and the efficient algorithm to accurately compute the matrix exponential is still limited [10]. It is very meaningful and challenging to discuss and compare the ETD multi-step method and the BDF method in different models, spatial discretizations and iteration methods.

3. Solvability and Energy Dissipation Law

In this section, the unique solvability of the stabilized convex splitting BDF k ($k = 3, 4, 5$) scheme (2.5) can be proved by demonstrating that the auxiliary convex, coercive functional has the unique minimizer. The discrete dissipation law in a modified version will be built up by using the tools of the discrete gradient decompositions of the BDF formulas and explicit extrapolations.

We assume that the numerical value of the first $(k - 1)$ -level conserve the mass $\langle \phi^n, 1 \rangle = \langle \phi^0, 1 \rangle$ for $1 \leq n \leq k$ with $k = 3, 4, 5$. Thus, it is not difficult to obtain the mass conservation law of the numerical solution ϕ^n . Actually, taking the inner product with the numerical scheme (2.5) by 1, it leads to

$$\langle D_k \phi^j, 1 \rangle = -\kappa \langle \mu^j, 1 \rangle + S\tau^{k-1} \langle \Delta_h \delta_1 \phi^j, 1 \rangle = 0, \quad j \geq k. \quad (3.1)$$

Multiplying the both sides of the Eq. (3.1) by the DOC kernels $\theta_{n-j}^{(k)}$, summing the results in j from k to n , and applying the Eq. (2.2), one gets

$$0 = \sum_{j=k}^n \theta_{n-j}^{(k)} \langle D_k \phi^j, 1 \rangle = \left\langle \frac{1}{\tau} \delta_1 \phi^n + \frac{1}{\tau} \phi_1^{(k,n)}, 1 \right\rangle,$$

which implies $\langle \delta_1 \phi^n, 1 \rangle = 0$. Therefore, the mass conservation law, $\langle \phi^n, 1 \rangle = \langle \phi^0, 1 \rangle$ for $n \geq 1$, holds by a simple recurrence.

Next, we focus on the unique solvability of the proposed numerical schemes. As a preliminary, we define the space

$$\mathbb{V}_h^* = \{z \in \mathbb{V}_h \mid \langle z - \phi^{n-1}, 1 \rangle = 0\},$$

and introduce the notation

$$\mathcal{L}^{n-1} = \sum_{\ell=1}^{n-1} b_{n-\ell}^{(k)} \delta_1 \phi^\ell$$

for the index $n \geq k$ with $k = 3, 4, 5$.

Theorem 3.1. *The stabilized convex splitting BDF k ($k = 3, 4, 5$) scheme is uniquely solvable.*

Proof. For any time level index $n \geq k$, we present the discrete energy functional $G[z]$ on \mathbb{V}_h^* as follows:

$$\begin{aligned} G[z] &= \frac{b_0^{(k)}}{2\tau} \|z - \phi^{n-1}\|^2 + \frac{1}{\tau} \langle \mathcal{L}^{n-1}, z - \phi^{n-1} \rangle + \frac{S}{2} \tau^{k-1} \|\nabla_h(z - \phi^{n-1})\|^2 \\ &\quad + \frac{\kappa \epsilon^2}{2} \|\Delta_h z\|^2 + \frac{\kappa}{4} \|\nabla_h z\|_{l^4}^4 + \kappa \langle \Delta_h \hat{\phi}^{(n,k)}, z \rangle. \end{aligned}$$

For any $\lambda \in \mathbb{R}$ and $\psi \in \mathbb{V}_h$, one considers the second derivative of functional $G[z + \lambda\psi]$ with respect to λ at point $\lambda = 0$, namely

$$\frac{d^2}{d\lambda^2} G[z + \lambda\psi]_{\lambda=0} = \frac{b_0^{(k)}}{\tau} \|\psi\|^2 + S\tau^{k-1} \|\nabla_h \psi\|^2 + \kappa \epsilon^2 \|\Delta_h \psi\|^2 + 3\kappa \|\nabla_h z \nabla_h \psi\|^2 \geq 0,$$

which implies that the functional $G[z]$ is strictly convex. It is not difficult to show the functional $G[z]$ is coercive on \mathbb{V}_h , that is,

$$G[z] \geq \frac{b_0^{(k)}}{2\tau} \|z - \phi^{n-1}\|^2 - \frac{b_0^{(k)}}{4\tau} \|z - \phi^{n-1}\|^2 - \frac{1}{\tau b_0^{(k)}} \|\mathcal{L}^{n-1}\|^2$$

$$\begin{aligned}
& + \frac{\kappa\epsilon^2}{2} \|\Delta_h z\|^2 - \frac{\kappa\epsilon^2}{2} \|\Delta_h z\|^2 - \frac{\kappa}{2\epsilon^2} \|\hat{\phi}^{(n,k)}\|^2 \\
& = \frac{b_0^{(k)}}{4\tau} \|z - \phi^{n-1}\|^2 - \frac{1}{\tau b_0^{(k)}} \|\mathcal{L}^{n-1}\|^2 - \frac{\kappa}{2\epsilon^2} \|\hat{\phi}^{(n,k)}\|^2,
\end{aligned}$$

where the evaluation

$$\langle \Delta_h \hat{\phi}^{(n,k)}, z \rangle = \langle \hat{\phi}^{(n,k)}, \Delta_h z \rangle \leq \frac{\epsilon^2}{2} \|\Delta_h z\|^2 + \frac{1}{2\epsilon^2} \|\hat{\phi}^{(n,k)}\|^2$$

is applied in the first step of the above estimate.

Therefore, the functional $G[z]$ has a unique minimizer denoted by ϕ^n , if and only if it solves the following equation:

$$\begin{aligned}
0 = \frac{d}{d\lambda} G[z + \lambda\psi] \Big|_{\lambda=0} & = \left\langle \frac{b_0^{(k)}}{\tau} (z - \phi^{n-1}) + \frac{1}{\tau} \mathcal{L}^{n-1} - S\tau^{k-1} \Delta_h (z - \phi^{n-1}) \right. \\
& \quad \left. + \kappa\epsilon^2 \Delta_h^2 z - \kappa \nabla_h \cdot (|\nabla_h z|^2 \nabla_h z) + \kappa \Delta_h \hat{\phi}^{(n,k)}, \psi \right\rangle.
\end{aligned}$$

Notice that the above equation holds for any $\psi \in \mathbb{V}_h$. Therefore, the numerical scheme (2.5) is uniquely solvable. This completes the proof. \square

Furthermore, one applies the gradient structure of BDFk formula and the k -th order explicit extrapolation formula for constructing the energy dissipation law of the numerical scheme (2.5). Actually, for any sequence (w^n, \dots, w^1, w^0) , a gradient decomposition of the k -th order BDF formula is presented in the manner of

$$w^n \sum_{j=1}^n b_{n-j}^{(k)} w^j = \mathcal{G}_k[w^n] - \mathcal{G}_k[w^{n-1}] + \frac{\sigma_{Lk}}{2} (w^n)^2 + \mathcal{R}_k[w^n], \quad n \geq k, \quad (3.2)$$

where $\mathcal{G}_k[v]$ and $\mathcal{R}_k[v]$ are positive functionals defined by

- For $k = 3$, the constant $\sigma_{L3} = 95/48 \approx 1.979$,

$$\mathcal{G}_3[w^n] = \frac{1}{6} (w^n)^2 + \frac{1}{6} \left(\frac{7}{4} w^n - w^{n-1} \right)^2, \quad \mathcal{R}_3[w^n] = \frac{1}{6} \left(\delta_1^2 w^n + \frac{1}{4} w^{n-1} \right)^2.$$

- For $k = 4$, the constant $\sigma_{L4} = 4919/3072 \approx 1.601$,

$$\begin{aligned}
\mathcal{G}_4[w^n] & = \frac{13627}{43008} (w^n)^2 + \frac{7}{24} \left(\frac{65}{56} w^n - w^{n-1} \right)^2 + \frac{1}{8} \left(\frac{3}{2} \delta_1 w^n + w^{n-2} \right)^2, \\
\mathcal{R}_4[w^n] & = \frac{1}{8} \left(\delta_1^3 w^n + \frac{3}{2} \delta_1 w^{n-1} \right)^2 + \frac{1}{6} \left(\delta_1^2 w^n + \frac{35}{32} w^{n-1} \right)^2.
\end{aligned}$$

- For $k = 5$, the constant $\sigma_{L5} = 646631/1920000 \approx 0.3367$,

$$\begin{aligned}
\mathcal{G}_5[w^n] & = \frac{1198850903}{1678080000} (w^n)^2 + \frac{437}{900} \left(\frac{4931}{6992} w^n - w^{n-1} \right)^2 \\
& \quad + \frac{9}{40} \left(\frac{23}{18} \delta_1 w^n + w^{n-2} \right)^2 + \frac{1}{10} (2\delta_1 w^n + 2w^{n-2} - w^{n-3})^2, \\
\mathcal{R}_5[w^n] & = \frac{1}{10} (\delta_1^4 w^n + 2\delta_1^2 w^{n-1})^2 + \frac{1}{8} \left(\delta_1^3 w^n + \frac{23}{10} \delta_1 w^{n-1} \right)^2 + \frac{1}{6} \left(\delta_1^2 w^n + \frac{1787}{800} w^{n-1} \right)^2.
\end{aligned}$$

One refers to [15, 21, 26, 34] for more details. To handle the k -th order explicit extrapolation $\hat{\phi}^{(k,n)}$, we develop a class of gradient structures of the high order explicit extrapolations (together with the cubic polynomial nonlinear term). As a matter of convenience, we define functionals $\mathcal{F}_k, \mathfrak{R}_k$ (for the index $k = 3, 4, 5$) associated with $(w^n, w^{n-1}, \dots, w^1, w^0)$. For the purpose of simplicity, we introduce the notations as follows:

$$\mathcal{F}_k[w^n] \triangleq \mathcal{F}_k[w^n, w^{n-1}, \dots, w^0], \quad \mathfrak{R}_k[w^n] \triangleq \mathfrak{R}_k[w^n, w^{n-1}, \dots, w^0], \quad n \geq k.$$

For the index $k = 3, 4, 5$, the decomposition related to the explicit extrapolation is listed in the following lemma, and the proof will be presented in the Appendix.

Lemma 3.1. *For any sequence (v^n, \dots, v^1, v^0) , it holds that*

$$\begin{aligned} & [(v^n)^3 - \hat{v}^{(n,k)}] \delta_1 v^n \\ &= \frac{1}{4} [(v^n)^2 - 1]^2 - \frac{1}{4} [(v^{n-1})^2 - 1]^2 + \frac{1}{2} (v^n)^2 (\delta_1 v^n)^2 \\ & \quad + \frac{1}{4} [(v^n)^2 - (v^{n-1})^2]^2 + \mathcal{F}_k[\delta_1 v^n] \\ & \quad - \mathcal{F}_k[\delta_1 v^{n-1}] - \gamma_k (\delta_1 v^n)^2 + \mathfrak{R}_k[\delta_1 v^n], \quad n \geq k, \end{aligned} \quad (3.3)$$

where the positive constant γ_k , quadratic functionals $\mathcal{F}_k[w^n]$ and $\mathfrak{R}_k[w^n]$ are defined by

- For $k = 3$, the constant $\gamma_3 = 1$,

$$\mathcal{F}_3[w^n] = \frac{1}{2} (w^n)^2 + \frac{1}{2} (\delta_1 w^n)^2, \quad \mathfrak{R}_3[w^n] = \frac{1}{2} (\delta_2 w^n + w^{n-1})^2.$$

- For $k = 4$, the constant $\gamma_4 = 31/8$,

$$\begin{aligned} \mathcal{F}_4[w^n] &= \frac{13}{8} (w^n)^2 + \frac{5}{4} (w^{n-1})^2 + \frac{1}{2} (w^{n-2})^2 + \frac{3}{4} (\delta_1 w^n)^2, \\ \mathfrak{R}_4[w^n] &= \frac{3}{2} \left(\delta_2 w^n + \frac{3}{2} w^{n-1} \right)^2 + \frac{1}{2} (\delta_3 w^n + 3\delta_1 w^{n-1})^2. \end{aligned}$$

- For $k = 5$, the constant $\gamma_5 = 67/4$,

$$\begin{aligned} \mathcal{F}_5[w^n] &= \frac{39}{4} (w^n)^2 + \frac{19}{2} (w^{n-1})^2 + \frac{7}{2} (w^{n-2})^2 + \frac{3}{2} (w^{n-3})^2 + (\delta_1 w^n)^2, \\ \mathfrak{R}_5[w^n] &= 4 \left(\delta_2 w^n + \frac{7}{4} w^{n-1} \right)^2 + (\delta_2 w^{n-1} + 2w^{n-3})^2 \\ & \quad + 2(\delta_3 w^n + 3\delta_1 w^{n-1})^2 + \frac{1}{2} (\delta_4 w^n + 4\delta_2 w^{n-1})^2. \end{aligned}$$

Denote the discrete version of free energy (1.2) by

$$E[\phi^n] = \frac{\epsilon^2}{2} \|\Delta_h \phi^n\|^2 + \frac{1}{4} \|\ |\nabla_h \phi^n|^2 - 1 \|^2,$$

and the modified discrete energy by

$$\mathcal{E}_k[\phi^n] = E[\phi^n] + \frac{1}{\kappa\tau} \langle \mathcal{G}_k[\delta_1 \phi^n], 1 \rangle + \langle \mathcal{F}_k[\nabla_h \delta_1 \phi^n], 1 \rangle, \quad n \geq k, \quad k = 3, 4, 5. \quad (3.4)$$

Then we have the following discrete energy dissipation law.

Theorem 3.2. For $k = 3, 4, 5$, if the stabilized parameter S satisfies

$$S \geq \frac{4^{k-1} \kappa^k (1 + \gamma_k)^{3k-3} (k-2)^{k-2}}{[27\sigma_{Lk}\epsilon^2(k-1)]^{k-1}}, \quad (3.5)$$

the stabilized convex splitting BDFk scheme (2.5) preserves the modified energy dissipation law (3.4) at the discrete levels, namely

$$\mathcal{E}_k[\phi^n] \leq \mathcal{E}_k[\phi^{n-1}], \quad n \geq k.$$

Proof. Taking the inner product on both sides of (2.5) with $\delta_1 \phi^n / \kappa$, it follows that

$$\begin{aligned} & \frac{1}{\kappa} \langle D_k \phi^n, \delta_1 \phi^n \rangle + \epsilon^2 \langle \Delta_h^2 \phi^n, \delta_1 \phi^n \rangle \\ & + \langle |\nabla_h \phi^n|^2 \nabla_h \phi^n - \nabla_h \hat{\phi}^{(n,k)}, \nabla_h \delta_1 \phi^n \rangle \\ & + \frac{S}{\kappa} \tau^{k-1} \|\nabla_h \delta_1 \phi^n\|^2 = 0, \quad n \geq k. \end{aligned} \quad (3.6)$$

Based on the gradient structure (3.2) of the high order BDF formulas, the first term on the left-hand side of the above equality is handled by

$$\begin{aligned} \langle D_k \phi^n, \delta_1 \phi^n \rangle &= \frac{1}{\tau} \left\langle \sum_{j=k}^n b_{n-j}^{(k)} \delta_1 \phi^j, \delta_1 \phi^n \right\rangle \\ &\geq \frac{1}{\tau} \langle \mathcal{G}_k[\delta_1 \phi^n], 1 \rangle - \frac{1}{\tau} \langle \mathcal{G}_k[\delta_1 \phi^{n-1}], 1 \rangle + \frac{\sigma_{Lk}}{2\tau} \|\delta_1 \phi^n\|^2. \end{aligned} \quad (3.7)$$

By using simple identity $2a(a-b) = a^2 - b^2 + (a-b)^2$, the surface diffusion term is treated as

$$\langle \Delta_h^2 \phi^n, \delta_1 \phi^n \rangle = \langle \Delta_h \phi^n, \delta_1 \Delta_h \phi^n \rangle = \frac{1}{2} \|\Delta_h \phi^n\|^2 - \frac{1}{2} \|\Delta_h \phi^{n-1}\|^2 + \frac{1}{2} \|\delta_1 \Delta_h \phi^n\|^2. \quad (3.8)$$

Taking $v_n = \nabla_h \phi^n$ in Lemma 3.1, one deals with the cubic term together with the explicit extrapolation of the concave term as follows:

$$\begin{aligned} & \langle |\nabla_h \phi^n|^2 \nabla_h \phi^n - \nabla_h \hat{\phi}^{(n,k)}, \delta_1 \nabla_h \phi^n \rangle \\ & \geq \frac{1}{4} \|\nabla_h \phi^n\|^2 - 1 \|^2 - \frac{1}{4} \|\nabla_h \phi^{n-1}\|^2 - 1 \|^2 \\ & + \langle \mathcal{F}_k[\nabla_h \delta_1 \phi^n], 1 \rangle - \langle \mathcal{F}_k[\delta_1 \nabla_h \phi^{n-1}], 1 \rangle - \gamma_k \|\delta_1 \nabla_h \phi^n\|^2. \end{aligned} \quad (3.9)$$

The substitution of inequalities (3.7)-(3.9) into the equality (3.6) implies that

$$\mathcal{E}_k[\phi^n] + \left(\frac{S}{\kappa} \tau^{k-1} - \gamma_k \right) \|\delta_1 \nabla_h \phi^n\|^2 + \frac{\sigma_{Lk}}{2\kappa\tau} \|\delta_1 \phi^n\|^2 + \frac{\epsilon^2}{2} \|\delta_1 \Delta_h \phi^n\|^2 \leq \mathcal{E}_k[\phi^{n-1}] \quad (3.10)$$

for $n \geq k$. Notice the elementary inequality

$$1 + \frac{S}{\kappa} \tau^{k-1} = \sum_{i=1}^{k-2} \frac{1}{k-2} + \frac{S}{\kappa} \tau^{k-1} \geq \frac{k-1}{(k-2)^{\frac{k-2}{k-1}}} \left(\frac{S}{\kappa} \right)^{\frac{1}{k-1}} \tau.$$

Furthermore, applying the stabilized parameter setting (3.5), it holds that

$$\left[\frac{(k-1)\tau}{(k-2)^{\frac{k-2}{k-1}}} \left(\frac{S}{\kappa} \right)^{\frac{1}{k-1}} - 1 - \gamma_k \right] \|\delta_1 \nabla_h \phi^n\|^2 + \frac{\sigma_{Lk}}{2\kappa\tau} \|\delta_1 \phi^n\|^2 + \frac{\epsilon^2}{2} \|\delta_1 \Delta_h \phi^n\|^2$$

$$\begin{aligned}
&\geq \left[\frac{(k-1)\tau}{(k-2)^{\frac{k-2}{k-1}}} \left(\frac{S}{\kappa}\right)^{\frac{1}{k-1}} - 1 - \gamma_k + \sqrt{\frac{\sigma_{Lk}\epsilon^2}{\kappa\tau}} \right] \|\delta_1 \nabla_h \phi^n\| \\
&\geq \left\{ \left[\frac{27\sigma_{Lk}\epsilon^2}{4\kappa} \frac{(k-1)}{(k-2)^{\frac{k-2}{k-1}}} \left(\frac{S}{\kappa}\right)^{\frac{1}{k-1}} \right]^{\frac{1}{3}} - 1 - \gamma_k \right\} \|\delta_1 \nabla_h \phi^n\| \geq 0,
\end{aligned} \tag{3.11}$$

in which

$$\sqrt{\frac{\sigma_{Lk}\epsilon^2}{\kappa\tau}} \|\delta_1 \nabla_h \phi^n\|^2 \leq \sqrt{\frac{\sigma_{Lk}\epsilon^2}{\kappa\tau}} \|\delta_1 \phi^n\| \cdot \|\delta_1 \Delta_h \phi^n\| \leq \frac{\sigma_{Lk}}{2\kappa\tau} \|\delta_1 \phi^n\|^2 + \frac{\epsilon^2}{2} \|\delta_1 \Delta_h \phi^n\|^2$$

is used in the first step and the Young inequality is applied in the second step. A combination of (3.10) and (3.11) leads to the modified energy dissipation law. The proof is complete. \square

Remark 3.1. To balance the energy growth loss caused by the explicit treatment of concave term, we add the k -th order artificial Douglas-Dupont-type regularization term in the form of $S\tau^{k-1}\Delta_h\delta_1\phi^n$, which has the lower order than that of the surface diffusion term. It reveals that the higher order artificial diffusion term may cause additional numerical dissipation in the long time simulation [5].

The restriction of the stabilized parameter, $S = \mathcal{O}(\kappa^k/\epsilon^{2(k-1)})$, is required to obtain the modified energy dissipation law with no restriction on time step size. However, when we carried out the artificial stabilized term $S\tau^{k-1}\Delta_h^2\delta_1\phi^n$, the parameter setting becomes

$$S \geq \frac{\kappa^k(1+\gamma_k)^{2k-2}(k-2)^{k-2}}{2[\sigma_{Lk}(k-1)]^{k-1}} \frac{1}{(\epsilon^2)^{k-2}}$$

by using the similar derivation of the Theorem 3.2. Specifically, the parameter constraint is $S = \mathcal{O}(1/\epsilon^2)$ for $k = 3$, which is similar to the result in [13].

To facilitate the error analysis, an assumption is imposed on the numerical solution of the former $k-1$ levels. For any $k = 3, 4, 5$, it holds that $\mathcal{E}_k[\phi^n] \leq c_0$ ($1 \leq n \leq k-1$), where the positive constant c_0 mainly relies on the starting value $\phi^0, \phi^1, \dots, \phi^{k-1}$, but is independent of the spatial step h and the temporal step τ . With the help of the discrete Sobolev embedding inequality [32]

$$\|v\|_{l^6} \leq c_\Omega(\|v\| + \|\nabla_h v\|), \quad v \in \mathbb{V}_h, \tag{3.12}$$

and similarly to the proof of [18, Theorem 3.3], one gets the following theorem.

Theorem 3.3. *The numerical solution of the stabilized convex splitting BDFk scheme (2.5) is bounded in the manner of*

$$\|\nabla_h \phi^n\|_{l^6} \leq c_\Omega \sqrt{4c_0\epsilon^{-2} + (\epsilon^2 + 2)|\Omega|} =: c_1. \tag{3.13}$$

Overall, one obtains the unconditional energy stability of the numerical scheme, which listed in Theorem 3.2. Following the energy dissipation law, one gets the boundedness of the numerical solution, which will play a key role in the convergence analysis.

$$\sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} (w^\ell)^\top v^j \leq \varepsilon \sum_{\ell=k}^n (v^\ell)^\top v^j + \frac{\mathbf{m}_{3k}}{4\mathbf{m}_{1k}\varepsilon} \sum_{\ell=k}^n (w^\ell)^\top w^\ell.$$

Lemma 4.3. *For any real vector sequences $v^\ell, w^\ell \in \mathbb{R}^2$ ($k \leq \ell \leq n$), it holds*

$$\sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} (w^\ell)^\top v^j \leq \varepsilon \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} (w^\ell)^\top w^j + \frac{\mathbf{m}_{2k}\mathbf{m}_{3k}}{2\mathbf{m}_{1k}^2\varepsilon} \sum_{\ell=k}^n (v^\ell)^\top v^\ell, \quad \forall \varepsilon > 0.$$

Proof. Based on the property of the matrix Θ_k that its minimum eigenvalue has the positive lower bound $\mathbf{m}_{1k}/\mathbf{m}_{2k}$, it is natural to get

$$\sum_{\ell=k}^n (w^\ell)^\top w^\ell \leq \frac{2\mathbf{m}_{2k}}{\mathbf{m}_{1k}} \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} (w^\ell)^\top w^j. \quad (4.5)$$

It follows from the second inequality with $\varepsilon = \mathbf{m}_{2k}\mathbf{m}_{3k}/(2\mathbf{m}_{1k}^2\varepsilon)$ in Lemma 4.2 that the desired result holds. This ends the proof. \square

Lemma 4.4. *Suppose that any real vector sequences $v^\ell, z^\ell \in \mathbb{V}_h$ ($k \leq \ell \leq n$) and there exist nonnegative constants c_v such that $\|v^\ell\|_{l^3} \leq c_v$. Then, for any $\varepsilon > 0$, it holds that*

$$\begin{aligned} & \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle v^j z^j, z^\ell \rangle \\ & \leq \varepsilon \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \nabla_h z^j, \nabla_h z^\ell \rangle \\ & \quad + \left(\varepsilon + \frac{2c_v^2 c_\Omega^2 \mathbf{m}_{2k}^2 \mathbf{m}_{3k}}{\mathbf{m}_{1k}^3 \varepsilon} \right) \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle z^j, z^\ell \rangle. \end{aligned}$$

Proof. With the help of Lemma 4.3, the Hölder inequality and imbedding inequality (3.12), one obtains

$$\begin{aligned} & \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle v^j z^j, z^\ell \rangle \\ & \leq \varepsilon_1 \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle z^j, z^\ell \rangle + \frac{\mathbf{m}_{2k}\mathbf{m}_{3k}}{2\mathbf{m}_{1k}^2\varepsilon_1} \sum_{\ell=k}^n \|v^\ell z^\ell\|^2 \\ & \leq \varepsilon_1 \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle z^j, z^\ell \rangle + c_v^2 c_\Omega^2 \frac{\mathbf{m}_{2k}\mathbf{m}_{3k}}{\mathbf{m}_{1k}^2\varepsilon_1} \sum_{\ell=k}^n (\|z^\ell\|^2 + \|\nabla_h z^\ell\|^2). \end{aligned} \quad (4.6)$$

Applying the estimate (4.5) and taking $\varepsilon_1 = 2c_v^2 c_\Omega^2 \mathbf{m}_{2k}^2 \mathbf{m}_{3k}/(\mathbf{m}_{1k}^3 \varepsilon)$, it follows from the inequality (4.6) that the desired result holds. This completes the proof. \square

Lemma 4.5 ([24]). *For the index $k = 3, 4, 5$, the DOC kernels $\theta_j^{(k)}$ ($j \geq 0$) are positive definite and satisfy the decaying estimates*

$$|\theta_j^{(k)}| \leq \frac{\rho_k}{4} \left(\frac{k}{7} \right)^j,$$

where the constants $\rho_3 = 10/3, \rho_4 = 6, \rho_5 = 96/5$. Furthermore, there exist positive constants $c_{1k} \geq 1$ such that

$$\sum_{j=k}^n |\phi_1^{(k,j)}| \leq \frac{7c_{1k}\rho_k}{8(7-k)} \sum_{\ell=1}^{k-1} |\delta_1 \phi^\ell|, \quad n \geq k.$$

As a preliminary, we define the truncation errors and give their estimates. Let $\Phi_M = P_M \Phi$ be the L^2 projection of the exact solution Φ . Then, we obtain the semi-discrete system of Eq. (1.1) as follows:

$$\partial_t \Phi_M = -\kappa \mu_M + r_P, \quad \mu_M = \epsilon^2 \Delta_h^2 \Phi_M - \nabla_h \cdot (|\nabla_h \Phi_M|^2 \nabla_h \Phi_M) + \Delta_h \Phi_M, \quad (4.7)$$

where $r_P(\mathbf{x}_h, t)$ is the spatial consistency error

$$r_P = \partial_t \Phi_M - \partial_t \Phi + \kappa(\mu_M - \mu), \quad \mathbf{x}_h \in \Omega_h. \quad (4.8)$$

Denote $r_P^n = r_P(\mathbf{x}_h, t_n)$. For any $k = 3, 4, 5$, applying the k -th order BDF formula and explicit extrapolation formula to the semi-discrete approximation equation (4.7), adding the k -th order Douglas-Dupont type stabilization term, one obtains an approximation equation of (1.1)

$$\begin{aligned} D_k \Phi_M^n &= -\kappa \mu_M^n + S\tau^{k-1} \Delta_h \delta_1 \Phi_M^n + r_P^n + r_\Phi^n, \\ \mu_M^n &= \epsilon^2 \Delta_h^2 \Phi_M^n - \nabla_h \cdot (|\nabla_h \Phi_M^n|^2 \nabla_h \Phi_M^n) + \Delta_h \hat{\Phi}_M^{(n,k)}, \quad k \leq n \leq N, \end{aligned} \quad (4.9)$$

where r_Φ^n comes from the BDFk formula, k -th order extrapolation and stabilization term,

$$r_\Phi^n = D_k \Phi_M(t_n) - \partial_t \Phi_M(t_n) + \kappa [\Delta_h \hat{\Phi}_M^{(n,k)} - \Delta_h \Phi_M(t_n)] - S\tau^{k-1} \Delta_h \delta_1 \Phi_M(t_n). \quad (4.10)$$

For the convenience of error estimate, one defines the global spatial and temporal errors by

$$R_P^\ell = \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} r_P^j, \quad R_\Phi^\ell = \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} r_\Phi^j, \quad \ell \geq k. \quad (4.11)$$

Suppose that the exact solution of MBE problem satisfies $\Phi \in C^{k+1}([0, T]; H_{per}^{m+4})$ for certain nonnegative integer m . There exists positive constant C_Φ such that

$$|r_\Phi^j| \leq C_\Phi \tau^k \max_{t_k \leq t \leq T} \{|\partial_t^{k+1} \Phi(t)| + \kappa |\Delta \partial_t^k \Phi(t)| + S |\Delta \partial_t \Phi(t)|\} \leq C_\Phi \tau^k, \quad j \geq k. \quad (4.12)$$

It follows from the proof of [20, Theorem 3.1] that the estimate of spatial error satisfies $\|r_P^n\| \leq C_\Phi h^m$. Furthermore, by using Lemma 4.5, we have

$$\sum_{\ell=k}^n \tau \|R_\Phi^\ell\| \leq \frac{\rho_k t_{n-k+1}}{7-k} C_\Phi \tau^k, \quad \sum_{\ell=k}^n \tau \|R_P^\ell\| \leq \frac{\rho_k t_{n-k+1}}{7-k} C_\Phi h^m, \quad n \geq k. \quad (4.13)$$

It notes that C_Φ mentioned in the paper represents a generalized positive constant, which is not necessarily the same in different cases.

Theorem 4.1. *If the time step satisfies*

$$\tau \leq \min \left\{ \left(\frac{\kappa \epsilon}{3S} \right)^{\frac{1}{k-1}}, \left(\frac{\mathbf{m}_{1k}^2 \epsilon}{\mathbf{m}_{2k} \mathbf{m}_{3k} S} \right)^{\frac{1}{k}}, \frac{\mathbf{m}_{1k} \epsilon^2}{12\kappa C_4^2} \right\},$$

the numerical solution of the fully discrete stabilized convex splitting BDFk scheme (2.5) is convergent in the L^2 norm. In details, the following estimate holds for $k \leq n \leq N$ with $k = 3, 4, 5$:

$$\|\Phi^n - \phi^n\| \leq \exp(c_5 t_{n-k+1}) \left[c_6 \sum_{\ell=0}^{k-1} \|\Phi_M^\ell - \phi^\ell\| + C_\Phi t_{n-k+1} (\tau^k + h^m) \right],$$

where

$$c_5 = 6\kappa \frac{2c_4^2 \mathbf{m}_{1k} + \hat{C}_k \mathbf{m}_{2k} \mathbf{m}_{3k}}{\mathbf{m}_{1k}^2 \epsilon^2}, \quad c_6 = \frac{14c_{1k} \rho_k}{7-k} + \frac{6\kappa \mathbf{m}_{2k} \mathbf{m}_{3k} \hat{C}_k \tau}{\mathbf{m}_{1k} \epsilon^2}.$$

Proof. Let $\Phi_M^n = P_M \Phi^n$ be the L^2 projection of the exact solution at time $t = t_n$ and $e^n = \Phi_M^n - \phi^n$ be the error between the projection Φ_M^n and the numerical solution ϕ^n of the proposed numerical scheme (2.5). It is clear that the error between the exact solution and numerical solution can be estimated by the following triangle inequality:

$$\|\Phi^n - \phi^n\| \leq \|\Phi^n - \Phi_M^n\| + \|e^n\|, \quad k \leq n \leq N. \quad (4.14)$$

By applying Lemma 4.1, one finds that $\|\Phi^n - \Phi_M^n\| \leq C_\Phi h^m |\Phi^n|_{H^m}$. It remains to estimate the error between the projection solution and the numerical solution.

Subtracting the numerical scheme (2.5) from the approximation system (4.9), one has the error equations as follows:

$$\begin{aligned} D_k e^n &= -\kappa \mu_e^n + S\tau^{k-1} \Delta_h \delta_1 e^n + r_P^n + r_\Phi^n, \quad k \leq n \leq N, \\ \mu_e^n &= \epsilon^2 \Delta_h^2 e^n - \nabla_h \cdot (|\nabla_h \Phi_M^n|^2 \nabla_h \Phi_M^n - |\nabla_h \phi^n|^2 \nabla_h \phi^n) + \Delta_h \hat{e}^{(n,k)}. \end{aligned} \quad (4.15)$$

Replacing the index n with j and multiplying both sides of (4.15) by $\tau \theta_{\ell-j}^{(k)}$ and summing the index j from k to ℓ , we apply (2.2) with $\phi^\ell = e^\ell$ to get an equivalent convolution form of error system (4.15), that is

$$\begin{aligned} \delta_1 e^\ell &= -\kappa \epsilon^2 \tau \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \Delta_h^2 e^j + \kappa \tau \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \nabla_h \cdot (u^j \nabla_h e^j) - \kappa \tau \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \Delta_h \hat{e}^{(j,k)} \\ &\quad + S\tau^k \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \Delta_h \delta_1 e^j - e_1^{(k,\ell)} + \tau R_P^\ell + \tau R_\Phi^\ell, \quad k \leq n \leq N, \end{aligned} \quad (4.16)$$

where

$$u^j = (\nabla_h \Phi_M^j)^2 + \nabla_h \phi^j \nabla_h \Phi_M^j + (\nabla_h \phi^j)^2,$$

the global spatial error R_P^ℓ and temporal error R_Φ^ℓ are given by equality (4.11), $e_1^{(k,\ell)}$ represents the starting error of the numerical solution

$$e_1^{(k,\ell)} = \sum_{i=1}^{k-1} \delta_1 e^i \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} b_{j-i}^{(k)}, \quad \ell \geq k. \quad (4.17)$$

Considering the inner product of the Eq. (4.16) with $2e^\ell$ and summing the results in ℓ from k to n , it follows that

$$\begin{aligned} \|e^n\|^2 - \|e^{k-1}\|^2 &+ \sum_{\ell=k}^n \|\delta_1 e^\ell\|^2 \\ &= -2\kappa \tau \epsilon^2 \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \Delta_h e^j, \Delta_h e^\ell \rangle - 2\kappa \tau \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle u^j \nabla_h e^j, \nabla_h e^\ell \rangle \end{aligned}$$

$$\begin{aligned}
& -2\kappa\tau \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \Delta_h \hat{e}^{(j,k)}, e^\ell \rangle + 2S\tau^k \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \Delta_h \delta_1 e^j, e^\ell \rangle \\
& -2 \sum_{\ell=k}^n \langle e_1^{(k,\ell)}, e^\ell \rangle + 2\tau \sum_{\ell=k}^n \langle R_P^\ell + R_\Phi^\ell, e^\ell \rangle,
\end{aligned} \tag{4.18}$$

where the Green's formulas (2.4) and equality $2a(a-b) = a^2 - b^2 + (a-b)^2$ are applied. Based on the positive definiteness of the BDF k kernels, one knows that the first term on the right-hand side of the above equality is negative definite. It remains to estimate the other terms.

Following the energy dissipation law (1.3), it is not difficult to check that $\|\nabla_h \Phi_M^n\|_{l^6} \leq c_2$ (c_2 is a positive constant). Furthermore, we have

$$\|u^j\|_{l^3} \leq \|\nabla_h \Phi_M^n\|_{l^6}^2 + \|\nabla_h \Phi_M^n\|_{l^6} \|\nabla_h \phi^n\|_{l^6} + \|\nabla_h \phi^n\|_{l^6}^2 \leq c_1^2 + c_1 c_2 + c_2^2 = c_3.$$

With the help of Lemma 4.4 with $v^j = u^j$, $z^j = \nabla_h e^j$ and $\varepsilon = \varepsilon^2/6$, one obtains

$$\begin{aligned}
& -2\kappa\tau \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle v^j \nabla_h e^j, \nabla_h e^\ell \rangle \\
& \leq 2\kappa\tau \frac{\varepsilon^2}{6} \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \Delta_h e^j, \Delta_h e^\ell \rangle \\
& \quad + 2\kappa c_4 \tau \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \nabla_h e^j, \nabla_h e^\ell \rangle,
\end{aligned}$$

in which

$$c_4 = \frac{\varepsilon^2}{6} + \frac{12c_3^2 c_\Omega^2 m_{2k}^2 m_{3k}}{\varepsilon^2 m_{1k}^3}.$$

For the gradient term in the last step of the above inequality, it can be bounded in the manner of

$$\begin{aligned}
& 2\kappa c_4 \tau \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \nabla_h e^j, \nabla_h e^\ell \rangle \\
& = -2\kappa c_4 \tau \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \Delta_h e^j, e^\ell \rangle \\
& \leq \frac{\varepsilon^2}{6} 2\kappa\tau \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \Delta_h e^j, \Delta_h e^\ell \rangle + \frac{6c_4^2 \kappa\tau}{m_{1k} \varepsilon^2} \sum_{\ell=k}^n \|e^\ell\|^2,
\end{aligned}$$

where the first inequality in Lemma 4.2 is applied with $\varepsilon = \varepsilon^2/(6c_4)$ at the last step. Applying Lemma 4.3 with $\varepsilon = \varepsilon^2/3$ to the explicit extrapolation of concave term, it yields that

$$\begin{aligned}
& -2\kappa\tau \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \Delta_h \hat{e}^{(j,k)}, e^\ell \rangle \\
& = -2\kappa\tau \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \hat{e}^{(j,k)}, \Delta_h e^\ell \rangle \\
& \leq 2\kappa\tau \frac{\varepsilon^2}{3} \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \Delta_h e^j, \Delta_h e^\ell \rangle + \frac{3\kappa m_{2k} m_{3k}}{m_{1k}^2 \varepsilon^2} \tau \sum_{\ell=k}^n \|\hat{e}^{(\ell,k)}\|^2.
\end{aligned}$$

Again, with the help of Lemma 4.3 with $\varepsilon = \epsilon$, the stabilized term can be treated as

$$\begin{aligned} & 2S\tau^k \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \Delta_h \delta_1 e^j, e^\ell \rangle \\ & \leq 2S\tau^k \epsilon \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \Delta_h e^j, \Delta_h e^\ell \rangle + \frac{\mathbf{m}_{2k} \mathbf{m}_{3k} S}{\mathbf{m}_{1k}^2 \epsilon} \tau^k \sum_{\ell=k}^n \|\delta_1 e^\ell\|^2. \end{aligned}$$

There exists a constant \hat{C}_k such that

$$\sum_{\ell=k}^n \|\hat{e}^{(\ell,k)}\|^2 \leq \hat{C}_k \sum_{\ell=0}^{n-1} \|e^\ell\|^2$$

from the definition of explicit extrapolations. By collecting the estimates of the every term on the right-hand side of the inequality (4.18) and applying the Cauchy-Schwarz inequality, for $k \leq n \leq N$, one has

$$\begin{aligned} & \|e^n\|^2 - \|e^{k-1}\|^2 + \left(1 - \frac{\mathbf{m}_{2k} \mathbf{m}_{3k} S}{\mathbf{m}_{1k}^2 \epsilon} \tau^k\right) \sum_{\ell=k}^n \|\delta_1 e^\ell\|^2 \\ & \leq \left(2S\tau^k \epsilon - 2\kappa\tau \frac{\epsilon^2}{3}\right) \sum_{\ell=k}^n \sum_{j=k}^{\ell} \theta_{\ell-j}^{(k)} \langle \Delta_h e^j, \Delta_h e^\ell \rangle + \frac{6\kappa c_4^2}{\mathbf{m}_{1k} \epsilon^2} \tau \sum_{\ell=k}^n \|e^\ell\|^2 \\ & \quad + \frac{3\kappa \mathbf{m}_{2k} \mathbf{m}_{3k}}{\mathbf{m}_{1k}^2 \epsilon^2} \hat{C}_k \tau \sum_{\ell=0}^{n-1} \|e^\ell\|^2 + 2 \sum_{\ell=k}^n \|e_1^{(k,\ell)}\| \cdot \|e^\ell\| + 2\tau \sum_{\ell=k}^n \|R_P^\ell + R_\Phi^\ell\| \cdot \|e^\ell\|. \end{aligned}$$

Under the time step constraint

$$\tau \leq \min \left\{ \left(\frac{\kappa \epsilon}{3S}\right)^{\frac{1}{k-1}}, \left(\frac{\mathbf{m}_{1k}^2 \epsilon}{\mathbf{m}_{2k} \mathbf{m}_{3k} S}\right)^{\frac{1}{k}} \right\},$$

the above equality yields

$$\begin{aligned} \|e^n\|^2 & \leq \|e^{k-1}\|^2 + 2 \sum_{\ell=k}^n \|e_1^{(k,\ell)}\| \cdot \|e^\ell\| + \frac{6\kappa c_4^2}{\mathbf{m}_{1k} \epsilon^2} \tau \sum_{\ell=k}^n \|e^\ell\|^2 \\ & \quad + \frac{3\kappa \mathbf{m}_{2k} \mathbf{m}_{3k}}{\mathbf{m}_{1k}^2 \epsilon^2} \hat{C}_k \tau \sum_{\ell=0}^{n-1} \|e^\ell\|^2 + 2\tau \sum_{\ell=k}^n \|R_P^\ell + R_\Phi^\ell\| \cdot \|e^\ell\|. \end{aligned} \quad (4.19)$$

We select certain integer n_0 ($0 \leq n_0 \leq n$) such that $\|e^{n_0}\| = \max_{0 \leq \ell \leq n} \|e^\ell\|$. Taking $n = n_0$ in (4.19) and enlarging the sum upper bound n_0 to n , one can obtain

$$\begin{aligned} \|e^{n_0}\|^2 & \leq \|e^{k-1}\| \cdot \|e^{n_0}\| + 2 \sum_{\ell=k}^n \|e_1^{(k,\ell)}\| \cdot \|e^{n_0}\| + \frac{6\kappa c_4^2}{\mathbf{m}_{1k} \epsilon^2} \tau \sum_{\ell=k}^n \|e^\ell\| \cdot \|e^{n_0}\| \\ & \quad + \frac{3\kappa \mathbf{m}_{2k} \mathbf{m}_{3k}}{\mathbf{m}_{1k}^2 \epsilon^2} \hat{C}_k \tau \sum_{\ell=0}^{n-1} \|e^\ell\| \cdot \|e^{n_0}\| + 2\tau \sum_{\ell=k}^n \|R_P^\ell + R_\Phi^\ell\| \cdot \|e^{n_0}\|. \end{aligned}$$

Consequently, it follows from $\|e^n\| \leq \|e^{n_0}\|$ that

$$\|e^n\| \leq \|e^{k-1}\| + 2 \sum_{\ell=k}^n \|e_1^{(k,\ell)}\| + \left(\frac{6\kappa c_4^2 \tau}{\mathbf{m}_{1k} \epsilon^2} + \frac{3\kappa \mathbf{m}_{2k} \mathbf{m}_{3k}}{\mathbf{m}_{1k}^2 \epsilon^2} \hat{C}_k \tau\right) \sum_{\ell=k}^{n-1} \|e^\ell\|$$

$$+ \frac{6\kappa c_4^2 \tau}{\mathbf{m}_{1k} \epsilon^2} \|e^n\| + \frac{3\kappa \mathbf{m}_{2k} \mathbf{m}_{3k}}{\mathbf{m}_{1k}^2 \epsilon^2} \hat{C}_k \tau \sum_{\ell=0}^{k-1} \|e^\ell\| + 2\tau \sum_{\ell=k}^n \|R_P^\ell + R_\Phi^\ell\|.$$

Using Lemma 4.5, the starting term $e_1^{(k,\ell)}$ defined in (4.17) can be estimated by

$$\sum_{\ell=k}^n \|e_1^{(k,\ell)}\| \leq \frac{7c_{1k}\rho_k}{8(7-k)} \sum_{\ell=1}^{k-1} \|\delta_1 e^\ell\| \leq \frac{7c_{1k}\rho_k}{4(7-k)} \sum_{\ell=1}^{k-1} \|e^\ell\|, \quad n \geq k.$$

Thus, we have

$$\begin{aligned} \|e^n\| &\leq \left[\frac{7c_{1k}\rho_k}{7-k} + \frac{3\kappa \mathbf{m}_{2k} \mathbf{m}_{3k} \hat{C}_k \tau}{\mathbf{m}_{1k}^2 \epsilon^2} \right] \sum_{\ell=0}^{k-1} \|e^\ell\| + \frac{6\kappa c_4^2 \tau}{\mathbf{m}_{1k} \epsilon^2} \|e^n\| \\ &\quad + 3\kappa \tau \frac{2c_4^2 \mathbf{m}_{1k} + \hat{C}_k \mathbf{m}_{2k} \mathbf{m}_{3k}}{\mathbf{m}_{1k}^2 \epsilon^2} \sum_{\ell=k}^{n-1} \|e^\ell\| + 2\tau \sum_{\ell=k}^n \|R_P^\ell + R_\Phi^\ell\|, \end{aligned}$$

where we used the fact $1 \leq 7c_{1k}\rho_k/(2(7-k))$. Under the time step constraint $\tau \leq \mathbf{m}_{1k}\epsilon^2/(12\kappa c_4^2)$, we have

$$\begin{aligned} \|e^n\| &\leq \left[\frac{14c_{1k}\rho_k}{7-k} + \frac{6\kappa \mathbf{m}_{2k} \mathbf{m}_{3k} \hat{C}_k \tau}{\mathbf{m}_{1k} \epsilon^2} \right] \sum_{\ell=0}^{k-1} \|e^\ell\| \\ &\quad + 6\kappa \tau \frac{2c_4^2 \mathbf{m}_{1k} + \hat{C}_k \mathbf{m}_{2k} \mathbf{m}_{3k}}{\mathbf{m}_{1k}^2 \epsilon^2} \sum_{\ell=k}^{n-1} \|e^\ell\| + 4\tau \sum_{\ell=k}^n \|R_P^\ell + R_\Phi^\ell\|. \end{aligned}$$

Furthermore, applying the discrete Grönwall inequality, it leads to the estimate as follows:

$$\|e^n\| \leq \exp(c_5 t_{n-k+1}) \left[c_6 \sum_{\ell=0}^{k-1} \|e^\ell\| + 4\tau \sum_{\ell=k}^n (\|R_P^\ell\| + \|R_\Phi^\ell\|) \right], \quad k \leq n \leq N.$$

With the help of the estimates of the global errors (4.13) and the triangle inequality (4.14), it leads to the claimed result. This completes the proof. \square

5. Numerical Experiments

In this section, numerical experiments are presented to verify our theoretical analysis about the stabilized convex splitting BDF k ($k = 3, 4, 5$) scheme (2.5). To ensure the accuracy of the numerical scheme, we calculate the starting numerical values by the sixth order Gaussian collocation method [12]. The fixed-point iteration method with termination error 10^{-12} is employed to calculate the nonlinear algebraic equations at each time level. In the following practical computation, we always divide the spatial region Ω into 128×128 uniform lattices, and take the stabilized parameter $S = 1$.

We present an accuracy check for the stabilized convex splitting BDF k scheme. Let the discrete L^2 norm error be $E(N) = \|\Phi(T) - \phi^N\|$ and the temporal convergence order be $order = \log_2(e(N)/e(2N))$. We consider the model with an artificial forcing term $g(\mathbf{x}, t)$ as follows:

$$\partial_t \Phi = -\kappa \{ \epsilon^2 \Delta^2 \Phi - \nabla \cdot [(|\nabla \Phi|^2 - 1) \nabla \Phi] \} + g(\mathbf{x}, t), \quad \mathbf{x} \in \Omega = (0, 2\pi)^2$$

Table 5.1: Errors and orders of the BDF k schemes (2.5) with the artificial forcing term.

N	τ	BDF3 scheme		BDF4 scheme		BDF5 scheme	
		$E(N)$	$order$	$E(N)$	$order$	$E(N)$	$order$
10	1.00e-01	4.62e-04	-	6.11e-05	-	2.39e-05	-
20	5.00e-02	4.53e-05	3.35	3.86e-06	3.99	8.97e-07	4.74
40	2.50e-02	4.83e-06	3.23	2.26e-07	4.09	2.97e-08	4.91
80	1.25e-02	5.51e-07	3.13	1.35e-08	4.07	9.54e-10	4.96
160	6.25e-03	6.56e-08	3.07	8.21e-10	4.04	3.02e-11	4.98
320	3.13e-03	8.00e-09	3.04	5.04e-11	4.03	9.20e-13	5.03

Table 5.2: Errors and orders of the BDF k schemes (2.5) without the artificial forcing term.

N	τ	BDF3 scheme		BDF4 scheme		BDF5 scheme	
		$E(N)$	$order$	$E(N)$	$order$	$E(N)$	$order$
10	1.00e-01	5.39e-04	-	2.59e-04	-	2.04e-04	-
20	5.00e-02	7.23e-05	2.90	6.70e-06	5.27	6.47e-06	4.98
40	2.50e-02	9.78e-06	2.89	3.49e-07	4.26	2.75e-07	4.55
80	1.25e-02	1.30e-06	2.91	4.49e-08	2.96	1.92e-08	3.84
160	6.25e-03	1.69e-07	2.94	4.34e-09	3.37	9.99e-10	4.26
320	3.13e-03	2.17e-08	2.97	3.37e-10	3.69	3.76e-11	4.73

with the exact solution $\Phi(x, y, t) = \cos(t) \sin(x) \sin(y)$ and model parameters $\kappa = 1, \epsilon^2 = 0.5$. We use the proposed convex splitting BDF k scheme to compute the forced problem with time $T = 1$. Taking the number of grid nodes $N = 10, 20, 40, 80, 160, 320$ respectively, the experiment errors and convergence orders are summarized in Table 5.1. It demonstrates that the stabilized convex splitting BDF k scheme is of order k ($k = 3, 4, 5$), which is consistent with the convergence result in Theorem 4.1. We also use another example without forcing terms, i.e. $\Phi(x, y) = \sin(x) + \cos(y)$ with $\kappa = 0.2, \epsilon = 0.5, T = 1$ and $g(\mathbf{x}, t) = 0$. The reference solution is computed by $N_0 = 3200$ and let $\Phi(T) = \phi^{N_0}$ in the error $E(N)$. Table 5.2 lists the errors and convergence orders. We see that the BDF k scheme can achieve k -th order accuracy for $k = 3, 4, 5$.

To model the energy dissipation phenomenon of the MBE model with slope selection, we perform the standard model (1.1) with the parameters $\kappa = 0.25, \epsilon^2 = 0.1$, spatial domain $\Omega = (0, 2\pi)^2$ and initial value $\Phi(x, y, 0) = 0.1[\sin(3x) \sin(2y) + \sin(5x) \sin(5y)]$. Using the proposed BDF k schemes, we compute the problem (1.1) with fixed temporal step $\tau = 0.005$ until time $T = 100$. The numerical results of the original energy and mass are presented in Fig. 5.1. It shows that the energy decreases rapidly in the early stage and exhibits multi-scale behavior, and then it tends to a steady state. In addition, the curves of the numerical schemes almost overlap each other. We also find that the numerical solutions of the three numerical schemes conserve the mass. Furthermore, the snapshots of the numerical solution at the time $t = 0, 3, 7, 8, 10, 30, 50, 100$ are given in Fig. 5.2 by applying the stabilized convex splitting BDF5 scheme, and that of the BDF3 and BDF4 schemes have the similar evolutions, which will not be shown here.

More generally, we consider the numerical simulations of coarsening dynamics of the standard problem (1.1) with the parameters $\kappa = 0.25, \epsilon^2 = 0.1$, spatial domain $\Omega = (0, 12.8)^2$

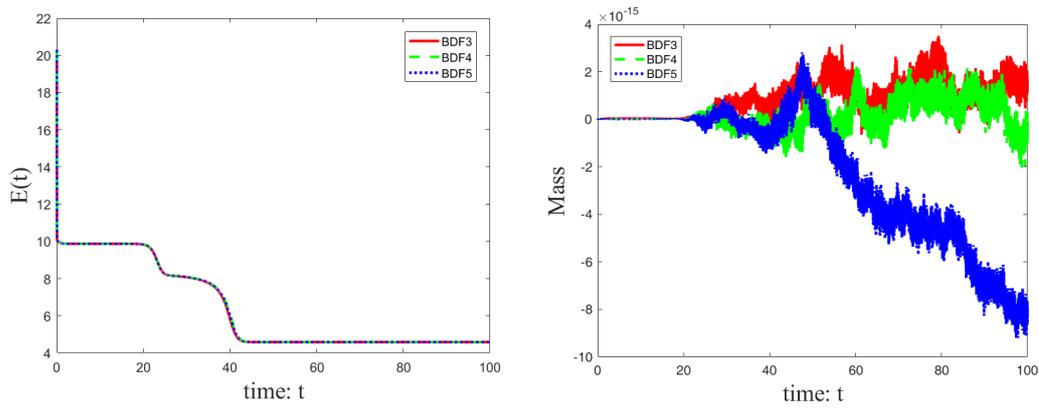


Fig. 5.1. Time evolutions of the energy and mass for the MBE model (1.1) with the initial data $\Phi(x, y, 0) = 0.1[\sin(3x) \sin(2y) + \sin(5x) \sin(5y)]$.

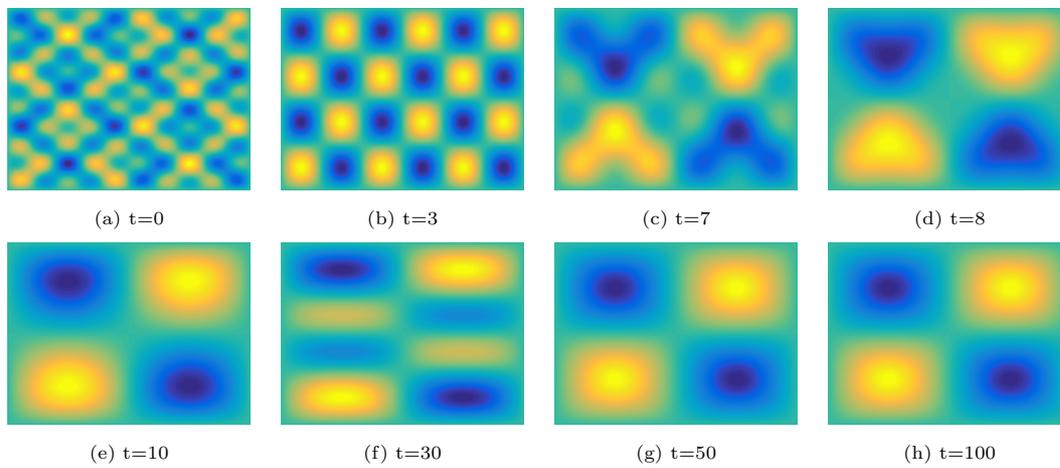


Fig. 5.2. Snapshots of the numerical solutions for the MBE model (1.1) with the initial data $\Phi(x, y, 0) = 0.1[\sin(3x) \sin(2y) + \sin(5x) \sin(5y)]$.

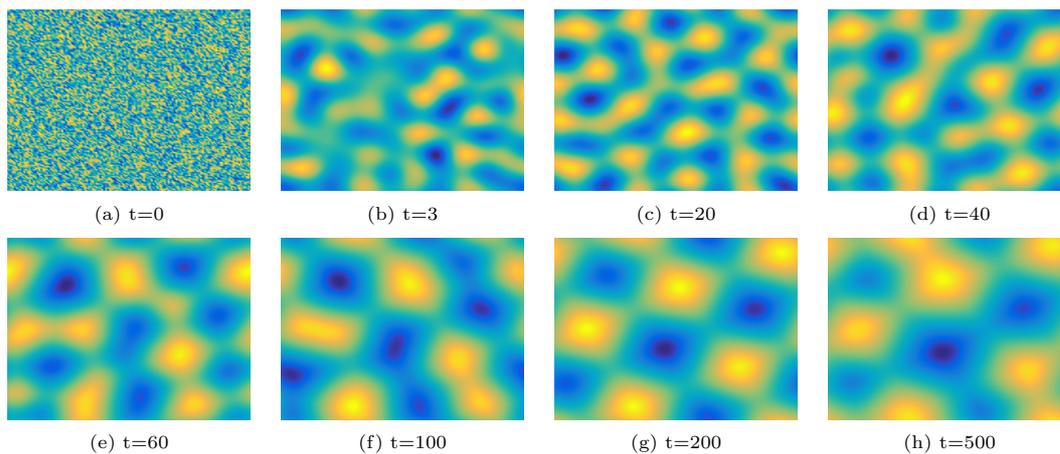


Fig. 5.3. The snapshots of numerical solutions for the MBE model (1.1) with the random initial data $\Phi(x, y, 0) = \text{rand}(x, y)$.

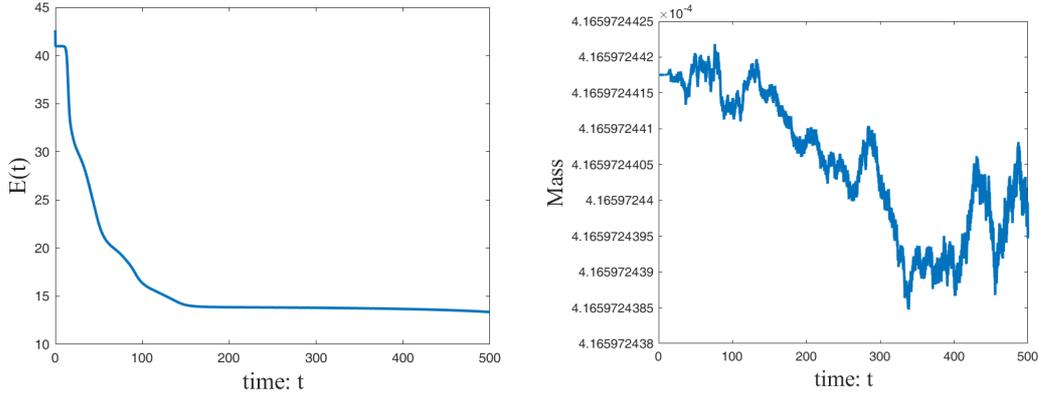


Fig. 5.4. Time evolutions of the energy and mass for the MBE model (1.1) with the random initial data $\Phi(x, y, 0) = \text{rand}(x, y)$.

and initial data $\Phi(x, y, 0) = \text{rand}(x, y)$, where $\text{rand}(x, y)$ creates random digits from -0.001 to 0.001 . The stabilized convex splitting BDF5 scheme is applied to calculate the numerical solutions until time $T = 500$ with the fixed time step $\tau = 0.005$. Fig. 5.3 shows the snapshots of numerical solutions, and Fig. 5.4 presents the energy dissipation law and mass conservation.

6. Conclusion

In this article, we discussed the error analysis of the stabilized convex splitting BDF k ($k = 3, 4, 5$) scheme for the MBE equation with slope selection (1.1). By adding a class of k -th order accurate Douglas-Dupont type stabilized terms, the stabilized scheme (2.5) was designed by combining the BDF k formula and the convex splitting method. We proved that the proposed schemes admit the modified energy dissipation law, which yields the boundedness of numerical solutions. Then the L^2 norm error estimate was established without supposing the Lipschitz continuity of the nonlinear term. At last, several numerical tests were carried out to verify our theoretical results.

As well known, the nonuniform BDF schemes combined with some adaptive time-stepping methods, are very efficient to solve gradient flow problems, see [14, 23]. We will consider the high order convex splitting BDF schemes with variable time steps in the future work. To obtain the energy dissipation law at the discrete levels, one should construct the gradient decomposition of the k -th order explicit extrapolation formula, which would be a challenging task.

Appendix A. Proof of Lemma 3.1

For simplicity, we first denote an auxiliary sequence $w^n = \delta_1 v^n$. Based on the elementary identity

$$4(a^3 - a)(a - b) = (a^2 - 1)^2 - (b^2 - 1)^2 - 2(1 - a^2)(a - b)^2 + (a^2 - b^2)^2,$$

it is not difficult to check the following equality:

$$\begin{aligned} & [(v^n)^3 - \hat{v}^{(n,k)}] \delta_1 v^n = [(v^n)^3 - v^n] \delta_1 v^n + [v^n - \hat{v}^{(n,k)}] \delta_1 v^n \\ &= \frac{1}{4} [(v^n)^2 - 1]^2 - \frac{1}{4} [(v^{n-1})^2 - 1]^2 - \frac{1}{2} [1 - (v^n)^2] [\delta_1 v^n]^2 \\ &\quad + \frac{1}{4} [(v^n)^2 - (v^{n-1})^2]^2 + J_k^n, \end{aligned} \quad (\text{A.1})$$

where J_k^n is defined by

$$J_k^n = \delta_k v^n (\delta_1 v^n) = w^n (\delta_{k-1} w^n), \quad 3 \leq k \leq 5.$$

To complete the proof, it is to decompose J_k^n into some quadratic terms. They can be obtained by simple computations with the basic identities $2a(a-b) = a^2 - b^2 + (a-b)^2$ and $2b(a-b) = a^2 - b^2 - (a-b)^2$. This type decomposition can also be found in the proof of Lemma 2.4, cf. [21, Appendix A]. For simplicity, we omit the lengthy derivations and write out the results directly, see the corresponding identities in [21, Eqs. (A.4), (A.9), (A.16)].

This proof is mainly to transfer the negative terms with higher order difference, such as $-(\delta_1 w^{n-1})^2$ and $-(\delta_2 w^{n-1})^2$ in (A.3) and $-(\delta_2 w^{n-1})^3$ in (A.9), to the zero order term $-(w^n)^2$ at the current time level t_n . In this reformulation process, the inverse decomposition formulas, see (A.4)-(A.6), play an important role.

(i) The case $k = 3$. It is not difficult to find that, also see [21, Eq. (A.4)],

$$\begin{aligned} J_3^n &= w^n \delta_2 w^n = \frac{1}{2} (\delta_1 w^n)^2 - \frac{1}{2} (\delta_1 w^{n-1})^2 + \frac{1}{2} (\delta_2 w^n)^2 + w^{n-1} \delta_2 w^n \\ &= \frac{1}{2} (\delta_1 w^n)^2 - \frac{1}{2} (\delta_1 w^{n-1})^2 + \frac{1}{2} (\delta_2 w^n + w^{n-1})^2 - \frac{1}{2} (w^{n-1})^2 \\ &= \mathcal{F}_3 [\delta_1 v^n] - \mathcal{F}_3 [\delta_1 v^{n-1}] - \frac{1}{2} (\delta_1 v^n)^2 + \mathfrak{R}_3 [\delta_1 v^n], \end{aligned} \quad (\text{A.2})$$

where the functionals

$$\mathcal{F}_3[w^n] = \frac{1}{2} (\delta_1 w^n)^2 + \frac{1}{2} (w^n)^2, \quad \mathfrak{R}_3[w^n] = \frac{1}{2} (\delta_2 w^n + w^{n-1})^2.$$

By inserting (A.2) into (A.1), the claimed identity (3.3) of $k = 3$ is verified with $\gamma_3 = 1$.

(ii) The case $k = 4$. One applies [21, Eq. (A.9)] to find

$$\begin{aligned} J_4^n &= w^n \delta_3 w^n = \frac{1}{2} (w^n)^2 - \frac{3}{2} (w^{n-1})^2 + \frac{3}{2} (w^{n-2})^2 - \frac{1}{2} (w^{n-3})^2 \\ &\quad - \frac{3}{2} (\delta_1 w^{n-1})^2 + \frac{3}{2} (\delta_1 w^{n-2})^2 + \frac{1}{2} (\delta_3 w^n)^2 - \frac{3}{2} (\delta_2 w^{n-1})^2. \end{aligned} \quad (\text{A.3})$$

It is to handle the last two terms (the underlined part). Notice that

$$2w^{n-1} \delta_2 w^n = (w^n)^2 - 2(w^{n-1})^2 + (w^{n-2})^2 - (\delta_1 w^n)^2 - (\delta_1 w^{n-1})^2$$

such that

$$-(\delta_1 w^{n-1})^2 = 2w^{n-1} \delta_2 w^n - (w^n)^2 + 2(w^{n-1})^2 - (w^{n-2})^2 + (\delta_1 w^n)^2, \quad (\text{A.4})$$

$$-(\delta_2 w^{n-1})^2 = 2\delta_1 w^{n-1} (\delta_3 w^n) - (\delta_1 w^n)^2 + 2(\delta_1 w^{n-1})^2 - (\delta_1 w^{n-2})^2 + (\delta_2 w^n)^2, \quad (\text{A.5})$$

$$-(\delta_3 w^{n-1})^2 = 2\delta_2 w^{n-1} (\delta_4 w^n) - (\delta_2 w^n)^2 + 2(\delta_2 w^{n-1})^2 - (\delta_2 w^{n-2})^2 + (\delta_3 w^n)^2. \quad (\text{A.6})$$

We apply (A.5) to find that

$$\begin{aligned}\tilde{J}_{41}^n &= \frac{1}{2}(\delta_3 w^n)^2 - \frac{3}{2}(\delta_2 w^{n-1})^2 \\ &= \frac{1}{2}(\delta_3 w^n)^2 + 3\delta_1 w^{n-1} \delta_3 w^n - \frac{3}{2}(\delta_1 w^n)^2 + 3(\delta_1 w^{n-1})^2 - \frac{3}{2}(\delta_1 w^{n-2})^2 + \frac{3}{2}(\delta_2 w^n)^2 \\ &= \frac{1}{2}(\delta_3 w^n + 3\delta_1 w^{n-1})^2 - \frac{3}{2}(\delta_1 w^n)^2 - \frac{3}{2}(\delta_1 w^{n-1})^2 - \frac{3}{2}(\delta_1 w^{n-2})^2 + \frac{3}{2}(\delta_2 w^n)^2.\end{aligned}$$

Substituting the above equality into (A.3), it arrives at

$$\begin{aligned}J_4^n &= \frac{1}{2}(w^n)^2 - \frac{3}{2}(w^{n-1})^2 + \frac{3}{2}(w^{n-2})^2 - \frac{1}{2}(w^{n-3})^2 + \frac{1}{2}(\delta_3 w^n + 3\delta_1 w^{n-1})^2 \\ &\quad - \frac{3}{2}(\delta_1 w^n)^2 - \frac{3}{4}(\delta_1 w^{n-1})^2 + \frac{3}{2}(\delta_2 w^n)^2 - \frac{9}{4}(\delta_1 w^{n-1})^2.\end{aligned}\quad (\text{A.7})$$

Now consider the last two terms (the underlined part). One applies (A.4) to derive that

$$\begin{aligned}\tilde{J}_{42}^n &= \frac{3}{2}(\delta_2 w^n)^2 - \frac{9}{4}(\delta_1 w^{n-1})^2 \\ &= \frac{3}{2}(\delta_2 w^n)^2 + \frac{9}{2}w^{n-1} \delta_2 w^n - \frac{9}{4}(w^n)^2 + \frac{9}{2}(w^{n-1})^2 - \frac{9}{4}(w^{n-2})^2 + \frac{9}{4}(\delta_1 w^n)^2 \\ &= \frac{3}{2}\left(\delta_2 w^n + \frac{3}{2}w^{n-1}\right)^2 - \frac{9}{4}(w^n)^2 + \frac{9}{8}(w^{n-1})^2 - \frac{9}{4}(w^{n-2})^2 + \frac{9}{4}(\delta_1 w^n)^2.\end{aligned}$$

Inserting it into (A.7), an elementary calculation leads to

$$\begin{aligned}J_4^n &= \left[\frac{13}{8}(w^n)^2 + \frac{5}{4}(w^{n-1})^2 + \frac{1}{2}(w^{n-2})^2 \right] - \left[\frac{13}{8}(w^{n-1})^2 + \frac{5}{4}(w^{n-2})^2 + \frac{1}{2}(w^{n-3})^2 \right] \\ &\quad - \frac{27}{8}(w^n)^2 + \frac{3}{4}(\delta_1 w^n)^2 - \frac{3}{4}(\delta_1 w^{n-1})^2 + \frac{3}{2}\left(\delta_2 w^n + \frac{3}{2}w^{n-1}\right)^2 + \frac{1}{2}(\delta_3 w^n + 3\delta_1 w^{n-1})^2 \\ &= \mathcal{F}_4[\delta_1 v^n] - \mathcal{F}_4[\delta_1 v^{n-1}] - \frac{27}{8}(\delta_1 v^n)^2 + \mathfrak{R}_4[\delta_1 v^n],\end{aligned}\quad (\text{A.8})$$

where the nonnegative quadratic functionals \mathcal{F}_4 and \mathfrak{R}_4 are defined by

$$\begin{aligned}\mathcal{F}_4[w^n] &:= \frac{13}{8}(w^n)^2 + \frac{5}{4}(w^{n-1})^2 + \frac{1}{2}(w^{n-2})^2 + \frac{3}{4}(\delta_1 w^n)^2, \\ \mathfrak{R}_4[w^n] &:= \frac{3}{2}\left(\delta_2 w^n + \frac{3}{2}w^{n-1}\right)^2 + \frac{1}{2}(\delta_3 w^n + 3\delta_1 w^{n-1})^2.\end{aligned}$$

Inserting (A.8) into (A.1), we obtain the claimed identity (3.3) of $k = 4$ with $\gamma_4 = 31/8$.

(iii) The case $k = 5$. One applies [21, Eq. (A.16)] to get

$$\begin{aligned}J_5^n &= w^n \delta_4 w^n = \frac{1}{2}(w^n)^2 - 2(w^{n-1})^2 + 3(w^{n-2})^2 - 2(w^{n-3})^2 + \frac{1}{2}(w^{n-4})^2 \\ &\quad - 2(\delta_1 w^{n-1})^2 + 4(\delta_1 w^{n-2})^2 - 2(\delta_1 w^{n-3})^2 - 2(\delta_2 w^{n-1})^2 \\ &\quad + 3(\delta_2 w^{n-2})^2 + \frac{1}{2}(\delta_4 w^n)^2 - 2(\delta_3 w^{n-1})^2.\end{aligned}\quad (\text{A.9})$$

For the last two terms (the underlined part), we apply (A.6) to derive that

$$\begin{aligned}\tilde{J}_{51}^n &= \frac{1}{2}(\delta_4 w^n)^2 - 2(\delta_3 w^{n-1})^2 \\ &= \frac{1}{2}(\delta_4 w^n)^2 + 4\delta_2 w^{n-1} \delta_4 w^n - 2(\delta_2 w^n)^2 + 4(\delta_2 w^{n-1})^2 - 2(\delta_2 w^{n-2})^2 + 2(\delta_3 w^n)^2 \\ &= \frac{1}{2}(\delta_4 w^n + 4\delta_2 w^{n-1})^2 - 2(\delta_2 w^n)^2 - 4(\delta_2 w^{n-1})^2 - 2(\delta_2 w^{n-2})^2 + 2(\delta_3 w^n)^2.\end{aligned}$$

Thus it follows that

$$\begin{aligned}J_5^n &= \frac{1}{2}(w^n)^2 - 2(w^{n-1})^2 + 3(w^{n-2})^2 - 2(w^{n-3})^2 + \frac{1}{2}(w^{n-4})^2 \\ &\quad - 2(\delta_1 w^{n-1})^2 + 4(\delta_1 w^{n-2})^2 - 2(\delta_1 w^{n-3})^2 - 2(\delta_2 w^n)^2 + (\delta_2 w^{n-2})^2 \\ &\quad + \frac{1}{2}(\delta_4 w^n + 4\delta_2 w^{n-1})^2 + \underline{2(\delta_3 w^n)^2 - 6(\delta_2 w^{n-1})^2}.\end{aligned}\tag{A.10}$$

We apply (A.5) to find that

$$\begin{aligned}\tilde{J}_{52}^n &= 2(\delta_3 w^n)^2 - 6(\delta_2 w^{n-1})^2 \\ &= 2(\delta_3 w^n + 3\delta_1 w^{n-1})^2 - 6(\delta_1 w^n)^2 - 6(\delta_1 w^{n-1})^2 - 6(\delta_1 w^{n-2})^2 + 6(\delta_2 w^n)^2.\end{aligned}$$

Inserting it into (A.10), one has

$$\begin{aligned}J_5^n &= \frac{1}{2}(w^n)^2 - 2(w^{n-1})^2 + 3(w^{n-2})^2 - 2(w^{n-3})^2 + \frac{1}{2}(w^{n-4})^2 - 6(\delta_1 w^n)^2 \\ &\quad - 8(\delta_1 w^{n-1})^2 + 4(\delta_2 w^n)^2 + 2(\delta_3 w^n + 3\delta_1 w^{n-1})^2 + \frac{1}{2}(\delta_4 w^n + 4\delta_2 w^{n-1})^2 \\ &\quad + \underline{(\delta_2 w^{n-2})^2 - 2(\delta_1 w^{n-2})^2 - 2(\delta_1 w^{n-3})^2}.\end{aligned}\tag{A.11}$$

For the underlined terms, one can apply (A.5) to obtain that

$$-(\delta_1 w^{n-3})^2 = 2w^{n-3} \delta_2 w^{n-2} - (w^{n-2})^2 + 2(w^{n-3})^2 - (w^{n-4})^2 + (\delta_1 w^{n-2})^2$$

such that

$$\begin{aligned}\tilde{J}_{53}^n &= (\delta_2 w^{n-2})^2 - 2(\delta_1 w^{n-2})^2 - 2(\delta_1 w^{n-3})^2 \\ &= (\delta_2 w^{n-2} + 2w^{n-3})^2 - 2(w^{n-2})^2 - 2(w^{n-4})^2.\end{aligned}$$

A substitution of the above equality into (A.11) leads to the following result:

$$\begin{aligned}J_5^n &= \frac{1}{2}(w^n)^2 - 2(w^{n-1})^2 + (w^{n-2})^2 - 2(w^{n-3})^2 - \frac{3}{2}(w^{n-4})^2 - 6(\delta_1 w^n)^2 \\ &\quad - (\delta_1 w^{n-1})^2 + (\delta_2 w^{n-2} + 2w^{n-3})^2 + 2(\delta_3 w^n + 3\delta_1 w^{n-1})^2 \\ &\quad + \frac{1}{2}(\delta_4 w^n + 4\delta_2 w^{n-1})^2 + \underline{4(\delta_2 w^n)^2 - 7(\delta_1 w^{n-1})^2}.\end{aligned}\tag{A.12}$$

In similar manner, one can apply (A.5) to handle the underlined terms as follows:

$$\begin{aligned}\tilde{J}_{54}^n &= 4(\delta_2 w^n)^2 - 7(\delta_1 w^{n-1})^2 \\ &= 4(\delta_2 w^n)^2 + 14w^{n-1} \delta_2 w^n - 7(w^n)^2 + 14(w^{n-1})^2 - 7(w^{n-2})^2 + 7(\delta_1 w^n)^2 \\ &= 4\left(\delta_2 w^n + \frac{7}{4}w^{n-1}\right)^2 - 7(w^n)^2 + \frac{7}{4}(w^{n-1})^2 - 7(w^{n-2})^2 + 7(\delta_1 w^n)^2.\end{aligned}$$

Then inserting it into (A.12) and recalling $w^n = \delta_1 v^n$, one has

$$\begin{aligned}
J_5^n &= -\frac{13}{2}(w^n)^2 - \frac{1}{4}(w^{n-1})^2 - 6(w^{n-2})^2 - 2(w^{n-3})^2 - \frac{3}{2}(w^{n-4})^2 + (\delta_1 w^n)^2 \\
&\quad - (\delta_1 w^{n-1})^2 + \mathfrak{R}_5[\delta_1 v^n] \\
&= \left[\frac{39}{4}(w^n)^2 + \frac{19}{2}(w^{n-1})^2 + \frac{7}{2}(w^{n-2})^2 + \frac{3}{2}(w^{n-3})^2 + (\delta_1 w^n)^2 \right] \\
&\quad - \left[\frac{39}{4}(w^{n-1})^2 + \frac{19}{2}(w^{n-2})^2 + \frac{7}{2}(w^{n-3})^2 + \frac{3}{2}(w^{n-4})^2 + (\delta_1 w^{n-1})^2 \right] \\
&\quad - \frac{65}{4}(w^n)^2 + \mathfrak{R}_5[\delta_1 v^n], \tag{A.13}
\end{aligned}$$

where \mathfrak{R}_5 is denoted by

$$\begin{aligned}
\mathfrak{R}_5[w^n] &= 4 \left(\delta_2 w^n + \frac{7}{4} w^{n-1} \right)^2 + (\delta_2 w^{n-2} + 2w^{n-3})^2 \\
&\quad + 2(\delta_3 w^n + 3\delta_1 w^{n-1})^2 + \frac{1}{2}(\delta_4 w^n + 4\delta_2 w^{n-1})^2.
\end{aligned}$$

It is not difficult to obtain that

$$J_5^n = \delta_5 v^n (\delta_1 v^n) = \mathcal{F}_5[\delta_1 v^n] - \mathcal{F}_5[\delta_1 v^{n-1}] - \frac{65}{4}(\delta_1 v^n)^2 + \mathfrak{R}_5[\delta_1 v^n], \tag{A.14}$$

where the nonnegative quadratic functional \mathcal{F}_5 is defined by

$$\mathcal{F}_5[w^n] = \frac{39}{4}(w^n)^2 + \frac{19}{2}(w^{n-1})^2 + \frac{7}{2}(w^{n-2})^2 + \frac{3}{2}(w^{n-3})^2 + (\delta_1 w^n)^2.$$

By inserting (A.14) into (A.1), the claimed inequality (3.3) of $k = 5$ follows with $\gamma_5 = 67/4$. The proof is complete. \square

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