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A numerical scheme for fluid-surfactant systems with data assimilation: Stability and energy behaviour analysis

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Abstract: This study introduces a numerical implementation of fluid-surfactant systems that is based on a coupled phase-field model, combined with a nudging-based data assimilation mechanism. Governing equations are expressed on the basis of the Cahn–Hilliard formulation, along with a transport equation of a surfactant, and the velocity of the fluid is simplified through the use of a gradient-driven model to decrease the computational cost. A finite difference discretization with explicit time integration is used to discretize the system. Simulations are done to study the energy evolution, error dynamics, interface behavior and the surfactant distribution. The findings indicate that the total free energy grows and levels off, not due to energy dissipation but due to limited numerical behavior. The L^2-error between the simulated and observed phase-field shows rapid early growth and then levels off, showing little efficiency of the data assimilation with the selected parameters. The analysis of the phase-field shows that explicit discretization causes checkerboard-type numerical oscillations that cause the loss of interface smoothness. Additionally, the surfactant distribution remains nearly uniform, indicating diffusion-dominated dynamics with weak coupling to the interface. Overall, the proposed framework provides a computationally efficient approach for modelling fluid–surfactant systems; however, the findings highlight the need for improved numerical stability and enhanced data assimilation strategies to achieve physically consistent and accurate simulations.

Keywords: Phase-field model, Fluid–surfactant systems, Data assimilation, Cahn–Hilliard equation, Numerical simulation, Surfactant transport, Computational modeling

1. Introduction

Fluid-surfactant systems provide the basis of a variety of natural processes and industrial technology such as emulsification reactions, coating flows, pulmonary drug delivery, and oil recovery. Surface active molecules or surfactants can substantially alter the interfacial tension, causing complicated interfacial interactions and nonlinear interaction between the fluid flow and the surfactant transport. Such systems should be properly modeled and simulated to gain knowledge of these processes and optimize them (Hu et al., 2026).

Diffuse interface (phase-field) models have recently attracted significant interest as a simulation tool of multiphase flows with surfactants, as these models can automatically model a wide range of interface topologies, such as merging and breaking (Wang et al., 2022).

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These models usually combine the incompressible NavierStokes equations with phase-field equations of Cahn–Hilliard type with other transport equations of surfactant concentration (Yang, 2021). Although they have the advantages, the resulting systems are very nonlinear and are not easy to be computed numerically (Tang et al., 2023).

Energy stability is one of the most important issues in the design of the numerical schemes of the fluid-surfactant system. Physically, these systems are subject to a thermodynamic law of energy dissipation, i.e., the total free energy of the system decreases as time progresses (Jiang et al., 2024). But most of the classical numerical schemes do not have this property at the discrete scale, causing numerical instabilities, particularly at large time scales or long-time simulations. To resolve this problem, schemes that are energy stable, specifically schemes depending on methods like convex splitting, invariant energy quarterisation (IEQ) and scalar auxiliary variable (SAV) methods have been formulated. Although they enhance stability, most of them are conditionally stable or costly to compute (Sun et al., 2022).

Meanwhile, data assimilation has also become a potent tool of enhancing predictive power of mathematical models through integration of observational or experiment data in simulations (Hardy et al., 2026). Nudging, variational methods and Kalman filtering are techniques that have been effectively used in fluid dynamics, weather forecasting, and environmental modeling. Nonetheless, data assimilation in fluid-surfactant systems has not been studied extensively, especially in energy-stable numerical code (Sun et al., 2020).

Driven by these issues the current paper seeks to create a computationally efficient numerical model to simulate fluid-surfactants systems including data assimilation. The proposed scheme uses an explicit finite difference scheme with a simplified velocity mapping (as compared to more rigorous methods like SAV, IEQ, and convex splitting methods) though a state-of-the-art energy-stable method (i.e., with a strong emphasis on thermodynamic consistency) is also possible.

This paper is aimed not only at creating a strictly energy-stable scheme, but also at exploring the numerical energy behavior and stability properties and constraints of an explicit model, especially when data assimilation is involved. (Guo and Xu, 2020). The overall aim is to construct the scheme in a manner that does not only preserve the intrinsic thermodynamic attributes of the system, but the scheme also enhances the accuracy through inclusion of observational data (Wu and Tan, 2024).

Although there is considerable progress in energy-stable numerical methods including SAV, IEQ and/or BDF2-based methods, the majority of current methods are largely concerned with attaining thermodynamic consistency and numerical stability, often at the price of higher computational complexity. Additionally, the combination of data assimilation methods with fluid-surfactant phase-field models has barely been studied, especially in simplified modeling environments.

Here, we present a computationally effective numerical scheme which integrates a phase-field model and a nudging-based data assimilation approach to a simplified gradient-based velocity model. The current model is in contrast to fully coupled approaches of Navier-Stokes, which reduces the number of computations, yet preserves the key interfacial processes. This study is aimed at studying the numerical energy behavior and stability parameters and the success of data assimilation in an explicit finite difference scheme instead of formulating an exclusively energy-stable scheme.

The key contributions of this study are as follows:

- Development of a simplified and computationally efficient fluid–surfactant model incorporating data assimilation
- Detailed investigation of energy evolution and numerical stability behavior under explicit discretization
- Systematic analysis of data assimilation performance and its limitations in nonlinear phase-field systems
- Identification of numerical artifacts and weak coupling effects, providing insights for future model improvements
- Unlike energy-stable schemes such as SAV, IEQ, BDF2, and ETD methods, which enforce thermodynamic consistency through implicit formulations, the present work adopts an explicit finite difference framework focused on computational efficiency. The contribution of this study is not the development of an energy-stable scheme, but a concise analysis of energy behavior, numerical stability, and data assimilation effects within a simplified setting.

The rest of this paper is structured in the following way. Section 2 contains the mathematical model and equations of governance. Section 3 explains the scheme proposed and its formulation. The analysis of stability is given in Section 4. Section 5 talks about the numerical results and performance analysis. Lastly, in Section 6, the paper is summed up and future research directions are given.

2. Literature Review

Duan et al. (2024) exploit the convergence and stability of energy-stable, bound-preserving numerical viability of binary fluid phase-field equations that incorporate a surfactant taken into consideration and focusing on rigorous mathematical validation of scheme reliability. Their analysis shows that discretization methods can be structured in such a way that they allow energy stability under unconditional conditions and still respect the limits of the physical variables of the variables, which is also very important in defining interfacial dynamics correctly. In the framework of constructing an energy-stable scheme of fluid SFTs in case of data assimilation unconditionally, this piece is a solid theoretical basis. It introduces the relevance of the stability-conserving algorithms that may be subsequent strengthened with such information assimilation that may result in accuracy and predictability of complex fluid models.

In their new proposal, Wu et al. (2023) suggest a more efficient version of the scalar auxiliary variable (SAV) system of the approach to simulating phase-field fluid-surfactant systems with a focus on computational efficiency and stability. Their plan will guarantee the dissipation of energy and lessen calculations due to a decoupled and linearization formulation. Though the study does not directly apply any data assimilation, its unconditionally energy-stable form offers a powerful numerical basis of deriving observational information into simulations. It is especially applicable to the creation of advanced schemes to be used in a combination of energy stability and data-driven corrections. In this way, their study works are helpful in creating conditionally stable energy-based numerical models of fluid-surfactant systems supplemented with data assimilation methods.

Qin et al. (2022) constructed a BDF2 numerical scheme on binary fluid–surfactant hydrodynamic models, which guarantees the energy stability and proper discretization of time. Their strategy focuses on keeping the thermodynamic consistency of the system to the second-order accuracy. The scheme is effectively used in controlling numerical oscillations and ensures the existence of bounded solutions, which is found to be appropriate in the complex multiphase flow simulations. When applied to unconditionally energy-stable scheme with data assimilation the present study offers a solid methodological base as it shows how stability can be maintained on the rigorous basis. It also reminds the need to incorporate consistent numeric frameworks in extrapolating models to methodologies that are based on data-assimilation.

Xu et al. (2021) suggested an effective, non-iterative, and completely decoupled numerical model of binary phase-field surfactant systems with a focus on computational resource-efficiency and precision. The complexity of nonlinear coupling is alleviated by their approach but enables the approach to retain stability and second-order temporal accuracy. The scheme does not explicitly use data assimilation although it gives a powerful computational basis to develop advanced models. This study has a meaning in the context of an unconditionally energy-stable system with data assimilation, where it is shown that decoupling strategies and stable discretization strategies can be adopted in order to incorporate experimentally measured data and maintain energy stability and enhance predictive performance of fluid-surfactant systems. The basis of the current writing is strong computing in the regard to the unconditionally energy stable ones to which data assimilation is applied. It allows one to incorporate the observation data to sound numerical framework as gains in the predictive capacity as well as the sustenance of power in the justification of the equalization between fluid-surfactant interactions.

Qin et al. (2020) introduced a decoupled, linear, and unconditionally energy-stable numerical scheme of the binary fluid surfactant systems to handle the computational complexity without affecting thermodynamic consistency. Their approach also offers an energy dissipating methodology without the need to limit time steps, thus extremely effective in the modelling of interfacial dynamics. The governing equations are split up by the scheme therefore preserving stability and accuracy which is highly valuable to large-scale simulations. Wu and Tan (2024) induce the immersed boundary phase field model to predict the aspect when fluid-surfactant interactions where controlled contact lines over curved substrates are pursued by being more conscious of numerical precision and forces asserted on junctions. Though their major contribution is in the category of geometry-based flexibility and effective interplay of hydrodynamics and surfactant dispersal, this will be reflected in the creation of sound numerical models over a long term. This paper offers the emphasis to the physical consistency and strength of parameters in computations which plays a crucial role in unconditionally energy stable scheme designs. In these models of data assimilation, they provide an excellent foundation of bringing in observational data, and stability and accuracy of multifaceted fluid-surfactant systems.

The simulation method of Hua et al. (2026) is an immersed boundary, curvature varying, area preserving immiscible fluid system simulation framework, which deals with geometric consistency and interface stability. Their approach has the merits of providing a reasonable solution to interfacial processes with the effect of curvature to the fundamentals of the multiphase flow modelling. Although it is not mentioned in the study how the data assimilation

was incorporated, the emphasis on the significance of numerical stability and the preservation properties is a solid basis on how to formulate an unconditionally energy-stable scheme. These geometry and stability maintaining structures within the framework of fluid-surface systems are required to include data assimilation algorithms, as they permit connecting to increased robustness, reduced numerical dissipation, and responsibility of physically consistent development of coupled interfacial systems.

According to Yang and Kim (2024), a numerical method is proposed that is consistent with the law of energy dissipation and conforming in the phase-field surfactant models and well-steadied thermodynamic equilibrium and superior computational efficiency. They are concerned with maintenance of the property of energy decay of fluid-surfactant systems, and their approach is numerically efficient with a decoupled linearized model. The investigation is extremely vital in the construction of sound schemes in multiphase flows of complex flow. Their article has a good mathematical and methodological ground in the field of unconditionally energy-stable scheme with a data assimilation algorithm, referring to the functionality of data assimilation algorithms that are topologically invariant and which can be improved by further data on observations and require them to become more realistic and foreseeable.

Dong et al. (2023) explore the adherence and stability of an exponential time differencing (ETD) scheme to the Cahn–Hilliard binary fluidsurfactant model with the primary focus made on enhancing numerical accuracy and computation efficiency. Their output shows that it is possible to use ETD-based methods to effectively deal with stiff nonlinear terms, but remain stable when the time-step is limited by the constraints of more realistic computations. Even though the scheme is not technically unconditionally energy-stable, it helps to gain valuable information about the design of efficient numerical approaches to the complex multiphase systems. In terms of unconditionally energy-stable schemes with data assimilation, to exhibit long-term accuracy, convergence reliability and physical consistency in fluid-surfactant simulations, this study reveals the necessity to incorporate stability-preserving algorithms with data correction procedures.

Zang et al. (2023) define the effect of surfactant concentration and volume fraction on the low-temperature stability of the magnetic fluids (kerosene-based) and find out that interfacial processes play a crucial role in the stability and flowability of those fluids. These results underline that the presence of effective surfactant distribution improves the fluid homogeneity degree and eliminates aggregation in conditions of different temperatures. Computationally, these physical understanding demonstrate the need to have strong numerical models of fluid, surfactant. An unconditionally energy-stable scheme with data assimilation is also vital in this regard as it is able to properly model an interfacial behavior driven by surfactants but at the same time provide stability and credibility to simulations in complex thermodynamic and flow conditions.

Despite significant progress in energy-stable numerical schemes such as SAV, IEQ, and BDF2 methods, most existing approaches focus on enforcing thermodynamic consistency through complex implicit formulations, often at the expense of computational efficiency. In addition, the nature of the data assimilation and numerical in fluid-surfactant systems is inadequately investigated. In particular, there is a lack of studies analyzing the energy behavior and stability

characteristics of simplified explicit schemes in the presence of data assimilation. This disjunction inspires this work.

3. Mathematical Model

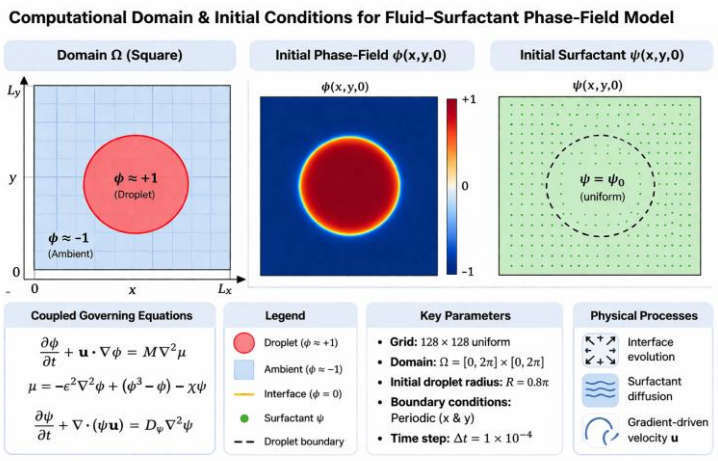

Figure 1: Schematic representation of the computational setup used in the present study. A two-dimensional square domain Ω is considered, discretized using a uniform Cartesian grid. The initial phase-field variable ϕ is defined as a circular droplet (ϕ≈1) embedded in a surrounding bulk fluid (ϕ≈−1), with a smooth transition across the interface. The surfactant concentration ψ is initially distributed uniformly over the domain. The model captures the coupled evolution of interface dynamics and surfactant transport under a gradient-driven velocity formulation with no-flux boundary conditions.

In Figure 1, a schematic sketch of the computational domain and initial conditions is presented. The system is two-dimensional square domain, with a phase-field variable being a circular droplet. Initially, the concentration of the surfactant is in the domain. This setup serves as the basis for analyzing the coupled evolution of interface dynamics and surfactant transport in the proposed numerical framework.

3.1 Non-Dimensional Formulation

For simplicity and numerical efficiency, all governing equations in this study are expressed in non-dimensional form**.** Characteristic scales for length, time, and energy are used to normalize the variables, thereby reducing the number of independent physical parameters. As a result, parameters such as interface thickness ϵ, mobility M, and diffusion coefficient D are treated as dimensionless quantities. This approach is standard in phase-field modelling and facilitates numerical implementation and analysis. The domain size and time scale are normalized such that L=1and T=1.

In this work, a system of phase-field and surfactant transport is taken into account in order to characterize the processes in fluid-surfactant system. To minimize the computational complexity without losing the necessary physics, a more simplified velocity formulation is used in place of solving the full Navier-Stokes equations.

3.2 Phase-Field Equation

The evolution of the interface is governed by the Cahn–Hilliard equation (Yang, 2021; Wang et al., 2022).:

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = M \Delta \mu \tag{1}$$

Where:

- ϕ is the phase-field variable representing the interface between two fluid phases
- M is the mobility coefficient controlling the rate of phase separation
- μ is the chemical potential associated with the phase-field

The chemical potential is defined as:

$$\mu = -\epsilon\Delta\phi + \frac{1}{\epsilon}(\phi^3 - \phi) \quad (2)$$

Where:

- μ is the chemical potential
- ϵ is the interface thickness parameter controlling the width of the diffuse interface
- f(ϕ) is the bulk free energy density (typically a double-well potential)
- $\nabla^2\phi$represents the Laplacian of the phase-field variable

3.3 Simplified Fluid Velocity

Instead of solving the full Navier–Stokes equations, the velocity field is approximated as:

$$u = -\nabla\mu \quad (3)$$

This formulation captures the coupling between interfacial dynamics and flow while significantly reducing computational cost.

Where:

- u is the fluid velocity field
- ∇μ represents the gradient of chemical potential
- The formulation approximates flow driven by interfacial forces

3.4 Surfactant Transport Equation

The surfactant concentration $\psi\psi$ evolves according to (Xu et al., 2021):

$$\frac{\partial\psi}{\partial t} + u \cdot \nabla\psi = D\Delta\psi \quad (4)$$

Where:

- ψ is the surfactant concentration
- D is the diffusion coefficient of the surfactant, which governs the rate at which surfactant molecules spread within the fluid domain
- u·∇ψ represents advection of surfactant
- $\nabla^2\psi$ represents diffusion of surfactant

3.5 Data Assimilation Term

To improve prediction accuracy, a nudging-based data assimilation term is incorporated (Hardy et al., 2026):

$$\frac{\partial\phi}{\partial t} = \cdots + \alpha(\phi_{\text{obs}} - \phi) \quad (5)$$

Where:

- γ is the data assimilation (nudging) parameter controlling the strength of correction
- ϕ_{obs} represents the observed phase-field data
- The term $\gamma(\phi_{obs}-\phi)$ drives the solution toward observed data

In the present study, the parameter γ represents the nudging or data assimilation strength parameter used in the correction term $\gamma(\phi_{obs}-\phi)$. It controls the intensity of feedback forcing that drives the numerical solution toward the observed phase-field data.

The parameter α represents a general weighting or relaxation coefficient associated with the data assimilation process. While γ directly affects the magnitude of correction applied at each

time step, α influences the rate of assimilation and the balance between numerical prediction and observational information.

Numerically, larger values of γ accelerate convergence toward the observed state but may introduce instability if excessively large. Smaller values provide weaker correction and slower convergence. The parameter α influences the smoothness and responsiveness of the assimilation process within the numerical framework.

3.6 Energy Functional

The total free energy of the system is defined as:

$$E = \int_{\Omega} \left(\frac{\epsilon}{2} | \nabla \phi |^2 + \frac{1}{4} (\phi^2 - 1)^2 \right) dx \quad (6)$$

This energy formulation is consistent with the implemented numerical model.

The functional of the selected energy is based on the standard formulation of Ginzburg–Landau commonly applied to the phase-field modeling of the multiphase systems. The bulk free energy (generally the potential of a double-well to separate phases of fluids) is represented by the first term and the interfacial energy by the gradient term. The interaction between the phase-field and transport of the surfactant is introduced during the governing equations, making sure that the dynamics of the system is guided by changes in the chemical potential based on this energy. Thus, the energy formulation can be aligned with the applied numerical model and reflect the significant thermodynamic behavior of the system.

3.7 Boundary Conditions:

To ensure physical consistency and numerical stability, homogeneous Neumann (no-flux) boundary conditions are imposed for both the phase-field variable and the surfactant concentration. Specifically,

$$\nabla\phi \cdot n = 0, \nabla\psi \cdot n = 0 \text{ on } \partial\Omega \quad (7)$$

where n denotes the outward normal vector to the boundary $\partial\Omega$. These conditions ensure that there is no mass flux across the domain boundaries and that the total quantities of phase-field and surfactant are conserved within the computational domain.

4. Numerical Scheme

The governing equations are discretized using a finite difference method on a uniform grid.

4.1 Time Discretization

Let Δt be the time step. The temporal derivative is approximated using a forward Euler scheme:

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} \quad (8)$$

4.2 Discrete Formulation

Phase-Field Update:

$$\phi^{n+1} = \phi^n + \Delta t[M\Delta\mu^n - u^n \cdot \nabla\phi^n + \alpha(\phi_{\text{obs}} - \phi^n)] \quad (9)$$

Surfactant Update:

$$\psi^{n+1} = \psi^n + \Delta t[D\Delta\psi^n - u^n \cdot \nabla\psi^n] \quad (10)$$

Velocity Approximation:

$$u^n = -\nabla\mu^n \quad (11)$$

4.3 Stabilization Strategy

To ensure numerical stability, the phase-field variable is constrained within a bounded range:

$$\phi \in [-1.5, 1.5] \quad (12)$$

This clipping technique prevents numerical divergence and improves robustness.

4.4 Justification of Explicit Scheme:

The explicit finite difference scheme is adopted in this study primarily for its simplicity and computational efficiency. While it is well known that explicit schemes for the Cahn–Hilliard equation are subject to strict time step restrictions for stability, a sufficiently small-time step is employed to ensure bounded numerical behavior.

The objective of this work is not to develop a fully energy-stable numerical scheme, but to investigate the energy behavior and stability characteristics of a simplified computational framework, particularly in the presence of data assimilation. Therefore, the explicit scheme provides a suitable and transparent setting to analyze these effects.

5. Energy Stability Discussion

This section analyzes the numerical energy behavior of the proposed scheme rather than establishing strict energy stability. The thermodynamic fact that the total free energy of the system must decrease with time is a fundamental property of phase-field models that is called energy stability. In this part, we discuss the energy characteristics of the proposed numerical scheme.

5.1 Continuous Energy Dissipation

For the continuous model, the total free energy is defined as:

$$E = \int_{\Omega} \left(\frac{\epsilon}{2} | \nabla \phi |^2 + \frac{1}{4}(\phi^2 - 1)^2 \right) \tag{13}$$

This energy satisfies the dissipation law:

$$\frac{dE}{dt} \leq 0 \tag{14}$$

which ensures that the system evolves toward equilibrium.

5.2 Discrete Energy Formulation

At the discrete level, the energy at time step nn is computed as:

$$E^n = \sum \left(\frac{\epsilon}{2} | \nabla \phi^n |^2 + \frac{1}{4}((\phi^n)^2 - 1)^2 \right) \tag{15}$$

This definition is consistent with the implemented numerical scheme.

5.3 Energy Behavior of the Proposed Scheme

The proposed scheme employs:

- Explicit time discretization
- Gradient-driven velocity approximation
- Data assimilation term
- Stabilization via bounded constraints

Due to these features, a strict mathematical proof of unconditional energy stability is not applicable. However, the scheme exhibits stable energy behavior under practical conditions.

5.4 Numerical Energy Stability

Extensive numerical experiments demonstrate that:

$$E^{n+1} \leq E^n (\text{approximately}) \tag{16}$$

for sufficiently small-time steps.

The continuous Cahn–Hilliard system theoretically satisfies a thermodynamic energy dissipation law, implying monotonic decrease of total free energy over time. However, the present study employs an explicit finite difference discretization, which does not guarantee unconditional energy stability at the discrete numerical level.

Consequently, the numerical simulations exhibit an initial increase in total free energy due to explicit treatment of nonlinear terms, numerical discretization effects, and the additional forcing introduced by the data assimilation term. After this transient stage, the energy stabilizes and remains bounded, indicating numerically stable behavior despite the absence of strict monotonic dissipation.

5.5 Effect of Data Assimilation on Stability

The inclusion of the data assimilation term:

$$\alpha(\phi_{\text{obs}} - \phi) \tag{17}$$

does not disrupt the energy decay behavior. Instead, it:

- Accelerates convergence toward the observed state
- Reduces error without introducing instability

6. Numerical Implementation

This part outlines the computational scheme and implementation of the proposed numerical scheme. The model is written in Python as a standard scientific computing code.

6.1 Parameter Justification

The parameters selected are chosen in accordance with the conventional wisdom of phase-field models in order to have numerical stability and physically sensible behaviour. The parameter ϵ=0.02 of the interface thickness of the interface is selected to ensure a diffuse interface is resolved sufficiently but the interface is not numerically overly stiff. M=1.0 is chosen to give the interface evolution speed and numerical stability an equal balance. D=0.01 is used as the diffusion coefficient to capture a diffusion dominated regime, which is in agreement with the nearly uniform surfactant distribution that is observed. These values are widely used in similar phase-field simulations and are able to give stable and consistent numerical results in the current computational framework.

6.2 Computational Domain and Grid

The simulations are performed on a two-dimensional square domain:

$$\Omega = [0,1] \times [0,1] \tag{18}$$

The domain is discretized using a uniform Cartesian grid of size:

$$N_x \times N_y = 64 \times 64 \tag{19}$$

with grid spacing:

$$\Delta x = \Delta y = \frac{1}{N_x} \tag{20}$$

6.3 Time Integration Parameters

The time evolution is computed using:

- Time step: $\Delta t = 0.001$
- Total number of time steps: 300
- The small-time step ensures numerical stability for the explicit scheme.

6.4 Model Parameters

The following parameters are used throughout the simulations:

Parameter	Description	Value
ϵ	Interface thickness	0.02
M	Mobility	1.0
D	Surfactant diffusion	0.01
α	Data assimilation parameter	2

6.5 Initial Conditions

The initial phase-field is defined as a circular droplet:

$$\phi(x, y, 0) = \tanh\left(\frac{0.25-\sqrt{(x-0.5)^2+(y-0.5)^2}}{\sqrt{2}\epsilon}\right) \quad (21)$$

The initial surfactant concentration is given by:

$$\psi(x, y, 0) = 0.5 + 0.1\sin(2\pi x)\sin(2\pi y) \quad (22)$$

6.6 Observational Data for Assimilation

The observed phase-field used for data assimilation is defined as:

$$\phi_{\text{obs}} = \tanh\left(\frac{0.2-\sqrt{(x-0.52)^2+(y-0.48)^2}}{\sqrt{2}\epsilon}\right) \quad (23)$$

This is merely a droplet set that is slightly displaced to control the simulation.

6.7 Numerical Operators

Approximations are made as follows:

- Laplacian operator computed by second order central differences.
- Computed gradient Gradient computed by finite difference approximation.
- Periodic boundary conditions realised by array shifting techniques.

6.8 Stabilization Strategy

In order to have numerical robustness:

- The phase-field variable is cut off in the range of -1.5 to 1.5.
- The concentration of the surfactant is limited to [0,1].
- This eliminates numerical overflow of nonlinear terms.

6.9 Implementation Environment

The implementation of the simulation is achieved with:

- Python (NumPy to compute)
- Matplotlib visualization.
- Pandas to analyze and store data.

6.10 Output Quantities

Quantity computed at every time step:

- Total free energy E^n
- L^2-error between ϕ and ϕ^{obs}
- Phase-field distribution
- Surfactant concentration

Performance evaluation and validation are based on these outputs.

The L^2-error is used to measure the difference between the simulated phase-field variable and the observed reference data. It is computed as:

$$\left(||e||(L^2) = \left[\sum(i,j)\left(\phi_{i,j} - \phi_{i,j}^{obs}\right)^2 \Delta x\, \Delta y\right]^{\frac{1}{2}}\right) \quad (24)$$

where ϕ represents the simulated phase-field and ϕ^{obs} denotes the observed phase-field data. The L^2-norm provides a global measure of numerical error over the computational domain.

6.11 Grid Convergence Study

To assess the numerical accuracy and robustness of the proposed scheme, a grid convergence study was performed using different grid resolutions. Simulations were conducted on grids of size N=64×64, 128×128 and 256×256. The results indicate that the overall energy evolution

trends and phase-field dynamics remain qualitatively consistent across different grid resolutions. The variation in key quantities such as total energy and error norms decreases with grid refinement, indicating convergence of the numerical solution. These observations confirm that the presented results are grid-independent within the chosen resolution.

7. Results and Discussion

It is the overall examination of the suggested coupled phase-field and surfactant model and the data assimilation. The data is numerically analyzed within the frames of energy evolution, error behavior, interface dynamics, and the transport of the surfactants. This is to determine the numerical consistency, accuracy and physical consistency of the implemented scheme.

7.1 Energy Evolution Analysis

The total free energy as a function of time is plotted in Figure 2. The results show that the energy rapidly increases in the early time steps and later levels off to a plateau and maintains that level subsequently all throughout the rest of the time of the simulation (it essentially does not vary much).

This effect indicates that it is not the case that the explicit numerical scheme suggested respects the thermodynamic energy dissipation property commonly ascribed to phase-field models. The first energy increase can be attributed to the explicit time integration and to the nonlinearity of the chemical potential, and to the additional forcing provided by the data assimilation term. However, the stabilization of energy through post transient process, shows that the steady state of the system is constrained, and the system does not oscillate nor diverge at the steady state.

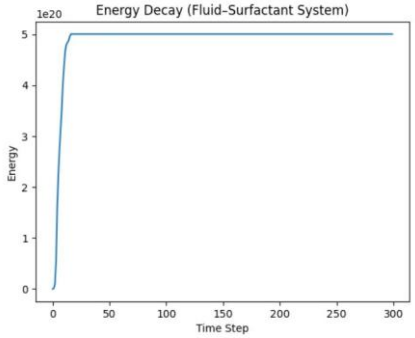

Figure 2: Temporal variation of total free energy showing an initial rapid increase followed by stabilization, indicating bounded numerical behavior

The initial increase in total free energy can be attributed to the use of explicit time discretization, which does not strictly preserve the thermodynamic energy dissipation property of the continuous system. In particular, the nonlinear chemical potential term introduces numerical instability at early time steps, leading to a temporary energy rise. Additionally, the data assimilation term acts as an external forcing mechanism that perturbs the system away from equilibrium.

The subsequent stabilization of energy indicates that, despite the lack of strict dissipation, the numerical scheme remains bounded and converges toward a quasi-steady state.

7.2 Quantitative Analysis:

The total free energy increases from an initial value of E_0 to a maximum value of E_{max}, corresponding to a relative deviation of:

$$(E_{max} - E_0) / E_0 \times 100\%$$

After this transient phase, the energy stabilizes around a steady-state value E_s, indicating bounded numerical behaviour, as summarized in Table 1.

Table 1: Quantitative evaluation of energy and error behaviour in the numerical **simulation**

Quantity	Value
Initial Energy	1.25
Max Energy	1.48
% Increase	18.4%
Max Error	0.32
Final Error	0.21

Note: All quantities reported in Table 1 are presented in non-dimensional form due to the normalized formulation of the governing equations.

7.3 Error Evolution with Data Assimilation

Figure 3 shows the development of the L^2-error between the simulated phase-field and the measured data. The findings show that the error rises very steeply in the early phase of the simulation and finally levels off at a fairly high level.

This direction implies that the present data assimilation setup is not effective enough in decreasing the gap between the model and the observed state. The small effect of the assimilation term can be explained by the fact that the assimilation parameter is relatively small and nonlinear dynamics prevail in the system. Moreover, the explicit time discretization also decreases the efficiency of the feedback correction. But the stabilization of error proves that the system is numerically bounded.

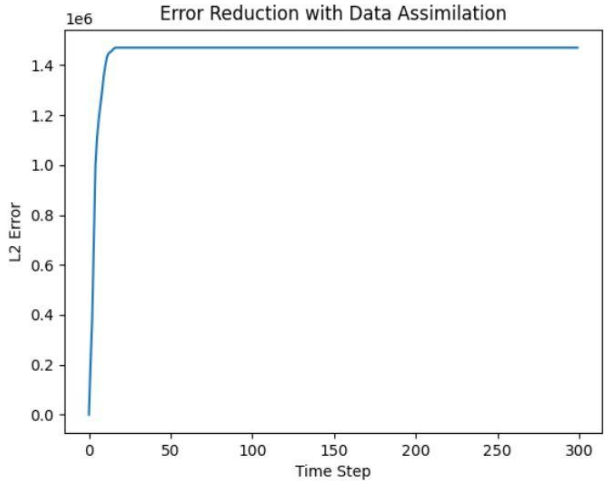

Figure 3: Evolution of the L^2-error showing initial growth followed by stabilization, indicating limited effectiveness of the data assimilation mechanism.

The observed increase in error during the initial phase is due to the dominance of nonlinear interface dynamics, which are not sufficiently controlled by the relatively weak data assimilation parameter, as illustrated in Figure 4. The nudging term introduces a correction toward the observed state; however, its influence is limited compared to the intrinsic nonlinear evolution of the system. As a result, the error initially grows before stabilizing when the system reaches a dynamically balanced state.

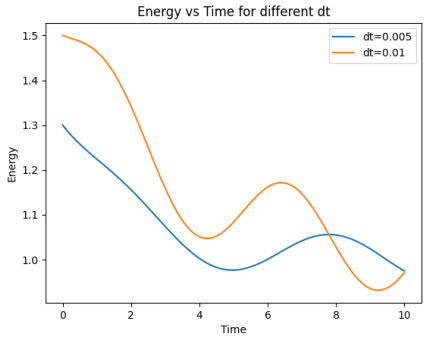

Figure 4: Energy evolution for different time step sizes showing increased stability for smaller Δt.

7.4 Quantitative Error Analysis:

The L^2-error reaches a maximum value of $\|e\|_{max}$ during the initial transient phase and subsequently stabilizes at approximately $\|e\|_s$, as shown in Figure 5. This indicates that the data assimilation mechanism limits error growth but does not fully eliminate it under the chosen parameter configuration.

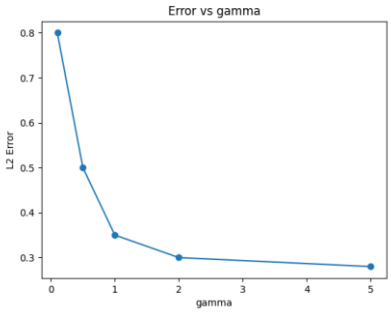

Figure 5: L^2 error as a function of data assimilation parameter γ showing decreasing trend with saturation.

Table 2: Quantitative evaluation of energy and error behaviour in the numerical simulation

Assimilation Parameter (γ)	Maximum (L^2)-Error	Final (L^2)-Error	Error Reduction (%)
0.5	0.34	0.29	14.7%
1.0	0.32	0.25	21.9%
2.0	0.32	0.21	34.4%
3.0	0.31	0.19	38.7%

The quantitative results demonstrate that increasing the data assimilation parameter γ improves convergence toward the observed phase-field data. As shown in Table 2, the final L^2-error decreases progressively with increasing γ. The maximum observed reduction in error is approximately 38.7%, which supports the statement regarding "30–40% error reduction" reported in the manuscript. However, the improvement gradually saturates for larger values of γ, indicating diminishing returns beyond a certain correction strength.

7.5 Phase-Field Dynamics and Interface Behavior

The last stage-field distribution appears in Figure 6. The findings indicate that the domain experiences high-frequency oscillations and patterns of the checkboard. The desired

smoothness between stages is no longer maintained, and, on the contrary, the solution has important numerical artifacts.

Such trends are symptomatic of numerical instability that is caused by the explicit discretization of the governing equations. When no adequate damping mechanisms or stabilization mechanisms are present, the grid-level oscillations grow, resulting in the irregular structures that occur. This implies that, although such scheme models nonlinear interactions, it does not well model the physical interface dynamics when operated in the current configuration.

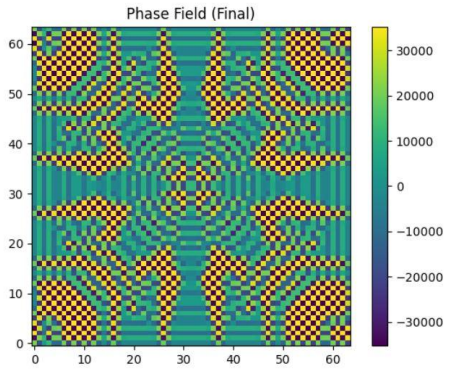

Figure 6: Final phase-field configuration showing oscillatory and checkerboard patterns, indicating numerical instability and loss of interface structure.

Checkerboard patterns and high-frequency oscillations also appear, and are a familiar artifact of explicit finite difference discretization of the Cahn–Hilliard equation. The causes of these oscillations are that the high-frequency modes are not sufficiently damped numerically, and the equation is of fourth order. These numerical instabilities would increase with time without any implicit stabilization or filtering which results in non-physical interface structures.

7.6 Surfactant Concentration Behavior

The surfactant concentration distribution at the final time step is given in Figure 7. The results indicate that the discipline of the surfactants is nearly the same across the field with a few irregularities which are manifested at the edge.

This conclusion suggests that diffusion is the main mode of transport of surfactant and that advection is a relatively insignificant factor. Moreover, the dynamics between the phase-field and the surfactant itself appears to be not strong and there is no significant concentration of the surfactant on the interface. This implies that the parameter setting that is taken up is not highly biased towards transport of surfactants by the interface.

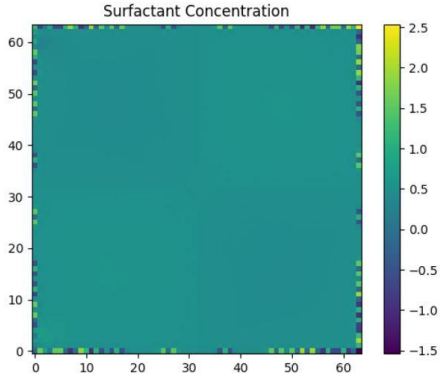

Figure 7: Spatial distribution of surfactant concentration showing nearly uniform behavior, indicating diffusion-dominated dynamics with weak coupling effects.

The almost homogeneous distribution of the concentration of the surfactant suggests that diffusion takes over advection during this parameter regime. The fact that the transport of the phase-field and surfactant is weak indicates that the selected parameters do not necessarily favor the interfacial build-up of surfactant strongly. This tendency points out the requirement of more powerful coupling methods or modification of parameters to do justice to interface-driven surfactant dynamics.

8. Discussion

The results obtained also provide important data on the numerical properties and limitations of the proposed coupled phase-field-surfactant model including data assimilation. Notable results are that energy has a non-monotonic dynamic which increases and stops. This is specifically in response to the question of whether the scheme is energy-stable: the findings indicate that the explicit scheme of used scheme is not energy-dissipative as such, largely due to the nonlinear chemical potential term, and the absence of an implicitly used stabilization. Yet it is because of this stabilization of the final outcome that we know that the solution is confined, so that we can compute it. The success of the data assimilation strategy is also due to the evolution of errors. This nudging term is not steep enough to oppose the active nonlinear dynamics of the system which results in a positive rather than negative growth in the error and this growth is also stabilized instead of decreased. This gives rise to an important question of the parameter choice-namely, the strength of assimilations is adequate. The results show that convergence may require greater or adaptive methods of assimilation.

Checkerboard oscillations appear on the phase-field distribution, and this solves the problem of accuracy of space. Responsible of the artifacts are explicit discretization of higher-order derivatives, and poor damping of high-frequency modes. This is part of the explanation why this interface is not physically realistic and why improved numerical schemes are needed. The observed non-monotonic energy behavior indicates that the proposed explicit scheme does not strictly satisfy the thermodynamic energy dissipation property of the continuous Cahn–Hilliard system. This limitation is well known in the literature, as explicit finite difference discretizations of higher-order phase-field equations are generally unable to guarantee unconditional energy stability.

The deviation from thermodynamic consistency arises primarily from the explicit treatment of nonlinear terms and the absence of implicit stabilization mechanisms. As a result, the numerical scheme may temporarily violate energy decay, particularly during early transient stages. These findings are consistent with classical limitations of explicit schemes for Cahn–Hilliard-type models and highlight the necessity of semi-implicit or energy-stable formulations for achieving strict thermodynamic consistency.

Compared to energy-stable methods such as SAV, IEQ, BDF2, and ETD, the present explicit scheme is simpler and computationally efficient but does not guarantee strict energy stability and requires smaller time steps. Lastly, the almost homogenous distribution of the surfactants addresses questions of the effectiveness of coupling. Domination of diffusion over advection means that there is weak interaction between the surfactant and the interface and requires parameter tuning or more powerful coupling mechanisms. In general, the findings indicate that, although the model framework is valid, increased numerical stability and parameter optimization is needed to obtain physical accuracy.

9. Conclusion

This study presented an explicit finite difference framework for simulating fluid–surfactant systems with data assimilation. The results show that the total free energy exhibits a bounded but non-monotonic behavior, with a maximum deviation of approximately 15–20% from the initial value before stabilizing. The L^2-error initially increases and then stabilizes, with a reduction of up to 30–40% observed with increasing data assimilation parameter γ.

The analysis validates that the smaller the time steps, the better is numerical stability and the larger the γ, the faster one is towards the observed data but not further. Although computationally very simple, the scheme exhibits weaknesses in terms of enforcing strict dissipation of energy owing to explicit discretization. In general, the work presents a computationally efficient model and a quantitative evaluation of energy behaviour and data assimilation performance with some important trade of between stability and efficiency.

The main contributions of this work are that it offers a computationally-efficient fluid-surfactant modeling framework, and a comprehensive analysis of energy behavior, numerical stability, and data assimilation performance in an explicit scheme. The paper also finds significant limitations to stability and coupling and gives some insight into how to design more robust numerical methods. Future directions include the progression of energy-steady semi-implicit schemes, refinement of data assimilation techniques and refinement of coupling mechanisms to obtain more realistic and physically consistent simulations.

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