IMA Journal of Numerical Analysis (1996) **16**, 111–139

Numerical analysis of a model for phase separation of a multi-component alloy

J. F. BLOWEY

Department of Mathematical Sciences, South Road, Durham DH1 3LE, UK

M. I. M. COPETTI

Departamento de Mathemática, Universidade Federal de Santa Maria, 97119 Santa Maria – RS, Brazil

AND

C. M. ELLIOTT

Centre for Mathematical Analysis and its Applications, University of Sussex, Falmer, Brighton BN1 9QH, UK

[Received 1 July 1994 and in revised form 20 February 1995]

We consider a fully discrete implicit finite-element approximation of a model for the phase separation of a multi-component alloy. We prove existence, uniqueness and stability of the numerical solution for a sufficiently small time step. We prove convergence to the solution of the associated continuous problem. We perform a linear stability analysis of the equation and describe some numerical experiments.

1. Introduction

The purpose of this work is to consider a finite-element approximation of the model studied in Elliott & Luckhaus (1991) for isothermal phase separation of a multi-component ideal mixture with $N \geqslant 2$ components, occupying an isolated domain $\Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$. It is concerned with finding the vector pair $\{\boldsymbol{u}(\boldsymbol{x}, t), \boldsymbol{w}(\boldsymbol{x}, t)\} \in \mathbb{R}^N \times \mathbb{R}^N$ for $\boldsymbol{x} \in \Omega$ and $t > 0$ solving the system of non-linear diffusion equations given by

$$\boldsymbol{u}_t - L\Delta \boldsymbol{w} = \boldsymbol{0}, \tag{1.1a}$$

$$\boldsymbol{w} = -\gamma\Delta\boldsymbol{u} + \theta\boldsymbol{\phi}(\boldsymbol{u}) - A\boldsymbol{u} - \boldsymbol{1}\sum[\theta\boldsymbol{\phi}(\boldsymbol{u}) - A\boldsymbol{u}], \tag{1.1b}$$

$$\frac{\partial \boldsymbol{u}}{\partial \nu} = \frac{\partial \boldsymbol{w}}{\partial \nu} = \boldsymbol{0} \quad \text{on } \partial\Omega, \tag{1.1c}$$

$$\boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{u}^0(\boldsymbol{x}). \tag{1.1d}$$

Here θ and γ are positive constants, ν is the normal unit vector pointing out of

Ω and A and L are symmetric $N \times N$ matrices. We use the notation η_l to be the lth component of $\boldsymbol{\eta} \in \mathbb{R}^N$ and for $l = 1,\dots,N$ set

$$\left\{\frac{\partial \boldsymbol{u}}{\partial \nu}\right\}_l = \frac{\partial u_l}{\partial \nu}, \qquad \{\nabla \boldsymbol{\eta}\}_l = \nabla \eta_l, \qquad \sum \boldsymbol{\eta} := \frac{1}{N}\sum_{l=1}^{N} \eta_l,$$

$$\mathbf{1}_l := 1, \qquad \{\boldsymbol{\phi}(\boldsymbol{u})\}_l := \phi(u_l),$$

where $\phi(r) = \ln r$. The concentration of the component l is denoted by u_l so that the constraints

$$(a)\ 0 \leq u_l \leq 1 \qquad (b)\ N \sum \boldsymbol{u} = 1 \tag{1.2}$$

are satisfied. The non-negativity of u_l is a consequence of the fact that $\phi(\cdot)$ is infinite at 0. That (1.2b) is satisfied is a consequence of assuming L has a one-dimensional kernel such that $L\mathbf{1} = 0$ and $N \sum \boldsymbol{u}^0(\boldsymbol{x}) = 1$. We also assume that L is positive semi-definite. It then easily follows by summation from (1.1a–d) that (1.2b) holds and that

$$\sum \boldsymbol{w} = 0, \qquad \int_\Omega \boldsymbol{u}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \int_\Omega \boldsymbol{u}^0(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \boldsymbol{m}, \qquad \forall t. \tag{1.3}$$

Here we take initial values such that $\mathbf{0} < \boldsymbol{m} < \mathbf{1}\,|\Omega|$; the notation $\boldsymbol{\eta} \geq (>)\mathbf{0}$ means that the inequality holds component by component.

The collection of equations (1.1a–d) is a system of Cahn–Hilliard equations, see De Fontaine (1972, 1973), Hoyt (1989, 1990) and Eyre (1993).

REMARK 1.1 In the case $N = 2$, assuming that $A_{11} = A_{22}$, $L_{11} = L_{22} = \frac{1}{2}$, defining $u := u_2 - u_1$, $w := w_2 - w_1$ and $\theta_c = (A_{11} - A_{22})/2$ we obtain that $\{u, w\}$ satisfies the equations

$$u_t - \Delta w = 0, \qquad w = -\gamma \Delta u + 2\psi'(u), \tag{1.4}$$

where

$$\psi(u) = \frac{\theta}{2}\big((1+u)\log_e(1+u) + (1-u)\log_e(1-u)\big) - \frac{\theta_c}{2}u^2.$$

This is the Cahn–Hilliard equation, with logarithmic free energy, whose numerical analysis has been studied by Copetti & Elliott (1992).

It is convenient to introduce the homogeneous free-energy functional

$$\Psi(\boldsymbol{u}) = \theta \sum_{l=1}^{N} u_l \ln u_l - \tfrac{1}{2}\boldsymbol{u}^{\mathrm{T}} A \boldsymbol{u}, \tag{1.5}$$

so that $\theta\phi(u_l) = \{D\Psi(\boldsymbol{u})\}_l + \{A\boldsymbol{u}\}_l - \theta = \theta \ln u_l$ $(1 \leq l \leq N)$. From physical considerations, that being Ψ should have more than one local minimum, we shall assume that A is not negative definite, i.e. it has at least one positive eigenvalue.

From the properties of L, all of its eigenvalues are non-negative, the eigenvectors form a basis and there exists l_0 (the smallest positive eigenvalue) such that

$$\boldsymbol{\eta}^{\mathrm{T}} L \boldsymbol{\eta} \geq l_0 \left\| \boldsymbol{\eta} - \mathbf{1} \sum \boldsymbol{\eta} \right\|^2. \tag{1.6}$$

Here we take $\|\cdot\|$ to be the usual 2-norm for vectors. We take the matrix norm to be that induced by the vector 2-norm; for symmetric matrices, the value of the matrix norm is given by the spectral radius.

Throughout this paper we assume that Ω is a convex polygonal bounded domain in $\mathbb{R}^2$; however results also hold in convex domains in $\mathbb{R}^d$ $(d = 1, 2, 3)$ where $\partial\Omega$ is sufficiently smooth. We denote the norm of the Sobolev space $H^p(\Omega)$ $(p \geq 0)$ by $\|\cdot\|_p$, the semi-norm $\|D^p\eta\|_0$ by $|\eta|_p$. We introduce the spaces $\boldsymbol{L}^2(\Omega) = \{L^2(\Omega)\}^N$ and $\boldsymbol{H}^1(\Omega) = \{H^1(\Omega)\}^N$.

The layout of the paper is as follows: in Section 2 we consider a fully discrete implicit finite-element approximation proving existence and uniqueness of the numerical solution. In Section 3 we obtain sufficient stability estimates which enable us to show that the approximation converges to the solution of (1.1a–d). In Section 4 we perform a linear stability analysis of the equations. Further, we describe the iterative method and perform some numerical experiments; the two are compared.

2. A finite-element approximation

Let $\mathcal{T}^h$ be a regular family of triangulations of Ω, see Ciarlet (1978), so that $\bar{\Omega} = \bigcup_{\tau \in \mathcal{T}^h} \tau$ with mesh size h. Associated with $\mathcal{T}^h$ is the finite-element space $S^h \subset H^1(\Omega)$ of continuous functions on $\bar{\Omega}$ which are linear on each $\tau \in \mathcal{T}^h$. Let $\{\boldsymbol{x}_i\}_{i=1}^D$ be the set of nodes of $\mathcal{T}^h$ and $\{\chi_i\}_{i=1}^D$ be the cardinal basis for S^h. For our discrete inner product on $C(\bar{\Omega})$ we choose

$$(\chi, \eta)^h = \int_\Omega I^h(\chi(\boldsymbol{x})\eta(\boldsymbol{x}))\,\mathrm{d}\boldsymbol{x},$$

where $I^h : C(\bar{\Omega}) \to S^h$ is the interpolant defined by $I^h f(\boldsymbol{x}_i) = f(\boldsymbol{x}_i)$ $(i = 1, \ldots, D)$. The norm $|\cdot|_h := [(\cdot, \cdot)^h]^{1/2}$ on S^h is an equivalent norm to $|\cdot|_0 := [(\cdot, \cdot)]^{1/2}$ ($(\cdot,\cdot)$ is the usual L^2 inner product) satisfying $\forall \chi, \eta \in S^h$

$$|\chi|_0 \leq |\chi|_h \leq C_1 |\chi|_0 \qquad \text{and} \qquad |(\chi, \eta) - (\chi, \eta)^h| \leq Ch^{1+r} \|\chi\|_r \|\eta\|_1 \qquad (r = 0, 1) \tag{2.1}$$

see Ciavaldini (1975). We also define M and K to be the usual mass and stiffness matrices

$$M_{ij} = (\chi_i, \chi_j)^h, \qquad K_{ij} = (\nabla\chi_i, \nabla\chi_j),$$

where M is a diagonal matrix, $M_{ii} > 0$. Further, we assume that our triangulation is acute so that $K_{ij} \leq 0$ $(i \neq j)$, see Ciarlet & Raviart (1973). We shall make reference to $\boldsymbol{v} \in \boldsymbol{S}^h$ to mean $v_l \in S^h$ $(1 \leq l \leq N)$.

Given

$$\boldsymbol{f} \in \boldsymbol{S}_0^h := \left\{\boldsymbol{\chi} \in \boldsymbol{S}^h : (\chi_l, 1)^h = 0\ (1 \leq l \leq N),\ \sum \chi = 0\right\},$$

we define the Green operator $\mathcal{G}_N^h$ to be the unique solution of the problem: find $\mathcal{G}_N^h f \in S_0^h$ such that

$$(L\nabla\mathcal{G}_N^h f, \nabla\eta) = (f, \eta)^h \qquad \forall \eta \in S^h, \tag{2.2}$$

where

$$(\chi, \eta)^h := \sum_{l=1}^N (\chi_l, \eta_l)^h \qquad \text{and} \qquad (\nabla\chi, \nabla\eta) := \sum_{l=1}^N (\nabla\chi_l, \nabla\eta_l).$$

Existence of $\mathcal{G}_N^h f$ satisfying (2.2) follows from the Lax–Milgram theorem, by using (1.6) and the discrete Poincaré inequality

$$|f|_h \leq C_P\big(|(f, 1)^h| + |f|_1\big) \qquad \forall f \in S^h. \tag{2.3}$$

Notice that, from the Poincaré inequality and (2.1), (2.3) holds for h sufficiently small. It is convenient to define a norm on S_0^h to be

$$\|f\|_{-h}^2 := |L^{1/2}\nabla\mathcal{G}_N^h f|_0^2 = (L\nabla\mathcal{G}_N^h f, \nabla\mathcal{G}_N^h f) = (f, \mathcal{G}_N^h f)^h. \tag{2.4}$$

Using the discrete Poincaré inequality and (1.6) a calculation reveals

$$|L^{1/2}\mathcal{G}_N^h f|_1^2 \leq |f|_h\, |\mathcal{G}_N^h f|_h \leq C_P\, |f|_h\, |\mathcal{G}_N^h f|_1 \leq \frac{C_P}{l_0^{1/2}} |f|_h\, |L^{1/2}\mathcal{G}_N^h f|_1$$

to yield

$$\|f\|_{-h} \leq \frac{C_P}{l_0^{1/2}} |f|_h. \tag{2.5}$$

Finally, it is necessary to introduce the following notation. Fix δ to be a non-negative number and define the sets K_δ^h and J_δ^h as follows:

$$J_\delta^h := \Big\{\chi \in S^h : \delta \leq \chi_l(x)\ (1 \leq l \leq N) \text{ and } N \sum \chi(x) = 1 \text{ for all } x \in \Omega\Big\},$$

$$K_\delta^h := \{\chi \in J_\delta^h : (1, \chi_l)^h = m_l\ (1 \leq l \leq N)\},$$

where

$$0 \leq \delta \leq \delta^* = \min_{1 \leq l \leq N} \frac{m_l}{|\Omega|}.$$

We note that J_δ^h and K_δ^h are both non-empty as they contain the trivial element $m/|\Omega|$.

The problem we wish to solve is the following: given $U^0 \in K_0^h$, for $1 \leq n \leq M$ find $\{U^n, W^n\} \in K_0^h \times S^h$ such that

$$(\partial U^n, \chi)^h + (L\nabla W^n, \nabla\chi) = 0 \qquad \forall \chi \in S^h, \tag{2.6a}$$

$$\gamma(\nabla U^n, \nabla\eta) + \big(\theta\phi(U^n) - AU^n, \eta\big)^h - \Big(\mathbf{1} \sum [\theta\phi(U^n) - AU^n], \eta\Big)^h$$
$$= (W^n, \eta)^h \qquad \forall \eta \in S^h, \tag{2.6b}$$

where $\partial U^n := (U^n - U^{n-1})/\Delta t$ and $\Delta t = T/M$. Due to the use of the discrete L^2

inner product, implicit in (2.6b) is the inequality $\boldsymbol{U}^n(\boldsymbol{x}) > \boldsymbol{0}$, $\boldsymbol{x} \in \Omega$, $n > 0$, in order for $\boldsymbol{\phi}(\boldsymbol{U}^n)$ to be well defined at the nodes of the triangulation. Notice that the sequence $\{\boldsymbol{U}^n, \boldsymbol{W}^n\}$ inherits the properties

$$\sum \boldsymbol{W}^n = 0, \qquad (\boldsymbol{U}^n, 1)^h = (\boldsymbol{U}^0, 1)^h \qquad \text{and} \qquad N \sum \boldsymbol{U}^n = 1, \tag{2.7}$$

where $\{(\boldsymbol{\chi}, 1)^h\}_l := (\chi_l, 1)^h$ $(1 \leq l \leq N)$. Using (2.2) and (2.6a,b) we see that

$$\boldsymbol{W}^n = -\mathcal{G}_N^h \partial \boldsymbol{U}^n + \frac{1}{|\Omega|}(\theta\boldsymbol{\phi}(\boldsymbol{U}^n) - A\boldsymbol{U}^n, 1)^h - \frac{1}{|\Omega|}\Big(\sum [\theta\phi(\boldsymbol{U}^n) - A\boldsymbol{U}^n], 1\Big)^h.$$

Furthermore, using (2.4) and (2.6a), with $\boldsymbol{\chi} = \boldsymbol{W}^n$, we find

$$\|\partial \boldsymbol{U}^n\|_{-h}^2 = (\partial \boldsymbol{U}^n, \mathcal{G}_N^h \partial \boldsymbol{U}^n)^h = -(\partial \boldsymbol{U}^n, \boldsymbol{W}^n)^h = (L\nabla \boldsymbol{W}^n, \nabla \boldsymbol{W}^n). \tag{2.8}$$

REMARK 2.1 The numerical analysis of (1.4) has been studied by Copetti & Elliott (1992) in the form of the fully implicit finite-element approximation: find $\{U^n, W^n\} \in S^h \times S^h$ such that for all $\chi, \eta \in S^h$

$$(\partial U^n, \chi)^h + (\nabla W^n, \nabla \chi) = 0, \tag{2.9}$$

$$(W^n, \eta)^h = \gamma(\nabla U^n, \nabla \eta) + (\psi'(U^n), \eta)^h. \tag{2.10}$$

They proved existence, uniqueness and convergence of the numerical solution to the solution of the continuous problem. Some numerical experiments were performed.

If we attempt to prove existence to (2.6a,b) using the fact that these equations can be rewritten as the Euler–Lagrange equation of a minimization problem over the set $\boldsymbol{K}_0^h$ then, in calculating the Euler–Lagrange equation, we will need to know in advance that the minimizer is strictly positive. To avoid this problem, we will consider the same minimization over the set K_δ^h where $\delta > 0$ and sufficiently small. Thus, for n fixed it is convenient to consider the following constrained problems which are Euler–Lagrange equations:

(Q_δ^h) Given $\boldsymbol{U}^{n-1} \in \boldsymbol{K}_0^h$ and $0 < \delta \leq \delta^*$, find $\boldsymbol{U}^\delta \in \boldsymbol{K}_\delta^h$ such that for all $\boldsymbol{\chi} \in \boldsymbol{K}_\delta^h$

$$\frac{1}{\Delta t}(\mathcal{G}_N^h(\boldsymbol{U}^\delta - \boldsymbol{U}^{n-1}), \boldsymbol{\chi} - \boldsymbol{U}^\delta)^h + \gamma(\nabla \boldsymbol{U}^\delta, \nabla \boldsymbol{\chi} - \nabla \boldsymbol{U}^\delta)$$
$$+ \theta(\boldsymbol{\phi}(\boldsymbol{U}^\delta), \boldsymbol{\chi} - \boldsymbol{U}^\delta)^h - (A\boldsymbol{U}^\delta, \boldsymbol{\chi} - \boldsymbol{U}^\delta)^h \geq 0. \tag{2.11}$$

(P_δ^h) Given $\boldsymbol{U}^{n-1} \in \boldsymbol{K}_0^h$ and $0 < \delta \leq \delta^*$, find $\{\boldsymbol{U}^\delta, \boldsymbol{W}^\delta\} \in \boldsymbol{J}_\delta^h \times \boldsymbol{S}^h$ such that for all $\boldsymbol{\eta} \in \boldsymbol{S}^h$ and $\boldsymbol{\chi} \in \boldsymbol{J}_\delta^h$

$$\frac{1}{\Delta t}(\boldsymbol{U}^\delta - \boldsymbol{U}^{n-1}, \boldsymbol{\eta})^h + (L\nabla \boldsymbol{W}^\delta, \nabla \boldsymbol{\eta}) = 0,$$

$$\gamma(\nabla \boldsymbol{U}^\delta, \nabla \boldsymbol{\chi} - \nabla \boldsymbol{U}^\delta) + (\theta\boldsymbol{\phi}(\boldsymbol{U}^\delta) - A\boldsymbol{U}^\delta, \boldsymbol{\chi} - \boldsymbol{U}^\delta)^h \geq (\boldsymbol{W}^\delta, \boldsymbol{\chi} - \boldsymbol{U}^\delta)^h. \tag{2.12}$$

LEMMA 2.2 Let λ_A be the largest positive eigenvalue of the matrix A. For $0 < \Delta t < 4\gamma/(\lambda_A^2 \|L\|)$ there exist unique solutions to (Q_δ^h) and (P_δ^h), where W^δ is unique up to the addition of a constant vector.

Proof. First we prove existence to (Q_δ^h). Consider the minimization problem

$$\min_{\chi \in K_\delta^h} \frac{1}{2\,\Delta t} \|\chi - U^{n-1}\|_{-h}^2 + \mathscr{E}^h(\chi) =: \mathscr{J}(\chi), \tag{2.13}$$

where

$$\mathscr{E}^h(\chi) := (\Psi(\chi), 1)^h + \frac{\gamma}{2} |\chi|_1^2. \tag{2.14}$$

We now prove a useful inequality. Using matrix properties, (2.2) and Young's inequality, a calculation yields for $\eta \in S_0^h$ and $\alpha > 0$

$$\begin{aligned}(A\eta, \eta)^h &\leq \lambda_A |\eta|_h^2 = \lambda_A(L\nabla\eta, \nabla\mathscr{G}_N^h\eta) \\ &\leq \lambda_A \|L\|^{1/2} |\eta|_1 \|\eta\|_{-h} \leq \frac{\alpha\,\Delta t\lambda_A^2 \|L\|}{4} |\eta|_1^2 + \frac{1}{\alpha\,\Delta t} \|\eta\|_{-h}^2. \end{aligned} \tag{2.15}$$

Setting $\alpha = 1 + \varepsilon$ and $\eta = \chi - m/|\Omega| \in S_0^h$, where $\varepsilon > 0$ and $\chi \in K_\delta^h$, we see that

$$(A\chi, \chi)^h - \lambda_A \frac{\|m\|^2}{|\Omega|} \leq \frac{1}{(1+\varepsilon)\,\Delta t} \left\| \chi - \frac{m}{|\Omega|} \right\|_{-h}^2 + \frac{\Delta t \lambda_A^2 \|L\| (1+\varepsilon)}{4} |\chi|_1^2. \tag{2.16}$$

Since

$$\left\| \chi - \frac{m}{|\Omega|} \right\|_{-h}^2 \leq (1+\varepsilon) \|\chi - U^{n-1}\|_{-h}^2 + (1 + 1/\varepsilon) \left\| U^{n-1} - \frac{m}{|\Omega|} \right\|_{-h}^2,$$

we obtain from (2.16)

$$\begin{aligned}(A\chi, \chi)^h \leq \frac{1}{\Delta t} \|\chi - U^{n-1}\|_{-h}^2 + \frac{(1+1/\varepsilon)}{\Delta t(1+\varepsilon)} \left\| U^{n-1} - \frac{m}{|\Omega|} \right\|_{-h}^2 \\ + \frac{\Delta t \lambda_A^2 \|L\| (1+\varepsilon)}{4} |\chi|_1^2 + \lambda_A \frac{\|m\|^2}{|\Omega|}.\end{aligned}$$

Using the inequality $0 \geq x \ln x \geq -e^{-1}$, where $0 \leq x \leq 1$, we obtain

$$\mathscr{J}(\chi) \geq \frac{1}{2}\left(\gamma - \frac{\Delta t \lambda_A^2 (1+\varepsilon) \|L\|}{4}\right) |\chi|_1^2 - C(m, U^{n-1}, \varepsilon, \Delta t, \lambda_A, \theta).$$

It follows from the Poincaré inequality that for $\varepsilon > 0$ sufficiently small, we can extract a minimizing subsequence $\{\chi^k\} \subset K_\delta^h$ converging to $U^\delta \in K_\delta^h$ which minimizes $\mathscr{J}(\cdot)$. We note that a minimizer of $\mathscr{J}(\cdot)$ satisfies the variational inequality (2.11), thus proving existence.

We now turn to the proof of uniqueness for solutions of (2.11). Let U_1^δ, U_2^δ be two different solutions to (2.11) and $\Theta^U := U_1^\delta - U_2^\delta$. In the usual way, we obtain

$$\frac{1}{\Delta t}(\mathscr{G}_N^h \Theta^U, \Theta^U)^h + \gamma |\Theta^U|_1^2 + \theta(\phi(U_1^\delta) - \phi(U_2^\delta), \Theta^U)^h - (A\Theta^U, \Theta^U)^h \leq 0.$$

Using the monotonicity of ϕ, setting $\boldsymbol{\eta} = \boldsymbol{\Theta}^U$ and $\alpha = 1$ in (2.15) yields the inequality

$$\left(\gamma - \frac{\Delta t \lambda_A^2 \, \|L\|}{4}\right) |\boldsymbol{\Theta}^U|_1^2 \leqslant 0.$$

Uniqueness follows immediately from the Poincaré inequality. Applying the Kuhn–Tucker conditions, we obtain a Lagrange multiplier, $\boldsymbol{\lambda}^\delta$, for the mass constraint, so that setting

$$\boldsymbol{W}^\delta = -\frac{1}{\Delta t}\mathcal{G}_N^h(\boldsymbol{U}^\delta - \boldsymbol{U}^{n-1}) + \boldsymbol{\lambda}^\delta,$$

existence for (P_δ^h) is proved. □

A consequence of this lemma is that (Q_δ^h) and (P_δ^h) are equivalent in the sense that they have the same solution.

In the next lemma, we obtain bounds on $\{\boldsymbol{U}^\delta\}$ which are independent of δ. If we can prove that $\liminf_{\delta\to 0} \min_{1\leqslant l\leqslant N} \inf_{\boldsymbol{x}\in\Omega} U_l^\delta(\boldsymbol{x}) > 0$, then we may extract a convergent subsequence and pass to the limit in δ.

LEMMA 2.3 The following stability estimate holds:

$$\frac{1}{4\,\Delta t}\left\|\boldsymbol{U}^\delta - \frac{\boldsymbol{m}}{|\Omega|}\right\|_{-h}^2 + \frac{1}{2\,\Delta t}\|\boldsymbol{U}^\delta - \boldsymbol{U}^{n-1}\|_{-h}^2 + \left(\gamma - \frac{\Delta t\,\|L\|\,\lambda_A^2}{4}\right)|\boldsymbol{U}^\delta|_1^2 \leqslant C, \quad (2.17)$$

where the constant C is independent of δ.

Proof. Setting $\boldsymbol{\chi} = (1/|\Omega|)\boldsymbol{m}$ in (2.11) we obtain

$$\frac{1}{\Delta t}\left(\mathcal{G}_N^h(\boldsymbol{U}^\delta - \boldsymbol{U}^{n-1}), \frac{\boldsymbol{m}}{|\Omega|} - \boldsymbol{U}^\delta\right)^h - \gamma\,|\boldsymbol{U}^\delta|_1^2 + \left(\theta\boldsymbol{\phi}(\boldsymbol{U}^\delta) - A\boldsymbol{U}^\delta, \frac{\boldsymbol{m}}{|\Omega|} - \boldsymbol{U}^\delta\right)^h \geqslant 0. \quad (2.18)$$

Noting the definition of $\boldsymbol{\Psi}$ and using the trivial inequality $\forall x \geqslant 0,\ y > 0$

$$x \log x \geqslant y \log y + (1 + \log y)(x - y), \quad (2.19)$$

it follows that

$$\Psi\left(\frac{\boldsymbol{m}}{|\Omega|}\right) \geqslant \Psi(\boldsymbol{U}^\delta) + (D\Psi(\boldsymbol{U}^\delta))^{\mathrm{T}}\left(\frac{\boldsymbol{m}}{|\Omega|} - \boldsymbol{U}^\delta\right) - \frac{1}{2}\left(\frac{\boldsymbol{m}}{|\Omega|} - \boldsymbol{U}^\delta\right)^{\mathrm{T}} A\left(\frac{\boldsymbol{m}}{|\Omega|} - \boldsymbol{U}^\delta\right). \quad (2.20)$$

Substitution into (2.18) and the identity $2a(a-b) = a^2 + (a-b)^2 - b^2$ yields

$$\frac{1}{2\,\Delta t}\left\|\boldsymbol{U}^\delta - \frac{\boldsymbol{m}}{|\Omega|}\right\|_{-h}^2 + \frac{1}{2\,\Delta t}\|\boldsymbol{U}^\delta - \boldsymbol{U}^{n-1}\|_{-h}^2 + \gamma\,|\boldsymbol{U}^\delta|_1^2 + (\Psi(\boldsymbol{U}^\delta), 1)^h$$
$$\leqslant \frac{1}{2\,\Delta t}\left\|\boldsymbol{U}^{n-1} - \frac{\boldsymbol{m}}{|\Omega|}\right\|_{-h}^2 + \left(\Psi\left(\frac{\boldsymbol{m}}{|\Omega|}\right), 1\right)^h + \frac{1}{2}\left(A\left(\frac{\boldsymbol{m}}{|\Omega|} - \boldsymbol{U}^\delta\right), \frac{\boldsymbol{m}}{|\Omega|} - \boldsymbol{U}^\delta\right)^h. \quad (2.21)$$

Noting that

$$(\Psi(U^\delta), 1)^h \geq \int_\Omega I^h\Big(-N\theta e^{-1} - \frac{\lambda_A}{2}\sum_{l=1}^N (U_l^\delta)^2\Big)\,\mathrm{d}x \geq -\Big(\theta e^{-1} + \frac{\lambda_A}{2}\Big)N\,|\Omega|,$$

and setting $\eta = (m/|\Omega|) - U^\delta$, $\alpha = 2$ in (2.15), substitution into (2.21) and rearrangement yields (2.17) where

$$C = \Big(\theta e^{-1} + \frac{\lambda_A}{2}\Big)N\,|\Omega| + \frac{1}{2\,\Delta t}\Big\|U^{n-1} - \frac{m}{|\Omega|}\Big\|_{-h}^2 + \Big(\Psi\Big(\frac{m}{|\Omega|}\Big), 1\Big)^h. \qquad \square$$

From the stability results obtained, we may extract a subsequence of $\{U^\delta\}$, denoted by the same sequence, with the property that $U^\delta \to U \in K_0^h$. To pass to the limit in (2.11), we need only prove that $U_l > 0$ and we do so using a finite-dimensional argument. Assume that $U_l(x_i) = 0$ at some node of the triangulation. Note that

$$-\Big(\phi(U^\delta), \frac{m}{|\Omega|} - U^\delta\Big)^h = -\sum_{k=1}^N \Big(\phi(U_k^\delta), \frac{m_k}{|\Omega|} - U_k^\delta\Big)^h$$

$$= -\sum_{k=1}^N \sum_{j=1}^D \phi(U_k^\delta(x_j))M_{jj}\Big(\frac{m_k}{|\Omega|} - U_k^\delta(x_j)\Big),$$

so when $j = i$ and $k = l$

$$-\lim_{\delta\to 0} \phi(U_l^\delta(x_i))M_{ii}\Big(\frac{m_l}{|\Omega|} - U_l^\delta(x_i)\Big) = +\infty.$$

Rewriting (2.11) with $\chi = m/|\Omega|$, using (2.17) and letting $\delta \to 0$, we obtain a contradiction due to the fact

$$-\theta\Big(\phi(U^\delta), \frac{m}{|\Omega|} - U^\delta\Big)^h \leq \frac{1}{\Delta t}\Big(\mathcal{G}_N^h(U^\delta - U^{n-1}), \frac{m}{|\Omega|} - U^\delta\Big)^h$$

$$- \gamma\,|U^\delta|_1^2 - \Big(AU^\delta, \frac{m}{|\Omega|} - U^\delta\Big)^h$$

$$\underset{+\infty}{\downarrow} \qquad \delta \to 0 \qquad \underset{C.}{\downarrow}$$

We deduce that there exists $0 < \delta^0$ such that $U \in K_\delta^h$ for all $\delta \leq \delta^0$ and hence that U is the solution to (Q_δ^h) for all $\delta \leq \delta^0$.

For $\delta \leq \delta^0$, we wish to pass to the limit in (2.11), however for technical reasons it is easier to pass to the limit in (2.12) where the problem is written with Lagrange multipliers. Our goal is to prove that all $\chi \in J_0^h$

$$\frac{1}{\Delta t}(\mathcal{G}_N^h(U - U^{n-1}), \chi - U)^h + \gamma(\nabla U, \nabla\chi - \nabla U) + \big(\theta\phi(U) - AU, \chi - U\big)^h$$

$$\geq \lambda^{\mathrm{T}}(1, \chi - U) \qquad (2.22)$$

for some $\lambda \in \mathbb{R}^N$. There are two mutually exclusive cases to consider.

- If $\chi \in J^h_\delta$ for δ sufficiently small, then (2.22) is automatically satisfied.
- If $\chi_l(x_i) = 0$ for N_i components then for δ sufficiently small define a new sequence χ^δ by

$$\chi^\delta_l(x_i) = \begin{cases} \delta & \text{if } \chi_l(x_i) = 0, \\ \chi_l(x_i) - N_i\delta & \text{if } l = \min\{j' : \chi_{j'}(x_i) = \max_j \chi_j(x_i)\}, \\ \chi_j(x_i) & \text{otherwise.} \end{cases}$$

So $\chi^\delta \to \chi$ and passage to the limit is immediate.

For $\Delta t < 4\gamma/(\lambda_A^2 \|L\|)$ uniqueness follows in a similar fashion to that shown for (2.11). Obviously, since $K^h_0 \subset J^h_0$ it follows that for all $\chi \in K^h_0$

$$\frac{1}{\Delta t}(\mathcal{G}^h_N(U - U^{n-1}), \chi - U)^h + \gamma(\nabla U, \nabla \chi - \nabla U) + (\theta\phi(U) - AU, \chi - U)^h \geq 0. \tag{2.23}$$

Let $\chi = U \pm \alpha\eta$ where $\eta \in S^h_0$ and $|\alpha|$ is sufficiently small so that $\chi \in K^h_0$. From (2.23) we obtain

$$\frac{1}{\Delta t}(\mathcal{G}^h_N(U - U^{n-1}), \eta)^h + \gamma(\nabla U, \nabla \eta) + (\theta\phi(U) - AU, \eta)^h = 0. \tag{2.24}$$

Let $\xi \in S^h$ be arbitrary. Then defining

$$\eta = \xi - \mathbf{1}\sum \xi - \frac{1}{|\Omega|}(\xi, 1)^h + \frac{\mathbf{1}}{|\Omega|}\left(\sum \xi, 1\right)^h \in S^h_0,$$

substitution into (2.24), noting $U \in K^h_0$, yields the equation

$$\begin{aligned} &\frac{1}{\Delta t}(\mathcal{G}^h_N(U - U^{n-1}), \xi)^h + \gamma(\nabla U, \nabla \xi) + (\theta\phi(U) - AU, \xi)^h \\ &= \left(\theta\phi(U) - AU, \mathbf{1}\sum \xi + \frac{1}{|\Omega|}(\xi, 1)^h - \frac{\mathbf{1}}{|\Omega|}\left(\sum \xi, 1\right)^h\right)^h \\ &= \left(\mathbf{1}\sum[\theta\phi(U) - AU] + \boldsymbol{\lambda}, \xi\right)^h, \end{aligned} \tag{2.25}$$

where

$$\lambda_l = \frac{1}{|\Omega|}(\theta\phi(U_l) - (AU)_l, 1)^h - \left(\frac{1}{|\Omega|}\sum[\theta\phi(U) - AU], 1\right)^h.$$

Setting $U^n = U$ and $W = -\mathcal{G}^h_N \partial U^n + \boldsymbol{\lambda}$ we have proven the following theorem.

THEOREM 2.4 Let $U^0 \in K^h_0$. Then for $\Delta t < 4\gamma/(\lambda_A^2 \|L\|)$, there exists a unique sequence $\{U^n, W^n\}$ satisfying (2.6a,b) with properties

$$\sum U^n = 1/N, \qquad \sum W^n = 0, \qquad (U^n, 1)^h = \boldsymbol{m}, \qquad \mathbf{0} < U^n < \mathbf{1}. \tag{2.26}$$

REMARK 2.5 In an analogous manner to Theorem 2.4, given $U^0 \in K_0^h$ and $\Delta t > 0$ there exists a unique sequence $\{U^n, W^n\}_{n=1}^M \in K_0^h \times S^h$ such that

$$(\partial U^n, \chi)^h + (L\nabla W^n, \nabla\chi) = 0 \qquad \forall \chi \in S^h, \tag{2.27a}$$

$$\gamma(\nabla U^n, \nabla\eta) + (\theta\phi(U^n) - AU^{n-1}, \eta)^h - \Big(1 \sum [\theta\phi(U^n) - AU^n], \eta\Big)^h = (W^n, \eta)^h$$
$$\forall \eta \in S^h, \tag{2.27b}$$

where (2.26) holds for each n.

3. Stability and convergence

In this section we follow Copetti & Elliott (1992) and prove convergence of the fully discrete numerical solution to the solution $\{u, w\}$ satisfying the following theorem proved in Elliott & Luckhaus (1991):

Let $T > 0$ and

$$u^0 \in K := \Big\{\eta \in H^1(\Omega) : N \sum \eta = 1,\ \eta \geqslant 0,\ |\Omega| ⨍ \eta = m\Big\}$$

where

$$0 < m < 1\,|\Omega| \qquad \text{and} \qquad |\Omega| ⨍ \eta = \int \eta(x)\,\mathrm{d}x.$$

Then there exists a unique pair $\{u, w\}$ such that

$$u \in C[0, T; (H^1(\Omega))'] \cap L^\infty(0, T; H^1(\Omega)),$$
$$\frac{\mathrm{d}u}{\mathrm{d}t} \in L^2(0, T; (H^1(\Omega))'), \qquad \sqrt{t}\,\frac{\mathrm{d}u}{\mathrm{d}t} \in L^2(0, T; H^1(\Omega)),$$
$$w \in L^2(0, T; H^1(\Omega)),$$
$$\sqrt{t}w \in L^\infty(0, T; H^1(\Omega)),$$
$$\sqrt{t}\theta\phi(u) \in L^\infty(0, T; L^2(\Omega)),$$
$$u(\cdot, 0) = u^0,$$
$$u(\cdot, t) \in K \quad \forall t > 0, \qquad ⨍ u(\cdot, t) = ⨍ u^0$$

and for all $\mu \in C[0, T]$ and $\eta \in H^1(\Omega)$

$$\int_0^T \mu(t)\Big\{\frac{\mathrm{d}}{\mathrm{d}t}\langle u, \eta\rangle + (L\nabla w, \nabla\eta)\Big\}\,\mathrm{d}t = 0, \tag{3.1a}$$

$$\int_0^T \mu(t)\Big\{\Big(w - \theta\phi(u) + Au + 1 \sum \theta\phi(u) - Au, \eta\Big) - \gamma(\nabla u, \nabla\eta)\Big\}\,\mathrm{d}t = 0, \tag{3.1b}$$

where $\langle\cdot,\cdot\rangle$ is the duality pairing between $(H^1(\Omega))'$ and $H^1(\Omega)$.

3.1 Stability

First we prove stability estimates which will enable us to pass to the limit in h and Δt.

LEMMA 3.1 Let $0 < \Delta t < 4\gamma/(\lambda_A^2 \|L\|)$ and $t^n := n\,\Delta t$ $(0 \leq n \leq M)$. Then for all $m \in [1, M]$

$$(\Psi(U^m), 1)^h + \frac{\Delta t}{2}\sum_{n=1}^{m} \|\partial U^n\|_{-h}^2 + \frac{\gamma}{2}|U^m|_1^2 + \frac{1}{2}\left(\gamma - \frac{\Delta t \lambda_A^2 \|L\|}{4}\right)\sum_{n=1}^{m}|U^n - U^{n-1}|_1^2 \leq C, \tag{3.2}$$

$$\frac{\Delta t}{2}\sum_{n=1}^{M}(L\nabla W^n, \nabla W^n) \leq C, \tag{3.3}$$

$$\frac{\Delta t}{2}\sum_{n=1}^{M}\|W^n\|_1^2 \leq C, \tag{3.4}$$

$$t^m(L\nabla W^m, \nabla W^m) + \gamma\,\Delta t\sum_{n=1}^{m} t^n|\partial U^n|_1^2 \leq C, \tag{3.5}$$

$$\theta\sum_{n=1}^{M}\Delta t\,|\phi(U^n)|_h^2 \leq C, \tag{3.6}$$

$$\theta t^m|\phi(U^m)|_h^2 \leq C, \tag{3.7}$$

where each constant C is independent of h and Δt.

Proof. Set $\eta = \partial U^n$ in (2.6*b*). Using (2.19) and (2.6*a*) with $\chi = \mathcal{G}_N^h(\partial U^n)$ we obtain

$$\frac{\gamma}{2\,\Delta t}(|U^n|_1^2 + |U^n - U^{n-1}|_1^2 - |U^{n-1}|_1^2) + \frac{1}{\Delta t}((\Psi(U^n), 1)^h - (\Psi(U^{n-1}), 1)^h) - \frac{\Delta t}{2}(A\,\partial U^n, \partial U^n)^h + \|\partial U^n\|_{-h}^2 \leq 0. \tag{3.8}$$

Setting $\eta = \partial U^n$ and $\alpha = 1$ in (2.15) we obtain

$$\frac{\gamma}{2\,\Delta t}(|U^n|_1^2 - |U^{n-1}|_1^2) + \frac{\Delta t}{2}\left(\gamma - \frac{\Delta t \lambda_A^2 \|L\|}{4}\right)|\partial U^n|_1^2 + \frac{1}{\Delta t}((\Psi(U^n), 1)^h - (\Psi(U^{n-1}), 1)^h) + \tfrac{1}{2}\|\partial U^n\|_{-h}^2 \leq 0, \tag{3.9}$$

and we see that $\mathscr{E}^h$ is a Lyapunov functional. Hence, multiplying (3.9) by Δt and summing from $n = 1,\ldots,m$ we obtain (3.2) where $C = \mathscr{E}^h(U^0)$. (3.3) follows immediately from (2.8).

We wish to show that W^n is bounded in $H^1(\Omega)$. Clearly by the equivalence of norms (2.1), the discrete Poincaré inequality (2.3) and (1.6)

$$\|W^n\|_1^2 = |W^n|_0^2 + |W^n|_1^2 = \left|W^n - \fint W^n\right|_0^2 + |\Omega| \left\|\fint W^n\right\|^2 + |W^n|_1^2$$

$$\leqslant |\Omega| \left\|\fint W^n\right\|^2 + C\,|W^n|_1^2 \leqslant |\Omega| \left\|\fint W^n\right\|^2 + \frac{C}{l_0}(L\nabla W^n, \nabla W^n).$$

Recalling (3.3), it is enough to bound $|\fint W_k^n|$ for all k. Since $\sum W^n = 0$, if $\max_k (W_k^n, 1)^h = 0$, then there is nothing to prove. Let $0 < (W_j^n, 1)^h = \max_k (W_k^n, 1)^h$. Setting $\eta = e^j - U^n$, where $e_k^j := \delta_{jk}$, in (2.6b) and using (2.19) so that

$$\frac{|\Omega|\,\|A\|}{2} \geqslant (\Psi(e^j), 1)^h$$

$$\geqslant (\Psi(U^n), 1)^h + (D\Psi(U^n), e^j - U^n)^h - \tfrac{1}{2}(A(e^j - U^n), e^j - U^n)^h,$$

it follows

$$\frac{|\Omega|\,\|A\|}{2} - \gamma\,|U^n|_1^2 - (\Psi(U^n), 1)^h + \tfrac{1}{2}(A(e^j - U^n), e^j - U^n)^h \geqslant (W^n, e^j - U^n)^h. \tag{3.10}$$

By definition

$$(W^n, e^j - U^n)^h = (W_j^n, 1)^h - (W^n, U^n)^h;$$

we estimate $(W^n, U^n)^h$. Using (2.2)

$$(W^n, U^n)^h = \sum_{k=1}^{N} (W_k^n, 1)^h \frac{m_k}{|\Omega|} + \left(W^n, U^n - \frac{m}{|\Omega|}\right)^h$$

$$\leqslant \sum_{\{k:(W_k^n,1)^h>0\}} (W_k^n, 1)^h \frac{m_k}{|\Omega|} + \left(L\nabla W^n, \nabla \mathscr{G}_N^h\left(U^n - \frac{m}{|\Omega|}\right)\right)$$

$$\leqslant (W_j^n, 1)^h \sum_{\{k:(W_k^n,1)^h>0\}} \frac{m_k}{|\Omega|} + |L^{1/2}W^n|_1 \left\|U^n - \frac{m}{|\Omega|}\right\|_{-h}$$

$$= (W_j^n, 1)^h\left(1 - \sum_{\{k:(W_k^n,1)^h\leqslant 0\}} \frac{m_k}{|\Omega|}\right) + |L^{1/2}W^n|_1 \left\|U^n - \frac{m}{|\Omega|}\right\|_{-h}$$

$$\leqslant (W_j^n, 1)^h\left(1 - \min_k \frac{m_k}{|\Omega|}\right) + |L^{1/2}W^n|_1 \left\|U^n - \frac{m}{|\Omega|}\right\|_{-h}$$

Hence

$$\min_k \frac{m_k}{|\Omega|} (W_j^n, 1)^h \leqslant (W^n, e^j - U^n)^h + |L^{1/2}W^n|_1 \left\|U^n - \frac{m}{|\Omega|}\right\|_{-h}.$$

so that substituting into (3.10) and using (2.5) we obtain

$$\min_k \frac{m_k}{|\Omega|}(W_j^n, 1)^h \leqslant \frac{\|A\|\,|\Omega|}{2} - \gamma\,|U^n|_1^2 - (\Psi(U^n), 1)^h$$

$$+ \tfrac{1}{2}(A(e^j - U^n), e^j - U^n)^h + \frac{C_P}{l_0^{1/2}}|L^{1/2}W^n|_1 \left|U^n - \frac{m}{|\Omega|}\right|_h.$$

Noting the uniform boundedness, (3.2), we have proved the inequality

$$(W_j^n, 1)^h \leqslant C_3 + C_4\,|L^{1/2}W^n|_1,$$

where C_3 and C_4 are independent of h and Δt. Let $(W_l^n, 1)^h = \min_k (W_k^n, 1)^h$, then

$$-(W_l^n, 1)^h \leqslant -\sum_{\{k:(W_k^n,1)^h<0\}} (W_k^n, 1)^h = \sum_{\{k:(W_k^n,1)^h\geqslant 0\}} (W_k^n, 1)^h$$

$$\leqslant (N-1)\max_k (W_k^n, 1)^h \leqslant (N-1)(C_3 + C_4\,|L^{1/2}W^n|_1).$$

Hence for all k

$$|(W_k^n, 1)^h| \leqslant (N-1)[C_3 + C_4\,|L^{1/2}W^n|_1]$$

and (3.4) follows from (3.3).

From (3.2) and (3.3), (3.5) clearly holds for $m = 1$. For $m \geqslant n \geqslant 2$, from (2.6$b$) with $\eta = \partial U^n$ and from the monotonicity of ϕ, it follows that

$$(\partial W^n, \partial U^n)^h = \gamma(\nabla\,\partial U^n, \nabla\,\partial U^n) + \left(\frac{\theta}{\Delta t}(\phi(U^n) - \phi(U^{n-1})) - A\,\partial U^n, \partial\, U^n\right)^h$$

$$\geqslant \gamma(\nabla\,\partial U^n, \nabla\,\partial U^n) - (A\,\partial U^n, \partial U^n)^h. \tag{3.11}$$

Using (2.6a) with $\chi = \partial W^n$ we see that

$$-(\partial W^n, \partial U^n)^h = (L\nabla W^n, \nabla\,\partial W^n)$$

$$= \frac{1}{2\,\Delta t}\left(|L^{1/2}\nabla W^n|_0^2 + |L^{1/2}\nabla(W^n - W^{n-1})|_0^2 - |L^{1/2}\nabla W^{n-1}|_0^2\right).$$

Taking $\eta = \partial U^n$ and $\alpha = 2\gamma/(\Delta t \lambda_A^2\,\|L\|)$ in (2.15), a calculation yields that

$$|L^{1/2}\nabla W^n|_0^2 - |L^{1/2}\nabla W^{n-1}|_0^2 + \Delta t\gamma\,|\partial U^n|_1^2 \leqslant \frac{\Delta t \lambda_A^2\,\|L\|}{\gamma}\,\|\partial U^n\|_{-h}^2.$$

Multiplying by t^n it results that

$$t^n\,|L^{1/2}\nabla W^n|_0^2 - t^{n-1}\,|L^{1/2}\nabla W^{n-1}|_0^2 + \Delta t\gamma t^n\,|\partial U^n|_1^2$$

$$\leqslant \frac{t^n\,\Delta t \lambda_A^2\,\|L\|}{\gamma}\,\|\partial U^n\|_{-h}^2 + \Delta t\,|L^{1/2}\nabla W^{n-1}|_0^2.$$

Summing from $n = 2,\dots,m$, noting that $t^n \leqslant T$, $W^{n-1} = -\mathcal{G}_N^h \partial U^{n-1} + \lambda^{n-1}$ and using (3.2), (3.3) we obtain

$$t^m |L^{1/2}\nabla W^m|_0^2 + \sum_{n=1}^{m} \Delta t \gamma t^n |\partial U^n|_1^2$$

$$\leqslant \left(\frac{T\lambda_A^2 \|L\|}{\gamma} + 1\right) \Delta t \sum_{n=1}^{m} \|\partial U^n\|_{-h}^2 + \Delta t |L^{1/2}\nabla W^1|_0^2 \leqslant C.$$

It remains to prove (3.6), (3.7). Setting

$$\eta = I^h\phi(U^n) - \frac{1}{|\Omega|}(\phi(U^n), 1)^h - \mathbf{1}\left(\sum I^h\phi(U^n) - \frac{1}{|\Omega|}\left(\sum \phi(U^n), 1\right)^h\right) \in S_0^h$$

in (2.6*b*) where $\{I^h\chi\}_l = I^h\chi_l$ and noting the inequality

$$0 \leqslant (\nabla\chi, \nabla I^h\phi(\chi)) \qquad \forall 0 < \chi \in S^h, \tag{3.12}$$

see Lemma 3.2 at the end of this subsection, we obtain

$$\theta |\eta|_h^2 \leqslant |W^n - (W^n, 1)^h|_h |\eta|_h + \|A\| |U^n|_h |\eta|_h,$$

so that using a kick-back argument, the Poincaré inequality, (1.6) and (3.5), we have proven

$$\theta \sum_{n=1}^{N} \Delta t \left|\phi(U^n) - \frac{1}{|\Omega|}(\phi(U^n), 1)^h - \mathbf{1}\left(\sum \phi(U^n) - \frac{1}{|\Omega|}\left(\sum \phi(U^n), 1\right)^h\right)\right|_h^2 \leqslant C, \tag{3.13}$$

$$\theta t^m \left|\phi(U^m) - \frac{1}{|\Omega|}(\phi(U^m), 1)^h - \mathbf{1}\left(\sum \phi(U^m) - \frac{1}{|\Omega|}\left(\sum \phi(U^m), 1\right)^h\right)\right|_h^2 \leqslant C. \tag{3.14}$$

It is a simple calculation to show that

$$\left|\phi(U^n) - \frac{1}{|\Omega|}(\phi(U^n), 1)^h - \mathbf{1}\left(\sum \phi(U^n) - \frac{1}{|\Omega|}\left(\sum \phi(U^n), 1\right)^h\right)\right|_h^2$$

$$= \left|\phi(U^n) - \mathbf{1}\sum \phi(U^n)\right|_h^2 - \frac{1}{|\Omega|}\left\|(\phi(U^n), 1)^h - \mathbf{1}\sum (\phi(U^n), 1)^h\right\|^2,$$

so given the bounds (3.13–3.14), it is sufficient to estimate

$$\left\|(\phi(U^n), 1)^h - \mathbf{1}\sum (\phi(U^n), 1)^h\right\|^2$$

appropriately. However, noting

$$(W^n, 1)^h = (\theta\phi(U^n) - AU^n, 1)^h - \mathbf{1}\left(\sum [\theta\phi(U^n) - AU^n], 1\right)^h,$$

(3.2) and that $(\boldsymbol{W}^n, \mathbf{1})^h$ has already been bounded, we are through. Hence

$$\left|\boldsymbol{\phi}(\boldsymbol{U}^n) - \mathbf{1}\sum \boldsymbol{\phi}(\boldsymbol{U}^n)\right|_h \leq C_3' + C_4' \, |L^{1/2}\boldsymbol{W}^n|_1,$$

and we have the stability estimates

$$\theta \sum_{n=1}^{M} \Delta t \left|\boldsymbol{\phi}(\boldsymbol{U}^n) - \mathbf{1}\sum \boldsymbol{\phi}(\boldsymbol{U}^n)\right|_h^2 \leq C, \tag{3.15}$$

$$\theta t^m \left|\boldsymbol{\phi}(\boldsymbol{U}^m) - \mathbf{1}\sum \boldsymbol{\phi}(\boldsymbol{U}^m)\right|_h^2 \leq C. \tag{3.16}$$

Noting the equality

$$\left|\boldsymbol{\phi}(\boldsymbol{U}^n) - \mathbf{1}\sum \boldsymbol{\phi}(\boldsymbol{U}^n)\right|_h^2 = |\boldsymbol{\phi}(\boldsymbol{U}^n)|_h^2 - N\left|\mathbf{1}\sum \boldsymbol{\phi}(\boldsymbol{U}^n)\right|_h^2,$$

in order to obtain (3.6) and (3.7), it is enough to bound $|\mathbf{1}\sum \mathbf{ln}\,(\boldsymbol{U}^n)|_h^2$ where $\{\mathbf{ln}\,(\boldsymbol{v})\}_l = \ln(v_l)$. Let us define

$$g_k^l = \ln U_k^n(\boldsymbol{x}_l) - \frac{1}{N}\sum_{j=1}^{N} \ln U_j^n(\boldsymbol{x}_l)$$

and

$$I_k = \left\{ i \in [1, D] : U_k^n(\boldsymbol{x}_i) = \max_j U_j^n(\boldsymbol{x}_i) \text{ where } U_j^n(\boldsymbol{x}_i) < U_k^n(\boldsymbol{x}_i), \text{ for } j < k \right\};$$

note that $I_1 \cup I_2 \cup \cdots \cup I_N = \{i : i \in [1, D]\}$. From the monotonicity of ln, for $i \in I_k$

$$g_k^l = \ln\left(\frac{U_k^n(\boldsymbol{x}_l)}{(\prod_{j=1}^{N} U_j^n(\boldsymbol{x}_l))^{1/N}}\right) \geq \ln 1 = 0.$$

Also, as $\sum_{j=1}^{N} U_j^n(\boldsymbol{x}_l) = 1$ it follows that

$$\ln U_k^n(\boldsymbol{x}_l) \geq \ln\frac{1}{N}.$$

Combining these inequalities

$$g_k^l \geq \left[\ln\frac{1}{N} - \frac{1}{N}\sum_{j=1}^{N} \ln U_j^n(\boldsymbol{x}_l)\right]_+,$$

where $[\cdot]_+ = \max\{\cdot, 0\}$. Thus, for k fixed

$$\sum_{l=1}^{D} M_{ll}(g_k^l)^2 \geq \sum_{l \in I_k} M_{ll}(g_k^l)^2 \geq \sum_{l \in I_k} M_{ll}\left[\ln\frac{1}{N} - \frac{1}{N}\sum_{j=1}^{N} \ln U_j^n(\boldsymbol{x}_l)\right]_+^2,$$

so that summing over k

$$\sum_{k=1}^{N}\sum_{i=1}^{D} M_{ii}(g_k^i)^2 \geq \sum_{i=1}^{D} M_{ii}\left[\ln\frac{1}{N}-\frac{1}{N}\sum_{j=1}^{N}\ln U_j^n(\boldsymbol{x}_i)\right]_+^2. \tag{3.17}$$

Next we prove a similar inequality in reverse. We claim that

$$\max g_k^i \geq \frac{1}{N}\left[\ln\max_j U_j^n(\boldsymbol{x}_i)-\ln\frac{1}{N}\right].$$

There are two cases to consider. If $\max_j U_j^n(\boldsymbol{x}_i)=1/N=\min_j U_j^n(\boldsymbol{x}_i)$ then the result is trivial. If $\max_j U_j^n(\boldsymbol{x}_i)>1/N>\min_j U_j^n(\boldsymbol{x}_i)$ then

$$\max_k g_k^i = \max_k \ln U_k^n(\boldsymbol{x}_i)-\frac{1}{N}\sum_{j=1}^{N}\ln U_j^n(\boldsymbol{x}_i) \geq \frac{1}{N}\left(\ln\max_j U_j^n(\boldsymbol{x}_i)-\ln\min_j U_j^n(\boldsymbol{x}_i)\right)$$

$$>\frac{1}{N}\left(\ln\max_j U_j^n(\boldsymbol{x}_i)-\ln\frac{1}{N}\right)>0.$$

Hence

$$\sum_{i=1}^{D} M_{ii}\left[\frac{1}{N}\sum_{j=1}^{N}\ln U_j^n(\boldsymbol{x}_i)-\ln\frac{1}{N}\right]_+^2 \leq \sum_{i=1}^{D} M_{ii}\left(\max_k \ln U_k^n(\boldsymbol{x}_i)-\ln\frac{1}{N}\right)^2$$

$$\leq N^2\sum_{i=1}^{D} M_{ii}\left(\max_k g_k^i\right)^2 \leq N^2\sum_{i=1}^{D} M_{ii}\sum_{k=1}^{N}(g_k^i)^2. \tag{3.18}$$

Combining (3.17–3.18) yields

$$\left|\mathbf{1}\left(\sum \ln \boldsymbol{U}^n-\ln\frac{1}{N}\right)\right|_h^2 = \sum_{k=1}^{N}\sum_{i=1}^{D} M_{ii}\left(\frac{1}{N}\sum_{j=1}^{N}\ln U_j^n(\boldsymbol{x}_i)-\ln\frac{1}{N}\right)^2$$

$$\leq N(N^2+1)\sum_{i=1}^{D} M_{ii}\sum_{k=1}^{N}(g_k^i)^2$$

$$= N(N^2+1)\left|\ln(\boldsymbol{U}^n)-\mathbf{1}\sum\ln(\boldsymbol{U}^n)\right|_h^2.$$

Implementing the inequality $(a-b)^2 \geq \frac{1}{2}a^2-b^2$, it results that

$$\frac{1}{2}\left|\mathbf{1}\sum\phi(\boldsymbol{U}^n)\right|_h^2 \leq N\left(\ln\frac{1}{N}\right)^2|\Omega| + N(N^2+1)(C_3'+C_4'|L^{1/2}\boldsymbol{W}^n|_1),$$

and (3.3), (3.5) yield (3.6–3.7). □

LEMMA 3.2 Let $\mathcal{T}^h$ be an acute regular family of triangulation of Ω. For $\boldsymbol{U}>\mathbf{0}$

$$(\nabla\boldsymbol{U}, \nabla\boldsymbol{I}^h\boldsymbol{\phi}(\boldsymbol{U})) \geq 0.$$

Proof. It is sufficient to prove the result for one component of the vector $\boldsymbol{U}$ which we denote U. Since the triangulation is acute $K_{ij}\leq 0$ when $i\neq j$. From the definition of the stiffness matrix K, it follows that

$$\sum_j K_{ij} = \sum_j (\nabla\chi_i, \nabla\chi_j) = \Big(\nabla\chi_i, \nabla\sum_j \chi_j\Big) = (\nabla\chi_i, \nabla 1) = 0$$

and K is symmetric. Defining $U(\boldsymbol{x}_j) = U_j$ and $\alpha_j = \phi(U_j)$ by monotonicity

$$\big(\nabla I^h\phi(U), \nabla U\big) = \sum_{i,j=1}^{D} \alpha_i K_{ij}(U_j - U_i) = \sum_{i,j=1}^{D} \alpha_j K_{ij}(U_i - U_j),$$

$$= \frac{1}{2}\sum_{i,j=1}^{D} -(\alpha_i - \alpha_j)K_{ij}(U_i - U_j) \geqslant 0. \qquad \square$$

3.2 *Convergence*

We will find it useful to define the following discrete operators. Let P_0^h be the discrete L^2 projection onto S^h: given $\eta \in L^2(\Omega)$, $P_0^h\eta$ is the unique solution of

$$(P_0^h\eta, \chi)^h = (\eta, \chi) \qquad \forall\chi \in S^h.$$

Given $\eta \in H^1(\Omega)$, $P_1^h\eta$ is the H^1 projection onto S^h such that $(P_1^h\eta, 1) = (\eta, 1)$ and

$$(\nabla P_1^h\eta, \nabla\chi) = (\nabla\eta, \nabla\chi) \qquad \forall\chi \in S^h.$$

Notice that due to the nature of projections, it follows that

$$P_1^h\eta \to \eta \quad \text{in } H^1(\Omega) \qquad \text{and} \qquad |P_1^h\eta|_1 \leqslant |\eta|_1.$$

Given $\boldsymbol{u}^0 \in \boldsymbol{H}^1(\Omega)$ satisfying

$$N\sum \boldsymbol{u}^0(\boldsymbol{x}) = 1, \qquad \boldsymbol{u}^0(\boldsymbol{x}) \geqslant \boldsymbol{0}, \qquad \boldsymbol{m} = \int_\Omega \boldsymbol{u}^0(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x},$$

we take $U_k^0 = P_0^h u_k^0$ $(k = 1,\dots,N)$. Automatically, $(\boldsymbol{U}^0, 1)^h = \boldsymbol{m}$ and since

$$U_k^0(\boldsymbol{x}_i) = \frac{(u_k^0, \chi_i)}{(1, \chi_i)^h} \geqslant 0,$$

where χ_i is an element of the cardinal basis for S^h, it follows that $\boldsymbol{U}^0 \geqslant \boldsymbol{0}$, $N\sum \boldsymbol{U}^0 = 1$. Hence $\boldsymbol{U}^0$ satisfies the assumptions of Theorem 2.4. Let $\{\boldsymbol{U}^n, \boldsymbol{W}^n\}_{n=1}^M$ be the sequence resulting from (2.6a,b). For $t \in (t^{n-1}, t^n)$, $n \in [1, M]$, define the piecewise constant sequences in time

$$\boldsymbol{u}_{\Delta t}^h(t) = \boldsymbol{U}^n, \qquad \boldsymbol{w}_{\Delta t}^h(t) = \boldsymbol{W}^n,$$

$$\boldsymbol{\phi}_{\Delta t}^h(t) = \boldsymbol{I}^h\boldsymbol{\phi}(\boldsymbol{U}^n), \qquad \mu_{\Delta t}(t) = \mu(t^{n-1}), \quad \mu \in C^\infty[0, T], \quad \mu(T) = 0,$$

and the piecewise linear sequences in time, such that for $n = 0,\dots, M$,

$$\bar{\boldsymbol{u}}_{\Delta t}^h(t^n) = \boldsymbol{U}^n, \qquad \bar{\mu}_{\Delta t}(t^n) = \mu(t^n).$$

From Lemma 3.1, these sequences satisfy

$$\|u^h_{\Delta t}\|_{L^\infty(0,T;H^1(\Omega))} + \|\bar{u}^h_{\Delta t}\|_{L^\infty(0,T;H^1(\Omega))} + \|w^h_{\Delta t}\|_{L^2(0,T;H^1(\Omega))} + \|\phi^h_{\Delta t}\|_{L^2(0,T;L^2(\Omega))}$$
$$+ \left\|\sqrt{t}\,\frac{\mathrm{d}}{\mathrm{d}t}\bar{u}^h_{\Delta t}\right\|_{L^2(0,T;H^1(\Omega))} + \|\sqrt{t}w^h_{\Delta t}\|_{L^\infty(0,T;H^1(\Omega))} + \|\sqrt{t}\phi^h_{\Delta t}\|_{L^\infty(0,T;L^2(\Omega))} \leq C,$$

where C is independent of h and Δt; we have used (2.1) so that

$$|I^h\phi(U^n)|_0 \leq C_1\,|\phi(U^n)|_h.$$

Let $\xi, \zeta \in H^1(\Omega)$ be arbitrary. Setting $\chi_l = P^h_1\zeta_l$ and $\eta_l = P^h_1\xi_l$ in (2.6a) and (2.6b) respectively, multiplying each equation by $\Delta t\mu(t^{n-1})$ and summing over n yields

$$0 = \int_0^T \left[-(u^h_{\Delta t}, P^h_1\zeta)^h \frac{\mathrm{d}}{\mathrm{d}t}\bar{\mu}_{\Delta t} + (L\nabla w^h_{\Delta t}, \nabla\zeta)\mu_{\Delta t}(t)\right]\mathrm{d}t - (u^0, P^h_1\zeta)^h\mu(0),$$

$$0 = \int_0^T \left[\gamma(\nabla u^h_{\Delta t}, \nabla\xi) + \left(\theta\phi^h_{\Delta t} - Au^h_{\Delta t}, P^h_1\xi - 1\sum P^h_1\xi\right)^h - (w^h_{\Delta t}, P^h_1\xi)^h\right]\mu_{\Delta t}\,\mathrm{d}t,$$

where $\{P^h_1\eta\}_l = P^h_1\eta_l$. By compactness we can extract subsequences such that

$$u^h_{\Delta t} \rightharpoonup u \quad \text{in} \quad L^2(0, T; H^1(\Omega)),$$
$$w^h_{\Delta t} \rightharpoonup w \quad \text{in} \quad L^2(0, T; H^1(\Omega)),$$
$$\bar{\mu}_{\Delta t} \to \mu \quad \text{in} \quad H^1(0, T),$$
$$\phi^h_{\Delta t} \rightharpoonup v \quad \text{in} \quad L^2(0, T; L^2(\Omega)),$$

as h, $\Delta t \to 0$. Furthermore, $\bar{u}^h_{\Delta t}$ is bounded in $H^1(\kappa, T; H^1(\Omega))$ for $0 < \kappa < T$, hence the compact injection into $L^2(\kappa, T; L^2(\Omega))$ guarantees the existence of a subsequence such that

$$\bar{u}^h_{\Delta t} \to u \quad \text{in} \quad L^2(\kappa, T; L^2(\Omega)).$$

From (3.2) we conclude that $\|\bar{u}^h_{\Delta t} - u^h_{\Delta t}\|_{L^2(\kappa,T;L^2(\Omega))} \to 0$ and it follows that

$$u^h_{\Delta t} \to u \quad \text{in} \quad L^2(\kappa, T; L^2(\Omega)).$$

Note that since $\phi^h_{\Delta t} \leq 0$ for all h and Δt, it follows that $v \leq 0$ a.e. We remark that $\{u, w\}$ satisfy the same regularity as proved in Elliott & Luckhaus (1991). Applying (2.1) we find that

$$\left|\int_0^T [(u^h_{\Delta t}, P^h_1\zeta)^h - (u^h_{\Delta t}, P^h_1\zeta)]\frac{\mathrm{d}}{\mathrm{d}t}\bar{\mu}_{\Delta t}(t)\,\mathrm{d}t\right|$$
$$\leq Ch^2\,\|u^h_{\Delta t}\|_{L^2(0,T;H^1(\Omega))}\,\|P^h_1\zeta\|_{H^1(\Omega)}\left\|\frac{\mathrm{d}}{\mathrm{d}t}\bar{\mu}_{\Delta t}(t)\right\|_{L^2(0,T)}$$

$$\left|\int_0^T [(\phi^h_{\Delta t}, P^h_1\xi)^h - (\phi^h_{\Delta t}, P^h_1\xi)]\mu_{\Delta t}(t)\,\mathrm{d}t\right|$$
$$\leq Ch\,\|\phi^h_{\Delta t}\|_{L^2(0,T;L^2(\Omega))}\,\|P^h_1\xi\|_{H^1(\Omega)}\,\|\mu_{\Delta t}\|_{L^2(0,T)}.$$

Using the convergence properties of the sequences above, we find that passing to the limit

$$0=\int_0^T\left[-(\boldsymbol{u},\boldsymbol{\zeta})\frac{d\mu}{dt}+(L\nabla\boldsymbol{w},\nabla\boldsymbol{\zeta})\mu(t)\right]dt-(\boldsymbol{u}^0,\boldsymbol{\zeta})\mu(0), \quad (3.19)$$

$$0=\int_0^T\left[\gamma(\nabla\boldsymbol{u},\nabla\boldsymbol{\xi})+\left(\theta\boldsymbol{v}-A\boldsymbol{u}-\mathbf{1}\sum(\theta\boldsymbol{v}-A\boldsymbol{u})-\boldsymbol{w},\boldsymbol{\xi}\right)\right]\mu(t)\,dt, \quad (3.20)$$

which implies that

$$0=\langle\boldsymbol{u}_t,\boldsymbol{\zeta}\rangle+(L\nabla\boldsymbol{w},\nabla\boldsymbol{\zeta}) \qquad \text{a.e. in } (0,T),$$

$$\gamma(\nabla\boldsymbol{u},\nabla\boldsymbol{\xi})+\left(\theta\boldsymbol{v}-A\boldsymbol{u}-\mathbf{1}\sum(\theta\boldsymbol{v}-A\boldsymbol{u})-\boldsymbol{w},\boldsymbol{\xi}\right)=0 \qquad \text{a.e. in } (0,T).$$

Also from (3.20), we deduce that $\boldsymbol{u}(t)\in\boldsymbol{H}^2(\Omega)$ for a.e. $t\in(0,T)$. And integration by parts of (3.19) gives

$$\left(\boldsymbol{u}(0)-\boldsymbol{u}^0,\boldsymbol{\zeta}\right)=0 \qquad \forall\boldsymbol{\zeta}\in\boldsymbol{H}^1(\Omega)$$

and therefore $\boldsymbol{u}(0)=\boldsymbol{u}^0$. It remains to prove

$$\boldsymbol{v}=\boldsymbol{\phi}(\boldsymbol{u}).$$

Here we use a different proof than that of Elliott & Luckhaus (1991). In fact we show that $u_l=\phi^{-1}(v_l)$ where $\phi^{-1}(v_l)=e^{v_l}$, which exists a.e. since $v_l\leqslant 0$ so that $e^{v_l}\in(0,1)$. Notice that

$$|\phi^{-1}(x)-\phi^{-1}(y)|\leqslant\phi^{-1}(\max\{x,y\})\,|x-y|. \quad (3.21)$$

We will show that for all $0<\kappa<T$

$$\int_\kappa^T\left(u_l-\phi^{-1}(v),\,v_l-v\right)\geqslant 0$$

where we assume that v is smooth, otherwise we approximate it by a smooth sequence and prove these results for the subsequent sequence. If the above inequality holds, then using Minty's lemma will yield the result; in fact the following argument is used. Setting $v=\lambda z+(1-\lambda)v_l$ $\big(\lambda\in(0,1)\big)$ so that

$$\int_\kappa^T\left(\mu_l-\phi^{-1}\big(\lambda z+(1-\lambda)v_l\big),\,v_l-z\right)\geqslant 0$$

taking $z=v_l\pm y$, letting $\lambda\to 0$ and noting (3.21), we have that

$$\int_\kappa^T\left(u_l-\phi^{-1}(v_l),\,y\right)dt=0$$

i.e. $u_l=\phi^{-1}(v_l)$. For the rest of the proof we identify u, v with u_l, v_l and $u^h_{\Delta t}$, $\phi^h_{\Delta t}$ with $\{\boldsymbol{u}^h_{\Delta t}\}_l$, $\{\boldsymbol{\phi}^h_{\Delta t}\}_l$. For $t\in(t^{n-1},t^n)$, let us define

$$v^h_{\Delta t}(t):=I^hv(t^n).$$

Note that

$$\int_\kappa^T |v_{\Delta t}^h(t)|_0^2\,\mathrm{d}t \leqslant \sum_{n=n_*}^{M} \int_{t^{n-1}}^{t^n} |I^h v(t^n)|_0^2\,\mathrm{d}t \leqslant C\,|v|^2_{L^\infty(0,T;L^\infty(\Omega))}$$

where $t^{n_*} \leqslant \kappa < t^{n_*+1}$ and

$$\begin{aligned}\int_\kappa^T |v_{\Delta t}^h(t) - v(t)|_0^2\,\mathrm{d}t &\leqslant \sum_{n=n_*}^{M} \int_{t^{n-1}}^{t^n} |I^h v(t^n) - v(t)|_0^2\,\mathrm{d}t \\ &\leqslant 2\sum_{n=n_*}^{M} \int_{t^{n-1}}^{t^n} (|I^h v(t^n) - I^h v(t)|_0^2 + |I^h v(t) - v(t)|_0^2)\,\mathrm{d}t \\ &\leqslant 2\sum_{n=n_*}^{M} \int_{t^{n-1}}^{t^n} \left(\left|\int_t^{t^n} v_t(s)\,\mathrm{d}s\right|^2_{L^\infty(\Omega)} + |I^h v(t) - v(t)|_0^2\right)\mathrm{d}t \\ &\leqslant C\Delta t^2\,\|v_t\|^2_{L^2(0,T;L^\infty(\Omega))} + Ch^4\,\|v\|^2_{L^2(0,T;H^2(\Omega))} \to 0\end{aligned}$$

as h, $\Delta t \to 0$, since the inequality $|I^h v - v|_0 \leqslant Ch^2\,\|v\|_{H^2(\Omega)}$ holds. Also, using (3.21), it follows that

$$\|\phi^{-1}(v_{\Delta t}^h) - \phi^{-1}(v)\|_{L^2(\kappa,T;L^2(\Omega))} \leqslant C\,\|v_{\Delta t}^h - v\|_{L^2(\kappa,T;L^2(\Omega))} \to 0.$$

Hence,

$$\int_\kappa^T \left(u_{\Delta t}^h - \phi^{-1}(v_{\Delta t}^h),\, \phi_{\Delta t}^h - v_{\Delta t}^h\right)\mathrm{d}t \to \int_\kappa^T \left(u - \phi^{-1}(v),\, v - v\right)\mathrm{d}t.$$

It is obvious that

$$\int_\kappa^T (u_{\Delta t}^h - I^h\phi^{-1}(v_{\Delta t}^h),\, \phi_{\Delta t}^h - v_{\Delta t}^h)^h \geqslant 0$$

since for each $t \in (t^{n-1}, t^n)$

$$\begin{aligned}&\left(u_{\Delta t}^h(t) - I^h\phi^{-1}(v_{\Delta t}^h(t)),\, \phi_{\Delta t}^h(t) - v_{\Delta t}^h(t)\right)^h \\ &\quad = \sum_{l=1}^{D} M_{ll}\left(\phi^{-1}(\phi(U^n(x_l))) - \phi^{-1}(v(x_l, t^n))\right)\left(\phi(U^n(x_l)) - v(x_l, t^n)\right) \geqslant 0.\end{aligned}$$

Finally

$$\begin{aligned}&\int_\Omega (\phi^{-1}(v_{\Delta t}^h) - I^h\phi^{-1}(v_{\Delta t}^h))(\phi_{\Delta t}^h - v_{\Delta t}^h)\,\mathrm{d}x \\ &\quad = \sum_{\tau\in\mathcal{T}^h} \int_\tau \left[\sum_{l:x_l\in\tau} (\phi^{-1}(v_{\Delta t}^h(x)) - \phi^{-1}(v_{\Delta t}^h(x_l)))\chi_l(x)\right](\phi_{\Delta t}^h - v_{\Delta t}^h)\,\mathrm{d}x \\ &\quad = \sum_{\tau\in\mathcal{T}^h} \int_\tau \left[\sum_{l:x_l\in\tau} (x - x_l)^{\mathrm{T}}\nabla v_{\Delta t}^h(\beta_l)\phi^{-1}(v_{\Delta t}^h(\beta_l))\chi_l(x)\right](\phi_{\Delta t}^h - v_{\Delta t}^h)\,\mathrm{d}x,\end{aligned}$$

where we have used the facts

$$I^h\phi^{-1}(v(\boldsymbol{x})) = \sum_{l:\boldsymbol{x}_l \in \tau} \phi^{-1}(v(\boldsymbol{x}_l))\chi_l(\boldsymbol{x}) \qquad \text{for } \boldsymbol{x} \in \tau,$$

$$\sum_{l:\boldsymbol{x}_l \in \tau} \chi_l(\boldsymbol{x}) = 1$$

and the mean value theorem.

Now, assembling all of these pieces together and using (2.1)

$$0 \leqslant \int_\kappa^T (u^h_{\Delta t} - I^h\phi^{-1}(v^h_{\Delta t}), \phi^h_{\Delta t} - v^h_{\Delta t})^h - \int_\kappa^T (u^h_{\Delta t} - I^h\phi^{-1}(v^h_{\Delta t}), \phi^h_{\Delta t} - v^h_{\Delta t})$$

$$+ \int_\kappa^T (\phi^{-1}(v^h_{\Delta t}) - I^h\phi^{-1}(v^h_{\Delta t}), \phi^h_{\Delta t} - v^h_{\Delta t}) + \int_\kappa^T (u^h_{\Delta t} - \phi^{-1}(v^h_{\Delta t}), \phi^h_{\Delta t} - v^h_{\Delta t})$$

$$\leqslant Ch \int_\kappa^T \|u^h_{\Delta t} - I^h\phi^{-1}(v^h_{\Delta t})\|_1 \, |\phi^h_{\Delta t} - v^h_{\Delta t}|_0$$

$$+ Ch\phi^{-1}(\|v^h_{\Delta t}\|_{L^\infty(0,T;L^\infty(\Omega))}) \int_\kappa^T \|v^h_{\Delta t}\|_{W^{1,\infty}(\Omega)} \, |\phi^h_{\Delta t} - v^h_{\Delta t}|_0$$

$$+ \int_\kappa^T (u^h_{\Delta t} - \phi^{-1}(v^h_{\Delta t}), \phi^h_{\Delta t} - v^h_{\Delta t})$$

$$\to \int_\kappa^T (u - \phi^{-1}(v), \nu - v)\, dt$$

and the result is proven.

REMARK 3.3 Convergence of the sequence $\{U^n, W^n\}$ satisfying (2.27*a,b*) to the continuous problem holds.

4. Numerical simulation

We consider a ternary system in one space dimension where $\Omega = (0, 1)$

$$L = \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

and

$$A = -\theta_c \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

Note that $\|L\| = 1$ and the largest positive eigenvalue of A is given by $\lambda_A = \theta_c$. It follows that

$$\Psi(u) = \theta(u_1 \ln u_1 + u_2 \ln u_2 + u_3 \ln u_3) + \theta_c(u_1u_2 + u_2u_3 + u_1u_3).$$

With L and A taken as above, noting that $u_1 + u_2 + u_3 = 1$, the partial differential equations (1.1a,b) we wish to solve may be written as

$$\boldsymbol{u}_t + \gamma \boldsymbol{u}_{xxxx} + \theta_c \boldsymbol{u}_{xx} - \theta\{L\boldsymbol{\phi}(\boldsymbol{u})\}_{xx} = \boldsymbol{0}. \tag{4.1}$$

4.1 *Linear stability analysis*

Let the mean concentration take the form $\boldsymbol{m} = (m_1, m_2, m_3)$ where $m_i > 0\ \forall i$ and $m_3 = 1 - m_1 - m_2$. We seek a solution of the form

$$u_i(x, t) = m_i + \sum_{n=1}^{\infty} c_i^n(t) \cos(n\pi x) \qquad (i = 1, 2, 3),$$

where $|c_i^n(t)| \ll 1$ $(i = 1, 2, 3;\ n = 1, 2, \ldots)$; note that $c_1^n(t) + c_2^n(t) + c_3^n(t) = 0$. Linearizing $\phi(u_i)$ about m_i and substituting into (4.1), up to first order we find that c_1^n and c_2^n must satisfy the ordinary differential equations

$$\frac{\mathrm{d}c_1^n}{\mathrm{d}t} + n^2\pi^2(n^2\pi^2\gamma - \theta_c)c_1^n + \theta n^2\pi^2\left(\frac{2c_1^n}{3m_1} - \frac{c_2^n}{3m_2} + \frac{c_1^n + c_2^n}{3(1 - m_1 - m_2)}\right) = 0$$

and

$$\frac{\mathrm{d}c_2^n}{\mathrm{d}t} + n^2\pi^2(n^2\pi^2\gamma - \theta_c)c_2^n + \theta n^2\pi^2\left(\frac{2c_2^n}{3m_2} - \frac{c_1^n}{3m_1} + \frac{c_1^n + c_2^n}{3(1 - m_1 - m_2)}\right) = 0.$$

In vector form we have

$$\frac{\mathrm{d}\boldsymbol{c}^n}{\mathrm{d}t} + n^4\pi^4\gamma\boldsymbol{c}^n + n^2\pi^2 B\boldsymbol{c}^n = \boldsymbol{0}$$

where $\boldsymbol{c}^n(t) = (c_1^n, c_2^n)^{\mathrm{T}}$,

$$B = \begin{pmatrix} \frac{2\theta}{3}\left(\frac{1}{m_1} + \frac{1}{2(1 - m_1 - m_2)}\right) - \theta_c & -\frac{2\theta}{3}\left(\frac{1}{2m_2} - \frac{1}{2(1 - m_1 - m_2)}\right) \\ -\frac{2\theta}{3}\left(\frac{1}{2m_1} - \frac{1}{2(1 - m_1 - m_2)}\right) & \frac{2\theta}{3}\left(\frac{1}{m_2} + \frac{1}{2(1 - m_1 - m_2)}\right) - \theta_c \end{pmatrix}$$

$$= \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} \end{pmatrix} H_{\Psi}.$$

Here H_Ψ is the Hessian of the free energy Ψ, with respect to the two independent concentrations, evaluated at $\boldsymbol{m}$ i.e.

$$\begin{pmatrix} \theta\left(\frac{1}{m_1}+\frac{1}{(1-m_1-m_2)}\right)-2\theta_c & \theta\frac{1}{(1-m_1-m_2)}-\theta_c \\ \theta\frac{1}{(1-m_1-m_2)}-\theta_c & \theta\left(\frac{1}{m_2}+\frac{1}{(1-m_1-m_2)}\right)-2\theta_c \end{pmatrix}.$$

The solution to the system of ODEs is given by

$$c^n(t)=\mathrm{e}^{-\gamma n^4\pi^4 t}\times \mathrm{e}^{-n^2\pi^2 Bt}c^n(0).$$

For interesting behaviour, i.e. growth of one or more of the components u_1, u_2, we want $c^n(t)\nrightarrow 0$ as t increases. A necessary condition is that at least one of the eigenvalues of B is smaller than $-\gamma\pi^2<0$. If λ_1 and λ_2 are the eigenvalues of B then from the identities

$$\lambda_1\times\lambda_2=\det B \qquad \text{and} \qquad \lambda_1+\lambda_2=\operatorname{trace} B$$

it is easy to find regions where both eigenvalues of B are positive and negative, in fact all we need do is solve the equation $\det B=0=\det H_\Psi$, this curve will obviously be θ dependent.

In the case where $m_2=m_1$, a calculation reveals that

$$\det H_\Psi=\frac{(\theta/\theta_c+6m_1^2-3m_1)(\theta/\theta_c-m_1)}{m_1^2(1-2m_1)}\theta_c^2 \tag{4.2}$$

The two curves $\theta/\theta_c=m_1$ and $\theta/\theta_c=3m_1-6m_1^2$ (see Fig. 1) defines four regions in which B is positive definite, negative definite or indefinite. It is easy to see that for $\theta/\theta_c<\frac{1}{3}$ we will have a negative definite region in which growth of phases may take place. For θ sufficiently small, the free energy Ψ has three equal minima; for $\theta<\theta_c/3$ a local maximum at $(\frac{1}{3},\frac{1}{3},\frac{1}{3})$. We notice that Ψ is defined on

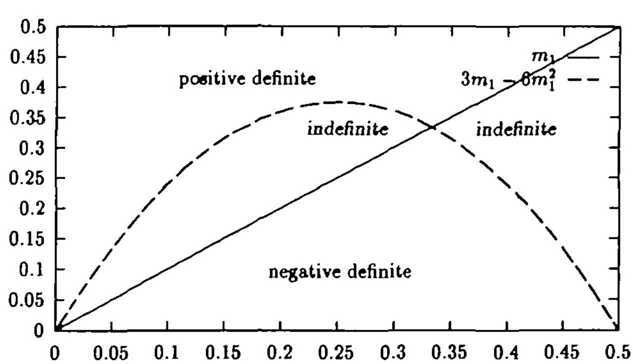

FIG. 1. m_1 against θ/θ_c.

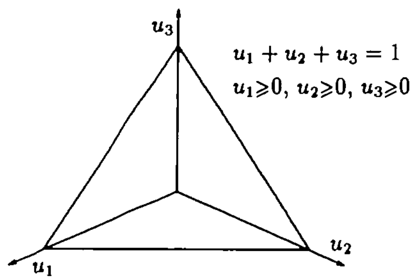

FIG. 2. Gibbs triangle.

the surface $u_1 + u_2 + u_3 = 1$ of the 3-simplex, known as the Gibbs triangle (see Fig. 2). For example, if we take $\theta = 0{\cdot}3$ and $\theta_c = 1$ then to calculate the regions where B is negative definite, positive definite and indefinite we solve $\det B = 0$ along the lines $(m_1, \alpha m_1, 1 - m_1 - \alpha m_1)$ of the Gibbs triangle, see Fig. 3. The black dots indicate the mean concentration used in the numerical experiments. To help explain this figure, given a point (u_1, u_2, u_3) on the Gibbs triangle, we define the affine mapping onto the x–y plane where

$$(x, y) = u_1\left(\frac{-1}{\sqrt{2}}, \frac{-1}{\sqrt{6}}\right) + u_2\left(\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{6}}\right) + u_3\left(0, \sqrt{\frac{2}{3}}\right).$$

Defining the origin on the Gibbs triangle to be $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ and the origin in the x–y plane to be $(0, 0)$ we notice that the Gibbs origin gets mapped to the x–y origin and the mapping preserves the distance from the relative origin.

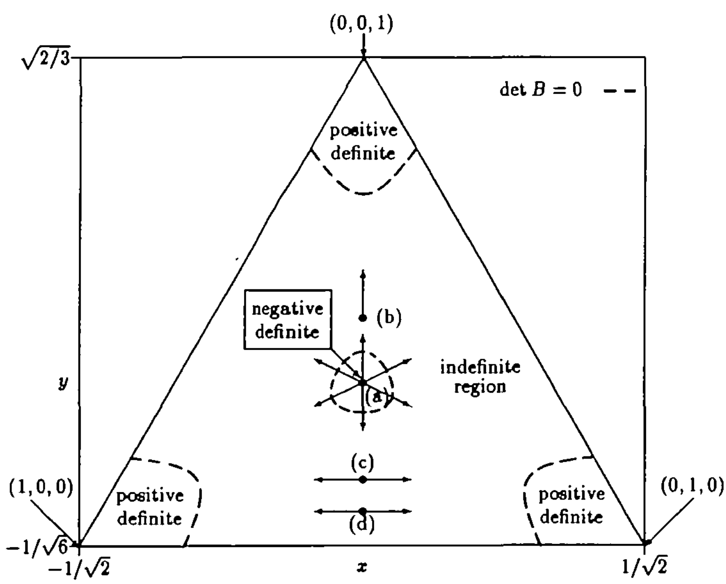

FIG. 3. Isothermal section of the phase diagram where $\theta = 0{\cdot}3$, $\theta_c = 1$.

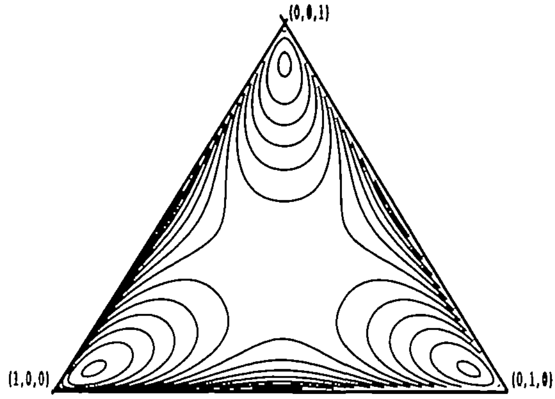

FIG. 4. Contour plot of the free energy Ψ on the Gibbs triangle.

From Fig. 3, it can be seen that if the mean concentration is near the middle of the Gibbs triangle, inside the negative definite region, then three phases may separate and if the mean concentration is near the edge of the Gibbs triangle, in the semi-definite region, then only two phases may separate. When the concentration is near a corner, in the positive definite region, then the homogeneous system is stable.

A contour of the free energy Ψ is shown in Fig. 4. The three minima of Ψ are approximately at $(0{\cdot}0551, 0{\cdot}0551, 0{\cdot}8898)$, the other two values being permutations. Also, Ψ has saddle points at approximately $(0{\cdot}3861, 0{\cdot}3861, 0{\cdot}2278)$ and two other points having permuted values.

The points where the line $\theta = 0{\cdot}3$ intersects the two graphs in Fig. 1 correspond to the three points intersecting $\det B = 0$ on the line $x = 0$, see Fig. 3. On Fig. 3, we also draw the direction of the eigenvectors associated with the eigenvalues. These give an indication of the directions in which we expect growth will take place.

4.2 *An iterative method*

Representing the solution of (2.6*a*,*b*) as a linear combination of the basis functions of S^h, i.e. for $j = 1, 2, 3$

$$\{U^n\}_j = U_j^n = \sum_{i=1}^{D} e_{ij}\chi_i, \qquad \{W^n\}_j = W_j^n = \sum_{i=1}^{D} f_{ij}\chi_i,$$

it follows that the discretized version of solving (4.1) is equivalent to solving $(j = 1, 2)$

$$(I + \Delta t\gamma M^{-1}KM^{-1}K - \Delta t\theta_c M^{-1}K)\boldsymbol{e}_j - \boldsymbol{e}_j^{n-1} + \theta\,\Delta t M^{-1}K\{\boldsymbol{\phi}(\boldsymbol{e})L\}_j = \boldsymbol{0}, \quad (4.3a)$$

$$\boldsymbol{e}_3 = \boldsymbol{1} - \boldsymbol{e}_2 - \boldsymbol{e}_1, \quad (4.3b)$$

where $\{\boldsymbol{e}_j\}_i := e_{ij}$ and $\{\boldsymbol{\phi}(\boldsymbol{e})L\}_j = \sum_i \boldsymbol{\phi}(\boldsymbol{e}_i)L_{ij}$. To numerically find the solution to the above set of non-linear equations, we use the following iterative technique:

given $\{e_1^0, e_2^0\}$, an initial guess to $\{e_1, e_2\}$, we use the non-linear Gauss–Seidel-type iteration: for $k \geq 1$

$$(I + \Delta t\gamma M^{-1}KM^{-1}K - \Delta t\theta_c M^{-1}K)e_1^k - e_1^{n-1}$$
$$+ \theta\, \Delta t M^{-1}K\{\tfrac{2}{3}\phi(e_1^{k-1}) - \tfrac{1}{3}\phi(e_2^{k-1}) - \tfrac{1}{3}\phi(1 - e_1^{k-1} - e_2^{k-1})\} = 0,$$
$$(I + \Delta t\gamma M^{-1}KM^{-1}K - \Delta t\theta_c M^{-1}K)e_2^k - e_2^{n-1}$$
$$+ \theta\, \Delta t M^{-1}K\{-\tfrac{1}{3}\phi(e_1^k) + \tfrac{2}{3}\phi(e_2^{k-1}) - \tfrac{1}{3}\phi(1 - e_1^k - e_2^{k-1})\} = 0,$$

where e_j^k denotes the kth iterate $(j = 1, 2)$ approximating e_j. For $\Delta t < 4\gamma/(\theta_c^2) = 4\gamma/(\lambda_A^2 \|L\|)$ the matrix multiplying e_j^k $(j = 1, 2)$ in the above equations is symmetric positive definite, hence the iterative sequence is uniquely defined. Provided that Δt was sufficiently small and $\{e_j^k\}$ $(j = 1, 2)$ were greater than zero and less than one, the iterative sequence was found to converge in each experiment.

4.3 *Numerical experiments*

We take $\theta = 0{\cdot}3$ and $\theta_c = 1$, corresponding to the choices of Section 4.1, see Figures 3 and 4. In each experiment, unless otherwise stated, we chose $h = \frac{1}{100}$, $\gamma = 5 \times 10^{-3}$ and $\Delta t = 10^{-4}$. The initial conditions were random perturbations of the uniform state $\boldsymbol{m}$ and the simulations were stopped when profiles were obtained which did not change for a long time.

In Fig. 5, we show the evolution where $\boldsymbol{m} = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ ($m_1 = \frac{1}{3}$ corresponds to

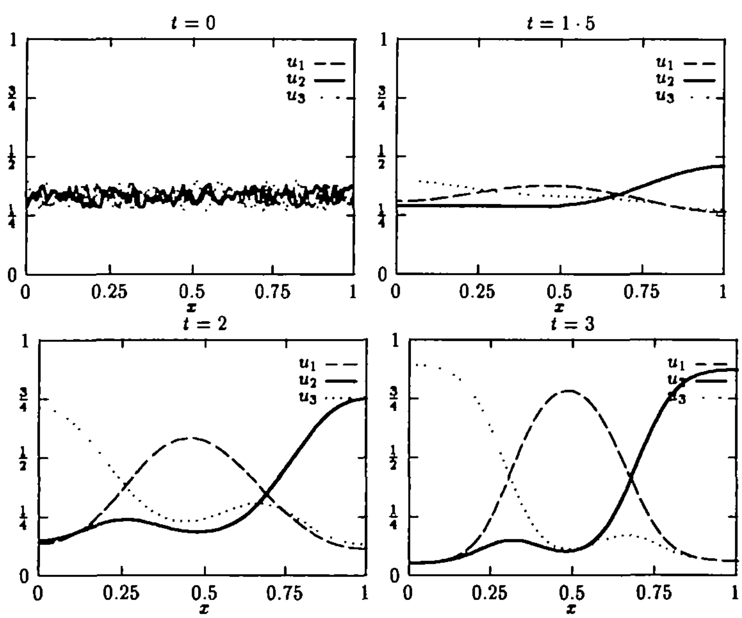

FIG. 5. $m_1 = 1/3$.

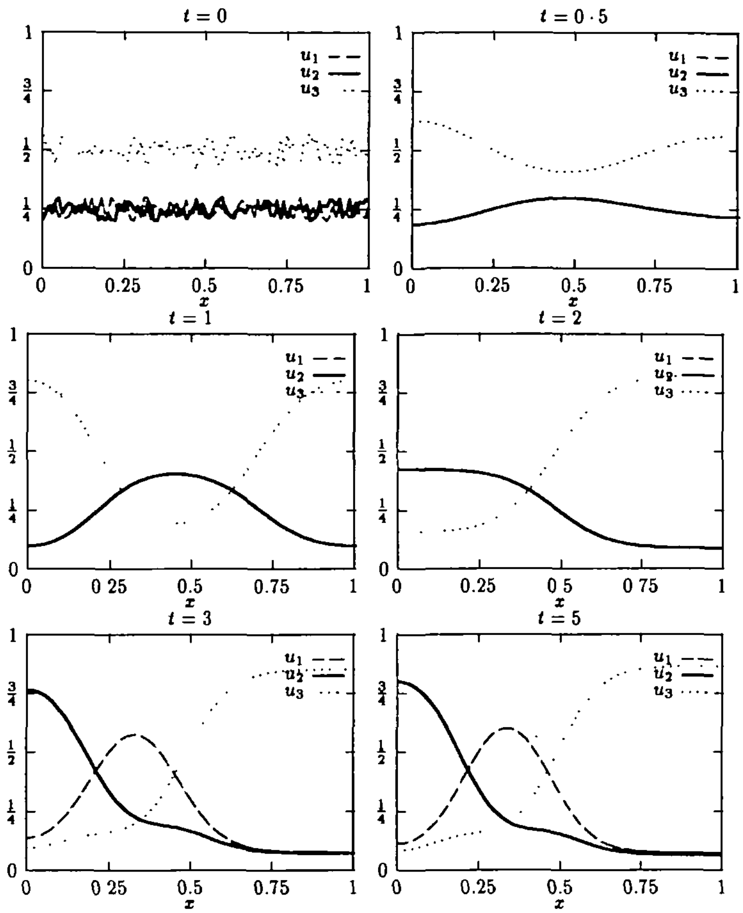

FIG. 6. Experiment 1: $m_1 = 1/4$.

point (a) in Fig. 3, inside the negative definite region). We observed three phases in the early stages of spinodal decomposition.

We performed three experiments with initial data inside the indefinite region, respectively taking $m_1 = 1/4$, $2/5$, $12/25$ (points (b), (c) and (d) in Fig. 3 respectively). In the first experiment with $m_1 = \frac{1}{4}$, initially the third phase u_3 dominates. Moreover, for some time the evolution is in the direction of $u_1 = u_2$ with a two-phase structure (see Fig. 6, $t = 1, 2$). However, at a time shortly after $t = 2$, the composition takes the value of a critical point of the free energy which is unstable to perturbations in the direction $u_1 = u_2$, and by $t = 3$ we see growth in the phases u_1 and u_2.

In the second experiment $m_1 = \frac{2}{5}$ and the evolution, after the quench, shows two phases with either u_1 or u_2 dominating (see Fig. 7, $t = 0{\cdot}5$, $1{\cdot}5$; decomposition proceeds like a binary alloy).

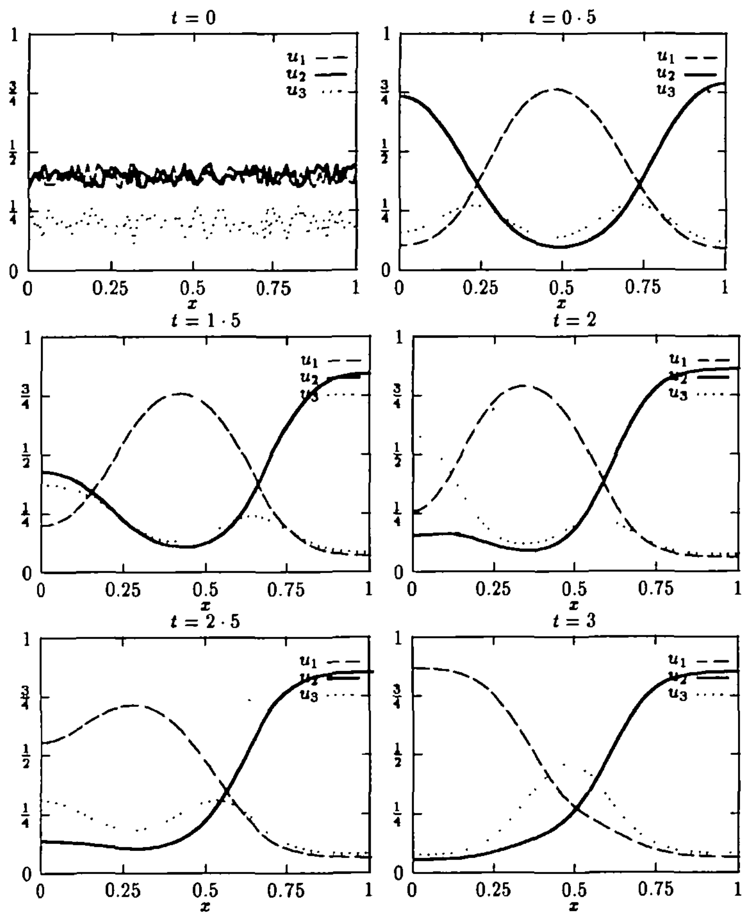

FIG. 7. Experiment 2: $m_1 = 2/5$.

In each of the above experiments, the system evolved into a three-phase structure with the concentration of the peaks, for some of the phases, very close to the value 0·89.

Figure 8 shows the time evolution of an almost binary system ($m_1 = 12/25$). As expected there are no spatial variations where u_3 is dominant; only phases u_1 and u_2 separated. We also set $\Delta t = 10^{-5}$.

We remark that in all experiments, the directions of decomposition observed at short times after the quench are in agreement with the direction of the eigenvectors for the negative eigenvalues. The results are consistent with numerical calculations performed by Eyre (1993) who investigated the evolution of ternary systems during spinodal decomposition using a finite-difference scheme.

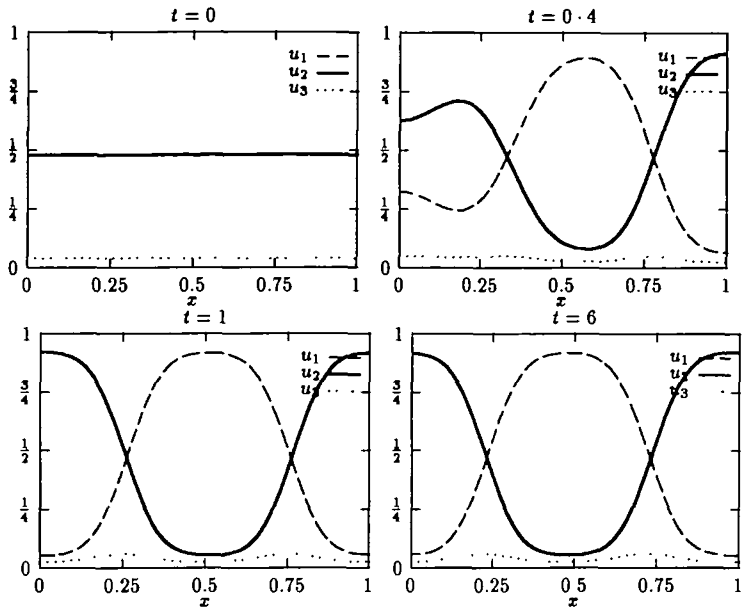

FIG. 8. Experiment 3: $m_1 = 12/25$.

Acknowledgements

This work was supported by the SERC (grant number GR/F85659) and CNPq (grant number 300766/92-0) when M. I. M. Copetti visited the University of Sussex in August 1992.

REFERENCES

CIARLET, P. G. 1978 *The Finite Element Method for Elliptic Problems*. Amsterdam: North-Holland.

CIARLET, P. G., & RAVIART, P. A. 1973 Maximum principle and uniform convergence for the finite element method. *Comput. Methods Appl. Mech. Eng.* **2,** 17–31.

CIAVALDINI, J. F. 1975 Analyse numérique d'un problème de Stefan à deux phases par une méthode d'elements finis. *SIAM J. Numer. Anal.* **12,** 464–487.

COPETTI, M. I. M., & ELLIOTT, C. M. 1992 Numerical analysis of the Cahn-Hilliard equation with logarithmic free energy. *Numerische Mathematik* **63,** 39–65.

DE FONTAINE, D. 1972 An analysis of clustering and ordering in multicomponent solid solutions—I. Stability criteria. *J. Phys. Chem. Solids* **33,** 297–310.

DE FONTAINE, D. 1973 An analysis of clustering and ordering in multicomponent solid solutions—II. Fluctuations and kinetics. *J. Phys. Chem. Solids* **34,** 1285–1304.

ELLIOTT, C. M., & LUCKHAUS, S. 1991 A generalised diffusion equation for phase separation of a multicomponent mixture with interfacial free energy. *Preprint Series 887,* IMA, University of Minnesota, 514 Vincent Hall, 206 Church Street S.E., Minneapolis, Minnesota 55455.

EYRE, D. J. 1993 Systems of Cahn-Hilliard equations. *SIAM J. Appl. Math.* **53,** 1686–1712.

HOYT, J. J. 1989 Spinodal decompositon in ternary alloys. *Acta Metall.* **37,** 2489–2497.

HOYT, J. J. 1990 Linear spinodal decomposition in a regular ternary alloy. *Acta Metall. Mater.* **38,** 227–231.