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AN ADI METHOD FOR HYSTERETIC REACTION-DIFFUSION SYSTEMS*

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Abstract. In this paper we consider a mathematical model motivated by patterned growth of bacterial cells. The model is a system of differential equations that consists of two subsystems. One is a system of ordinary differential equations and the other is a reaction-diffusion system. An alternating-direction implicit (ADI) method is derived for numerically solving the system. The ADI method given here is different from the usual ADI schemes for parabolic equations due to the special treatment of nonlinear reaction terms in the system. Stability and convergence of the ADI method are proved. We apply these results to the numerical solution of a problem in microbiology.

Key words. reaction-diffusion equations, hysteresis, accretion pattern formation, ADI methods

AMS subject classifications. 65N05, 65N15, 92-08, 92B05

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1. Introduction.

Reaction-diffusion systems are the main mathematical tools for studying various kinds of pattern formation in chemistry and biology [2, 13]. Different nonlinear reaction functions are responsible for different patterns [16]. In this paper, we consider the hysteretic reaction-diffusion systems which are closely related to reaction-diffusion systems. Hysteretic reaction-diffusion systems are useful for modeling accretion pattern formation in cell biology [12, 14]. Such systems were first proposed in [4] for concentric ring patterns formed by bacterial cells. Analytical results about the systems, e.g., existence and uniqueness of the solution, are given in [5]. The theory and the computer simulations show that hysteretic reaction-diffusion systems are interesting from a mathematical point of view as well as from a biological point of view [3, 9, 11]. In this paper we discuss the construction of an ADI method for solving a class of reaction-diffusion systems. This scheme is then adapted to give an ADI method for solving hysteretic reaction-diffusion systems.

Certain biological models divide nonmotile cells into different levels of torpor. Different torpors of cells can switch to each other in response to nutrition supply and environmental conditions. Let $\{u_1, u_2, \dots, u_\mu\}$ be cell concentrations of different torpors and $\{h_1, h_2, \dots, h_\nu\}$ be chemical concentrations (e.g., nutrient and oxygen). $\{h_1, h_2, \dots, h_\nu\}$ satisfy a reaction-diffusion system which models movement and chemical reactions. $\{u_1, u_2, \dots, u_\mu\}$ satisfy a hysteretic ordinary differential equation system which models growth of cells and switching between torpors, which has a hysteretic dependence on the conditions of $\{h_1, h_2, \dots, h_\nu\}$. The reaction-diffusion effect is recorded by the pattern formed by the total cell population $\sum_{i=1}^{\mu} u_i$, so we call these kind of patterns accretion patterns.

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Here, we consider a hysteretic reaction-diffusion system which involves only two levels of torpor, active and inactive cells, and two substrate concentrations, nutrient and buffer. Let u and v be the active and the inactive cell concentrations, respectively, H be the nutrient concentration, and G be the buffer concentration. Then the system is

$$\begin{cases} \dfrac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} -a & b \\ a & -b \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} fu \\ 0 \end{pmatrix}, \\ \dfrac{\partial}{\partial t}\begin{pmatrix} H \\ G \end{pmatrix} = \begin{pmatrix} D_H & 0 \\ 0 & D_G \end{pmatrix}\begin{pmatrix} \Delta H \\ \Delta G \end{pmatrix} + \begin{pmatrix} -fu/Y_H \\ -fu/Y_G \end{pmatrix}. \end{cases} \tag{1}$$

Here, $f = f(GH)$, $a = a(GH)$, and $b = b(GH)$ are three nonnegative functions depending on the product GH which is the combined concentration of nutrient and buffer. When $b > 0$, environmental conditions favor growth and inactive cells may become active. On the other hand, if $a > 0$, then the conditions are less favorable and active cells switch to the inactive state. The function f represents growth of cells by cell fission. $D_H > 0$ and $D_G > 0$ are diffusion constants. The two terms on the right-hand side of the second system describe loss of H and G due to uptake by active cells. $Y_H > 0$ and $Y_G > 0$ are two cell yield constant parameters. We assume that all cells at the start are active and that the distributions of u, H, and G at $t = 0$ are known. The initial conditions are then

$$u(x,0) = u_0(x) \ \geq\ 0 \ \text{ and } \ v(x,0) \ =\ 0. \tag{2}$$

$$H(x,0) = H_0(x) \ \text{ and } \ G(x,0) \ =\ G_0(x). \tag{3}$$

The boundary conditions for H and G are

$$\left.\frac{\partial H}{\partial n}\right|_{\partial\Omega} \ =\ \left.\frac{\partial G}{\partial n}\right|_{\partial\Omega} \ =\ 0. \tag{4}$$

The parameter functions f, a, and b are determined by the following criteria:

1. $f(\cdot)$ is monotone increasing and bounded, $f(0) = 0$.
2. When GH is large (acceptable environmental condition), $a = 0$ and $b > 0$.
3. When GH is small (unacceptable environmental condition), $a > 0$ and $b = 0$.
4. $a(\cdot)$ is monotone decreasing or zero, $b(\cdot)$ is monotone increasing or zero, and
$$b_{max} \ =\ \sup_{\alpha\geq 0} b(\alpha) \ =\ \lim_{\alpha\to\infty} b(\alpha) \ >\ 0.$$
5. There is a gap $[\alpha_1, \alpha_2]$, $\alpha_1 \leq \alpha_2$, such that
$$a(\alpha) \ =\ b(\alpha) \ =\ 0 \ \text{ for all } \alpha \in [\alpha_1, \alpha_2],$$
so active cells and inactive cells do not switch to each other when $GH \in [\alpha_1, \alpha_2]$. This property is exhibited in experiments, thus cells can have a hysteresis in growth depending on the combined concentration of nutrient and buffer [7].

An illustrative graph of f, a, and b is given in Figure 1.

Based on biological experiments [15], $f(\cdot)$ is defined by Monod's function

$$f(x) \ =\ \frac{V_0 x}{K_0 + x}, \quad x \geq 0,$$

where $V_0 > 0$ and $K_0 > 0$ are two parameters.

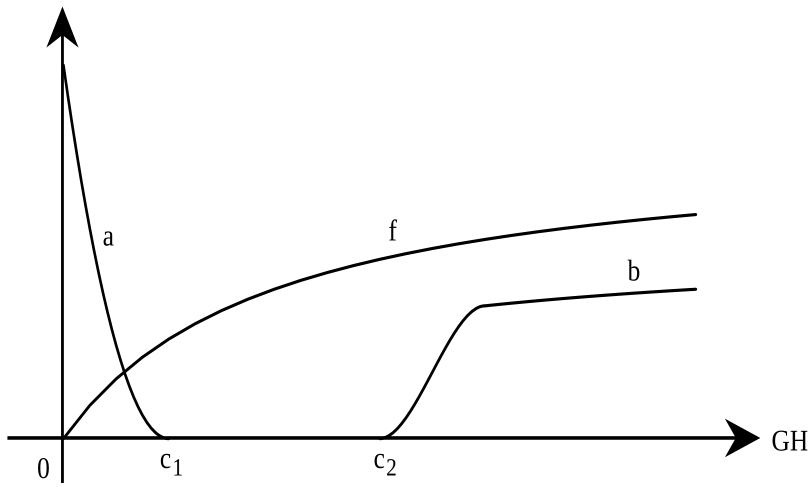

FIG. 1. *Graph of parameter functions $f(GH)$, $a(GH)$, and $b(GH)$.*

The simplest and the most straightforward numerical scheme for solving reaction-diffusion systems is the forward Euler scheme which is fully explicit and easy to implement. However, the forward Euler scheme requires the stability constraint

$$D\frac{\Delta t}{h^2} \; < \; \frac{1}{2}$$

to be satisfied, where D is the diffusion parameter, Δt is the time step size, and h is the spatial discretization size. Numerical experiments show that this condition results in extremely long run times. To avoid this problem, one may use the fully implicit backward Euler scheme. The analysis of this numerical scheme will parallel that of the continuous problem. While the stability constraint can be relaxed for the implicit scheme, one has to solve a (banded) system of nonlinear equations at each time step, which also results in long run times. A well-known class of efficient numerical methods for solving parabolic equations are the ADI methods [6, 17]. These methods do not require a strict stability condition like the one given above and only a tridiagonal linear system is solved at each time step. ADI schemes have traditionally been developed for linear parabolic equations, so a modification is required to accommodate the nonlinear reaction terms. In this paper, we present an alternating implicit technique with a judicious treatment of the reaction terms to achieve stability under minimal constraints. Our method will conserve the discrete mass, and we will also show that the numerical active cell density vanishes in the large time limit. It then follows that all of the cells will eventually become inactive, and a spatial pattern will form.

In section 2, we consider a general class of reaction-diffusion systems and construct an ADI method for solving this class of systems. Stability analysis and error estimates are given. Then in section 3 we apply the ADI method to the hysteretic reaction-diffusion system as given in (1). We will show some important properties of the numerical solution including positivity, conservation, and longtime behavior. Section 4 contains numerical experiment results. A summary is given in section 5.

2. An ADI method for a class of reaction-diffusion systems. In this section, we consider the following reaction-diffusion system:

$$\left\{ \begin{aligned} H_t \; &= \; D_H \Delta H \; - \; f_1(H,G), \\ G_t \; &= \; D_G \Delta G \; - \; f_2(H,G) \end{aligned} \right. \tag{5}$$

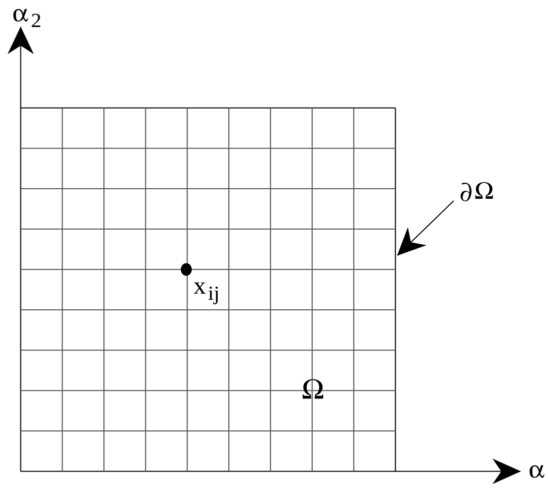

FIG. 2. *Uniform rectangular mesh of* Ω.

in a Lipschitz bounded domain $\Omega \in \Re^2$ with Neumann boundary conditions

$$\frac{\partial H}{\partial n}\bigg|_{\partial\Omega} \;=\; \frac{\partial G}{\partial n}\bigg|_{\partial\Omega} \;=\; 0. \tag{6}$$

Here, H and G model two chemical concentrations. $\partial\Omega$ is the boundary of Ω and n is its outward normal direction. The boundary condition (6) simulates zero flux of H and G at the boundary. Assume that the initial distributions of H and G are known as

$$H(x,0) \;=\; H_0(x) \quad \text{and} \quad G(x,0) \;=\; G_0(x). \tag{7}$$

In (5), $D_H > 0$ and $D_G > 0$ are two positive diffusion parameters; $f_1(H,G)$ and $f_2(H,G)$ are two parameter functions of the form

$$f_1(H,G) \;=\; F_1(H,G)H, \qquad\qquad f_2(H,G) \;=\; F_2(H,G)G, \tag{8}$$

where F_1 and F_2 are nonnegative and may depend upon the history $\{(G,H)(s)\,|\,0 \leq s \leq t\}$.

2.1. ADI scheme. ADI schemes are most effective for structured meshes, so for simplicity we consider a uniform rectangular mesh on the square $[-L,L]^2$ with mesh size $h = 2L/N$ (see Figure 2). Other geometries can be accommodated; however, approximation of the boundary conditions is less trivial [4]. Grid points are denoted by $x_{ij} = (ih, jh)$ and we adopt the standard notation $H^n_{ij} \approx H(x_{ij}, t^n)$, etc. A time step $t^{n+1} - t^n$ will be denoted by Δt^{n+1}, and for technical reasons, discussed in section 3, we allow for the possibility of variable time steps; however, it will always be assumed that the step size is monotone decreasing, i.e., $\Delta t^{n+1} \leq \Delta t^n$. An underscore will be used to denote a vector of mesh values $\underline{H}^n = \{H^n_{ij}\}$, etc., and we write $\underline{H}^n$ is bounded, or $\underline{H}^n \geq 0$, to convey that each component H^n_{ij} is bounded (uniformly in n) or nonnegative.

The basic ADI scheme is defined as

$$
(9) \qquad \begin{cases}
\frac{H_{ij}^{n+1/2}-H_{ij}^{n}}{\Delta t^{n+1}/2} &= D_H\left(\frac{\Delta_{xh}H_{ij}^{n+1/2}}{h^2}+\frac{\Delta_{yh}H_{ij}^{n}}{h^2}\right) - F_{1ij}^{n}H_{ij}^{n+1/2},\\
\frac{H_{ij}^{n+1}-H_{ij}^{n+1/2}}{\Delta t^{n+1}/2} &= D_H\left(\frac{\Delta_{xh}H_{ij}^{n+1/2}}{h^2}+\frac{\Delta_{yh}H_{ij}^{n+1}}{h^2}\right) - F_{1ij}^{n}H_{ij}^{n+1/2},\\
\frac{G_{ij}^{n+1/2}-G_{ij}^{n}}{\Delta t^{n+1}/2} &= D_G\left(\frac{\Delta_{xh}G_{ij}^{n+1/2}}{h^2}+\frac{\Delta_{yh}G_{ij}^{n}}{h^2}\right) - F_{2ij}^{n}G_{ij}^{n+1/2},\\
\frac{G_{ij}^{n+1}-G_{ij}^{n+1/2}}{\Delta t^{n+1}/2} &= D_G\left(\frac{\Delta_{xh}G_{ij}^{n+1/2}}{h^2}+\frac{\Delta_{yh}G_{ij}^{n+1}}{h^2}\right) - F_{2ij}^{n}G_{ij}^{n+1/2},
\end{cases}
$$

where Δ_{xh} and Δ_{yh} are the centered second-order difference operators such that

$$
(\Delta_{xh}+\Delta_{yh})H_{ij}^{n} = (H_{i+1j}^{n} - 2H_{ij}^{n} + H_{i-1j}^{n}) + (H_{ij+1}^{n} - 2H_{ij}^{n} + H_{ij-1}^{n}).
$$

The zero flux boundary condition is approximated by

$$
\begin{cases}
H_{iN+1}^{n} = H_{iN-1}^{n}, \quad H_{i(-1)}^{n} = H_{i1}^{n} \quad \text{for all } i,n, \quad \text{and}\\
H_{N+1j}^{n} = H_{N-1j}^{n}, \quad H_{(-1)j}^{n} = H_{1j}^{n} \quad \text{for all } j,n,
\end{cases}
$$

and similarly for G. In (9), the reaction terms are approximated by F_{1ij}^n and F_{2ij}^n, which will depend upon the discrete history $\{(G^m,H^m)\,|\,m=0,1/2,1,3/2,\ldots,n-1/2,n\}$.

The above scheme has two steps: one is implicit in x direction, and the next is implicit in y direction. While this is the basic idea of virtually all ADI schemes, the above decomposition of the reaction terms into an implicit and explicit part guarantees stability of the scheme.

The four equations in (9) can be expressed in matrix form as

$$
(10) \qquad \begin{cases}
(I + \delta^{n+1}A + D^n)\underline{H}^{n+1/2} = (I - \delta^{n+1}B)\underline{H}^{n},\\
(I + \delta^{n+1}B)\underline{H}^{n+1} = (I - \delta^{n+1}A - D^n)\underline{H}^{n+1/2},\\
(I + \delta'^{n+1}A + D'^n)\underline{G}^{n+1/2} = (I - \delta'^{n+1}B)\underline{G}^{n},\\
(I + \delta'^{n+1}B)\underline{G}^{n+1} = (I - \delta'^{n+1}A - D'^n)\underline{G}^{n+1/2},
\end{cases}
$$

where $\delta^{n+1} = D_H\Delta t^{n+1}/2h^2$ and $\delta'^{n+1} = D_G\Delta t^{n+1}/2h^2$, I is the identity matrix, D^n and D'^n are diagonal matrices whose diagonal elements are $\Delta t^{n+1}F_{1ij}^n/2$ and $\Delta t^{n+1}F_{2ij}^n/2$, respectively, and A and B are the standard discretization matrices obtained from finite difference operators $-\Delta_{xh}$, $-\Delta_{yh}$ with the zero flux boundary conditions. A and B are symmetric and nonnegative definite with respect to the discrete L^2 inner product $(.,.)_h$ on $\Re^{(N+1)\times(N+1)}$ determined by the midpoint rule

$$
(11) \qquad (G,H)_h = \sum_{i,j=0}^{N} h^2\gamma_i\gamma_j G_{ij}H_{ij},
$$

where $\gamma_i = 1/2$ if $i=0$ or $i=N$, and $\gamma_i = 1$ otherwise. The product $\gamma_i\gamma_j h^2$ is the area of the cell in Ω containing the point x_{ij}. In particular, $\|1\|_h^2 = |\Omega|$, where $\|.\|_h$ is the discrete L^2-norm associated with $(.,.)_h$.

2.2. Stability and convergence. To establish the stability of scheme (9), we recall the following well-known properties of real symmetric matrices. The proof can be obtained by following the same procedure as for the standard 2-norm [1].

LEMMA 2.1. *Let* $\mathtt{A}$ *be a real* $(M+1)\times(M+1)$ *matrix, symmetric with respect to the inner product* $(.,.)_h$*, and* $\{\lambda_i\}_{i=0}^M$ *be its eigenvalues. Then*

- $\|\mathtt{A}\|_h = \sigma(\mathtt{A}) = \max_{0\le i\le M}|\lambda_i|$.

And if, additionally, $\mathtt{A}$ *is nonnegative definite* ($\lambda_i \ge 0$)*, then*

- $(I-\mathtt{A})(I+\mathtt{A})^{-1}$ *is real symmetric,* $(I-\mathtt{A})(I+\mathtt{A})^{-1} = (I+\mathtt{A})^{-1}(I-\mathtt{A})$.
- $\sigma((I-\mathtt{A})(I+\mathtt{A})^{-1}) = \max_{0\le i\le M}|\frac{1-\lambda_i}{1+\lambda_i}| = \|(I-\mathtt{A})(I+\mathtt{A})^{-1}\|_h \le 1$.

We now establish stability of the ADI scheme (9).

LEMMA 2.2. *Solutions of the ADI scheme* (9) *satisfy*

(i) $\|(I+\delta^{n+1}B)\underline{H}^{n+1}\|_h \le \|(I+\delta^{n+1}B)\underline{H}^n\|_h$,

(ii) $\|(I+\delta'^{n+1}B)\underline{G}^{n+1}\|_h \le \|(I+\delta'^{n+1}B)\underline{G}^n\|_h$,

where $\delta^{n+1} = D_H\Delta t^{n+1}/h^2$, $\delta'^{n+1} = D_G\Delta t^{n+1}/h^2$*, and* B *is the matrix defined in* (10).

Proof. We will only show (i) since (ii) follows from the same line of argument. Let $\tilde{A}^n = \delta^{n+1}A + D^n$. Since A is nonnegative definite (with respect to $(.,.)_h$) and D^n is diagonal with nonnegative entries, $\tilde{A}^n$ is also symmetric and nonnegative definite. Combine the first two equations of (10) to get

$$\begin{aligned}(I+\delta^{n+1}B)\underline{H}^{n+1} &= (I-\tilde{A}^n)(I+\tilde{A}^n)^{-1}(I-\delta^{n+1}B)\underline{H}^n\\ &= (I-\tilde{A}^n)(I+\tilde{A}^n)^{-1}(I-\delta^{n+1}B)(I+\delta^{n+1}B)^{-1}(I+\delta^{n+1}B)\underline{H}^n.\end{aligned}$$

Taking the norm on both sides and using the Cauchy–Schwarz inequality, we have

$$\begin{aligned}\|(I+\delta^{n+1}B)\underline{H}^{n+1}\|_h \le \|(I-\tilde{A}^n)(I+\tilde{A}^n)^{-1}\|_h\|(I-\delta^{n+1}B)(I+\delta^{n+1}B)^{-1}\|_h\\ \cdot\|(I+\delta^{n+1}B)\underline{H}^n\|_h.\end{aligned}$$

The proof follows since Lemma 2.1 shows

$$\|(I-\tilde{A}^n)(I+\tilde{A}^n)^{-1}\|_h = \max_{1\le i\le (N+1)^2}\left|\frac{1-\mu_i}{1+\mu_i}\right| \le 1,$$

$$\|(I-\delta^{n+1}B)(I+\delta^{n+1}B)^{-1}\|_h = \max_{1\le i\le (N+1)^2}\left|\frac{1-\nu_i}{1+\nu_i}\right| \le 1,$$

where $\{\mu_i\}_{i=1}^{(N+1)^2}$ and $\{\nu_i\}_{i=1}^{(N+1)^2}$ are the nonnegative real eigenvalues of $\tilde{A}^n$ and $\delta^{n+1}B$, respectively. ∎

THEOREM 2.3 (stability). *Let* $\delta^n = D_H\Delta t^n/h^2$ *and* $\delta'^n = D_G\Delta t^n/h^2$*; then solutions of* (9) *satisfy*

(i) $\|\underline{H}^n\|_h \le \|(I+\delta^n B)\underline{H}^n\|_h \le \|(I+\delta^1 B)\underline{H}^0\|_h$,

(ii) $\|\underline{G}^n\|_h \le \|(I+\delta'^n B)\underline{G}^n\|_h \le \|(I+\delta'^1 B)\underline{G}^0\|_h$.

Remark. This theorem shows that $\underline{G}^n$ and $\underline{H}^n$ are bounded by a constant of order $\Delta t^1/h^2$. We then require $\Delta t^1/h^2 \le C$, where C is some constant. Note that this condition is quite different from the restriction $D\Delta t/h^2 < 1/2$ for the explicit scheme because we are allowed to choose a relatively large C (which can be much larger than $1/2D$). Computationally this makes a big difference. In our numerical experiments the difference is several days of computation versus several hours.

Proof. Again, we only need to show (i), since (ii) is proved similarly. Lemma 2.2 implies that

$$\|(I+\delta^n B)\underline{H}^n\|_h \le \|(I+\delta^n B)\underline{H}^{n-1}\|_h, \quad n = 1, 2, \ldots.$$

Since $\delta^n \le \delta^{n-1}$ we have

$$
\begin{aligned}
&\|(I+\delta^{n-1}B)\underline{H}^{n-1}\|_h^2\\
&= \|(I+\delta^n B)\underline{H}^{n-1} + (\delta^{n-1}-\delta^n)B\underline{H}^{n-1}\|_h^2\\
&= \|(I+\delta^n B)\underline{H}^{n-1}\|_h^2\\
&\quad +2(\delta^{n-1}-\delta^n)\left(B\underline{H}^{n-1},(I+\delta^n B)\underline{H}^{n-1}\right)_h + (\delta^{n-1}-\delta^n)^2\|B\underline{H}^{n-1}\|_h^2\\
&\ge \|(I+\delta^n B)\underline{H}^{n-1}\|_h^2.
\end{aligned}
$$

It follows that

$$\|(I+\delta^n B)\underline{H}^n\|_h \le \|(I+\delta^{n-1}B)\underline{H}^n\|_h \le \|(I+\delta^{n-1}B)\underline{H}^{n-1}\|_h \le \cdots \le \|(I+\delta^1 B)\underline{H}^0\|_h.$$

Note that $\|\underline{H}^n\|_h \le \|(I+\delta^n B)\underline{H}^n\|_h$, since B is symmetric and nonnegative definite, so that

$$\|\underline{H}^n\|_h \le \|(I+\delta^n B)\underline{H}^n\|_h \le \|(I+\delta^1 B)\underline{H}^0\|_h \quad \text{for all } n. \qquad \square$$

Letting $\tilde{H}(x_{ij},t^n)$ and $\tilde{G}(x_{ij},t^n)$ be the exact solutions at x_{ij} and t^n, the following lemma establishes the consistency of algorithm (9).

LEMMA 2.4 (consistency). *Assume that the solution of* (5) *is of class C^4; then*

$$
\text{(12)}\quad
\begin{cases}
\frac{\tilde{H}_{ij}^{n+1/2}-\tilde{H}_{ij}^n}{\Delta t^{n+1}/2} &= D_H\left(\frac{\Delta_{xh}\tilde{H}_{ij}^{n+1/2}}{h^2}+\frac{\Delta_{yh}\tilde{H}_{ij}^n}{h^2}\right) - \tilde{F}_{1ij}^n\tilde{H}_{ij}^{n+1/2} + r_{ij}^{n+1/2},\\
\frac{\tilde{H}_{ij}^{n+1}-\tilde{H}_{ij}^{n+1/2}}{\Delta t^{n+1}/2} &= D_H\left(\frac{\Delta_{xh}\tilde{H}_{ij}^{n+1/2}}{h^2}+\frac{\Delta_{yh}\tilde{H}_{ij}^{n+1}}{h^2}\right) - \tilde{F}_{1ij}^n\tilde{H}_{ij}^{n+1/2} + r_{ij}^{n+1},\\
\frac{\tilde{G}_{ij}^{n+1/2}-\tilde{G}_{ij}^n}{\Delta t^{n+1}/2} &= D_G\left(\frac{\Delta_{xh}\tilde{G}_{ij}^{n+1/2}}{h^2}+\frac{\Delta_{yh}\tilde{G}_{ij}^n}{h^2}\right) - \tilde{F}_{2ij}^n\tilde{G}_{ij}^{n+1/2} + s_{ij}^{n+1/2},\\
\frac{\tilde{G}_{ij}^{n+1}-\tilde{G}_{ij}^{n+1/2}}{\Delta t^{n+1}/2} &= D_G\left(\frac{\Delta_{xh}\tilde{G}_{ij}^{n+1/2}}{h^2}+\frac{\Delta_{yh}\tilde{G}_{ij}^{n+1}}{h^2}\right) - \tilde{F}_{2ij}^n\tilde{G}_{ij}^{n+1/2} + s_{ij}^{n+1},
\end{cases}
$$

where

$$s_{ij}^{n+1/2}, s_{ij}^{n+1}, r_{ij}^{n+1/2}, r_{ij}^{n+1} \simeq \begin{cases} O(\Delta t^{n+1}+h^2) & \textit{if } ij \textit{ is an interior point,}\\ O(\Delta t^{n+1}+h) & \textit{if } ij \textit{ is a boundary point.}\end{cases}$$

Remark. The above shows that the classical treatment of the Neumann boundary condition, while retaining symmetry of the discrete equations, results in a loss of accuracy. It is interesting to note that this problem does not arise in the finite element method due to the different treatment of the nonhomogeneous terms and nondiagonal "mass" matrix.

Proof. The proof follows directly by Taylor expansions.

$$\frac{\tilde{H}_{ij}^{n+1/2}-\tilde{H}_{ij}^n}{\Delta t^{n+1}/2} = (\tilde{H}_t)_{ij}^n + O(\Delta t^{n+1}) \quad \text{for all } ij,$$

$$\Delta_{xh}\tilde{H}_{ij}^n = \begin{cases} (\tilde{H}_{xx})_{ij}^n + O(h^2) & \text{if } i \text{ is an interior index,}\\ (\tilde{H}_{xx})_{ij}^n + O(h) & \text{if } i \text{ is a boundary index.}\end{cases}$$

Similar expansions also hold for $\Delta_{yh}\tilde{H}_{ij}^{n+\frac{1}{2}}$ as well as the other concentration function G. $\square$

THEOREM 2.5 (convergence). *Assume that a solution* $(\tilde{G}, \tilde{H})$ *of* (5) *is of class* C^4, *and let* (G, H) *denote the solution of the ADI scheme* (9), *where the time steps are nonincreasing* ($\Delta t^{n+1} \le \Delta t^n$). *Define the errors* $\underline{E}_H^n = \underline{\tilde{H}}^n - \underline{H}^n$, $\underline{E}_H^{n+1/2} = \underline{\tilde{H}}^{n+1/2} - \underline{H}^{n+1/2}$, *and* $\underline{E}_G^n$, $\underline{E}_G^{n+1/2}$ *similarly. Then for* $T > 0$ *fixed and any* n *such that* $\sum_{j=1}^n \Delta t^j \le T$,

$$\|\underline{E}_H^{n+1/2}\|_h + \|\underline{E}_H^{n+1}\|_h \le 2\|(I + \delta^1 B)\underline{E}_H^0\|_h + C\sum_{j=0}^{n} \Delta t^{j+1}\left(\|\underline{\tilde{F}}_1^j - \underline{F}_1^j\|_h + \epsilon^{j+1}\right),$$

$$\|\underline{E}_G^{n+1/2}\|_h + \|\underline{E}_G^{n+1}\|_h \le 2\|(I + \delta^1 B)\underline{E}_G^0\|_h + C\sum_{j=0}^{n} \Delta t^{j+1}\left(\|\underline{\tilde{F}}_2^j - \underline{F}_2^j\|_h + \epsilon^{j+1}\right),$$

where $C = C(\Omega, T, \tilde{G}, \tilde{H})$ *and* $\epsilon^j = O(\Delta t^j + h^{3/2})$.

Proof. Again, we only establish the estimates for H, since the estimates on G follow similarly. The consistency lemma shows that

$$\left\{\begin{array}{rcl} (I + \delta^{n+1}A + \tilde{D}^n)\underline{\tilde{H}}^{n+1/2} &=& (I - \delta^{n+1}B)\underline{\tilde{H}}^n + \Delta t^{n+1}\underline{R}^{n+1/2}, \\ (I + \delta^{n+1}B)\underline{\tilde{H}}^{n+1} &=& (I - \delta^{n+1}A - \tilde{D}^n)\underline{\tilde{H}}^{n+1/2} + \Delta t^{n+1}\underline{R}^{n+1}, \end{array}\right. \tag{13}$$

where $\tilde{D}^n$ is a diagonal matrix whose diagonal elements are $(1/2)\Delta t^{n+1}\tilde{F}_{1ij}^n$, and $R_{ij}^{n+1/2} = (1/2)r_{ij}^{n+1/2}$, $R_{ij}^{n+1} = (1/2)r_{ij}^{n+1}$. Then

$$\left\{\begin{array}{l} (I + \delta^{n+1}A + D^n)\underline{E}_H^{n+1/2} = (I - \delta^{n+1}B)\underline{E}_H^n - (\tilde{D}^n - D^n)\underline{\tilde{H}}^{n+1/2} + \Delta t^{n+1}\underline{R}^{n+1/2}, \\ (I + \delta^{n+1}B)\underline{E}_H^{n+1} = (I - \delta^{n+1}A - D^n)\underline{E}_H^{n+1/2} - (\tilde{D}^n - D^n)\underline{\tilde{H}}^{n+1/2} + \Delta t^{n+1}\underline{R}^{n+1}. \end{array}\right.$$

Writing

$$\underline{E}_H^{n+1/2} = (I + \tilde{A}^n)^{-1}\left[(I - \delta^{n+1}B)\underline{E}_H^n - (\tilde{D}^n - D^n)\underline{\tilde{H}}^{n+1/2} + \Delta t^{n+1}\underline{R}^{n+1/2}\right] \tag{14}$$

we obtain

$$\begin{aligned} &(I + \delta^{n+1}B)\underline{E}_H^{n+1} \\ &\quad = (I - \tilde{A}^n)(I + \tilde{A}^n)^{-1}(I - \delta^{n+1}B)(I + \delta^{n+1}B)^{-1}(I + \delta^{n+1}B)\underline{E}_H^n \\ &\qquad - \left[I + (I - \tilde{A}^n)(I + \tilde{A}^n)^{-1}\right](\tilde{D}^n - D^n)\underline{\tilde{H}}^{n+1/2} \\ &\qquad + \Delta t^{n+1}\left[(I - \tilde{A}^n)(I + \tilde{A}^n)^{-1}\underline{R}^{n+1/2} + \underline{R}^{n+1}\right]. \end{aligned}$$

Note that $\|(\tilde{D}^n - D^n)\underline{\tilde{H}}^{n+1/2}\|_h \le (1/2)\Delta t^{n+1}\|\underline{\tilde{H}}^{n+1/2}\|_\infty \|\underline{\tilde{F}}_1^n - \underline{F}_1^n\|_h$, and

$$\|\underline{R}^n\|_h^2 = \sum_{x_{ij}\in\Omega} h^2 (r_{ij}^n)^2 + \sum_{x_{ij}\in\partial\Omega} \gamma_i\gamma_j h^2 (r_{ij}^n)^2 = \left(O(\Delta t^n + h^{3/2})\right)^2,$$

since there are only $O(1/h)$ boundary points where $r_{ij}^n = O(\Delta t^n + h)$. Recalling Lemma 2.1, we now obtain

$$\begin{aligned} \|(I + \delta^{n+1}B)\underline{E}_H^{n+1}\|_h &\le \|(I + \delta^{n+1}B)\underline{E}_H^n\|_h + C\Delta t^{n+1}\left(\|\underline{\tilde{F}}_1^n - \underline{F}_1^n\|_h + \epsilon^{n+1}\right) \\ &\le \|(I + \delta^n B)\underline{E}_H^n\|_h + C\Delta t^{n+1}\left(\|\underline{\tilde{F}}_1^n - \underline{F}_1^n\|_h + \epsilon^{n+1}\right), \end{aligned}$$

where $\epsilon^{n+1} = \|(I - \tilde{A}^n)(I + \tilde{A}^n)^{-1}\underline{R}^{n+1/2} + \underline{R}^{n+1}\|_h = O(\Delta t^{n+1} + h^{3/2})$. Summing this gives

$$\|\underline{E}_H^{n+1}\|_h \leq \|(I+\delta^{n+1}B)\underline{E}_H^{n+1}\|_h \leq \|(I+\delta^1 B)\underline{E}_H^0\|_h + C\sum_{j=0}^{n} \Delta t^{j+1}\left(\|\underline{\tilde{F}}_1^j - \underline{F}_1^j\|_h + \epsilon^{j+1}\right).$$

Substituting this into (14), we obtain a similar bound on the half-step errors

$$\|\underline{E}_H^{n+1/2}\|_h \leq \|(I + \delta^1 B)\underline{E}_H^0\|_h + C\sum_{j=0}^{n} \Delta t^{j+1}\left(\|\underline{\tilde{F}}_1^j - \underline{F}_1^j\|_h + \epsilon^{j+1}\right). \qquad \square$$

COROLLARY 2.6. *Let F_1, $F_2 : \Re^2 \to \Re$ be Lipschitz functions; i.e., the reaction terms F_1 and F_2 depend only upon the current value of (G, H), and for $n = 1, 2, \ldots$ let*

$$\alpha_{n+1} = \|\underline{E}_H^{n+1}\|_h + \|\underline{E}_H^{n+1/2}\|_h + \|\underline{E}_G^{n+1}\|_h + \|\underline{E}_G^{n+1/2}\|_h,$$

and

$$\alpha_0 = 2\left(\|(I + \delta^1 B)\underline{E}_H^0\|_h + \|(I + \delta^1 B)\underline{E}_G^0\|_h\right).$$

Then for $T > 0$ fixed and any n such that $\sum_{j=0}^n \Delta t^{j+1} \leq T$

$$\alpha_n \leq (\alpha_0 + e^n)e^{CT},$$

where $e^n = TO(\Delta t + h^{3/2})$.

Proof. The Lipschitz hypothesis enables the conclusion of Theorem 2.5 to be written as

$$\alpha_j \leq \alpha_0 + C\sum_{j=0}^{n} \Delta t^{j+1}(\alpha_j + \epsilon^{j+1}).$$

Letting $e^{n+1} = C\sum_{j=0}^n \Delta t^{j+1}\epsilon^{j+1} = T\,O(\Delta t + h^{3/2})$, one has $e^{n+1} \geq e^n$ and

$$\alpha_{n+1} \leq (\alpha_0 + e^{n+1}) + C\sum_{j=0}^{n} \Delta t^{j+1}\alpha_j.$$

An elementary induction argument can now be used to establish the discrete Gronwall estimate

$$\alpha_{n+1} \leq (\alpha_0 + e^{n+1})\prod_{j=0}^{n}(1 + C\Delta t^{j+1}) \leq (\alpha_0 + e^{n+1})e^{CT}. \qquad \square$$

COROLLARY 2.7. *For $j = 1, 3, \ldots$ let*

$$\alpha_{n+1} = \|\underline{E}_H^{n+1}\|_h + \|\underline{E}_H^{n+1/2}\|_h + \|\underline{E}_G^{n+1}\|_h + \|\underline{E}_G^{n+1/2}\|_h,$$

and

$$\alpha_0 = 2(\|(I + \delta^1 B)\underline{E}_H^0\|_h + \|(I + \delta^1 B)\underline{E}_G^0\|_h).$$

Assume that there exists $\hat{\alpha}_0 \geq 0$ and $\hat{\epsilon}^j$ of size $O(\Delta t^j + h^{3/2})$ such that the error in the reaction terms is bounded by

$$\|\underline{\tilde{F}}_1^j - \underline{F}_1^j\|_h + \|\underline{\tilde{F}}_2^j - \underline{F}_2^j\|_h \leq \hat{\alpha}_0 + C\sum_{k=1}^{j} \Delta t^k(\alpha_k + \hat{\epsilon}^k).$$

Then for $T > 0$ fixed and any n such that $\sum_{j=1}^{n+1} \Delta t^j \le T$

$$\alpha_n \le (\alpha_0 + CT^2\hat{\alpha}_0 + e^n)e^{CT^2},$$

where $e^n = T\,O(\Delta t + h^{3/2})$.

Proof. Substituting the bound for the reaction terms into the estimates of Theorem 2.5 gives

$$\begin{aligned}\alpha_{n+1} &\le \alpha_0 + C\sum_{j=0}^{n}\Delta t^{j+1}\left(\hat{\alpha}_0 + C\sum_{k=1}^{j}\Delta t^k(\alpha_k + \hat{\epsilon}^k) + \epsilon^{j+1}\right)\\ &\le \alpha_0 + C\cdot T\hat{\alpha}_0 + e^{n+1} + C^2T\sum_{k=1}^{n}\Delta t^k\alpha_k,\end{aligned}$$

where

$$\begin{aligned}e^{n+1} &= C\sum_{j=0}^{n}\Delta t^{j+1}\epsilon^{j+1} + C^2\sum_{j=1}^{n}\Delta t^{j+1}\sum_{k=1}^{j}\Delta t^k\hat{\epsilon}^k\\ &\le C\sum_{j=0}^{n}\Delta t^{j+1}\epsilon^{j+1} + C^2T\sum_{k=1}^{n}\Delta t^k\hat{\epsilon}^k\\ &= T\cdot O(\Delta t + h^{3/2}).\end{aligned}$$

The estimate now follows from the discrete Gronwall inequality stated in the proof of the previous corollary. ∎

3. An ADI method for the 2×2 hysteretic reaction-diffusion systems.

In this section, we consider the 2×2 hysteretic reaction-diffusion system as given in the Introduction.

$$(15)\qquad \begin{cases} \dfrac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} -a & b \\ a & -b \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} + \begin{pmatrix} fu \\ 0 \end{pmatrix}, \\[2ex] \dfrac{\partial}{\partial t}\begin{pmatrix} H \\ G \end{pmatrix} = \begin{pmatrix} D_H & 0 \\ 0 & D_G \end{pmatrix}\begin{pmatrix} \Delta H \\ \Delta G \end{pmatrix} - \begin{pmatrix} fu/Y_H \\ fu/Y_G \end{pmatrix}. \end{cases}$$

We use the following ADI method for this system:

$$(16)\qquad \begin{cases} \frac{H_{ij}^{n+1/2} - H_{ij}^n}{\Delta t^{n+1}/2} = D_H\left(\frac{\Delta_{xh}H_{ij}^{n+1/2}}{h^2} + \frac{\Delta_{yh}H_{ij}^n}{h^2}\right) - \frac{u_{ij}^n p_{ij}^n}{Y_H}H_{ij}^{n+1/2}, \\ \frac{H_{ij}^{n+1} - H_{ij}^{n+1/2}}{\Delta t^{n+1}/2} = D_H\left(\frac{\Delta_{xh}H_{ij}^{n+1/2}}{h^2} + \frac{\Delta_{yh}H_{ij}^{n+1}}{h^2}\right) - \frac{u_{ij}^n p_{ij}^n}{Y_H}H_{ij}^{n+1/2}, \\ \frac{G_{ij}^{n+1/2} - G_{ij}^n}{\Delta t^{n+1}/2} = D_G\left(\frac{\Delta_{xh}G_{ij}^{n+1/2}}{h^2} + \frac{\Delta_{yh}G_{ij}^n}{h^2}\right) - \frac{u_{ij}^n q_{ij}^n}{Y_G}G_{ij}^{n+1/2}, \\ \frac{G_{ij}^{n+1} - G_{ij}^{n+1/2}}{\Delta t^{n+1}/2} = D_G\left(\frac{\Delta_{xh}G_{ij}^{n+1/2}}{h^2} + \frac{\Delta_{yh}G_{ij}^{n+1}}{h^2}\right) - \frac{u_{ij}^n q_{ij}^n}{Y_G}G_{ij}^{n+1/2}, \\ \frac{u_{ij}^{n+1} - u_{ij}^n}{\Delta t^{n+1}} = f_{ij}^{n+1/2}u_{ij}^n - a_{ij}^{n+1}u_{ij}^{n+1} + b_{ij}^{n+1}v_{ij}^n, \\ \frac{v_{ij}^{n+1} - v_{ij}^n}{\Delta t^{n+1}} = a_{ij}^{n+1}u_{ij}^{n+1} - b_{ij}^{n+1}v_{ij}^n. \end{cases}$$

The notation used here is the same as in the previous section, and

$$f_{ij}^n = f((G_{ij}^n)^+(H_{ij}^n)^+), \quad a_{ij}^n = a((G_{ij}^n)^+(H_{ij}^n)^+), \quad \text{and} \quad b_{ij}^n = b((G_{ij}^n)^+(H_{ij}^n)^+).$$

The terms p_{ij}^n, q_{ij}^n are given by

$$\begin{cases} p_{ij}^n \;=\; \frac{V_0(G_{ij}^n)^+}{K_0+(G_{ij}^n)^+(H_{ij}^n)^+}, \quad q_{ij}^n \;=\; \frac{V_0(H_{ij}^n)^+}{K_0+(G_{ij}^n)^+(H_{ij}^n)^+} & \text{if } f_{ij}^n = \frac{V_0(G_{ij}^n)^+(H_{ij}^n)^+}{K_0+(G_{ij}^n)^+(H_{ij}^n)^+} \neq 0, \\ p_{ij}^n \;=\; q_{ij}^n \;=\; 0 & \text{otherwise,} \end{cases}$$

and $f_{ij}^{n+1/2}$ is defined by

$$f_{ij}^{n+1/2} \;=\; \frac{1}{2}(p_{ij}^n H_{ij}^{n+1/2} \;+\; q_{ij}^n G_{ij}^{n+1/2}).$$

Here, the $+$ superscript indicates the positive part ($a^+ = a$ if $a \geq 0$ and zero otherwise). The first four equations in (16) can be expressed in matrix form as

$$(17) \qquad \begin{cases} (I \,+\, \delta^{n+1}A \,+\, D^n)\underline{H}^{n+1/2} \;=\; (I \,-\, \delta^{n+1}B)\underline{H}^n, \\ (I \,+\, \delta^{n+1}B)\underline{H}^{n+1} \;=\; (I \,-\, \delta^{n+1}A \,-\, D^n)\underline{H}^{n+1/2}, \\ (I \,+\, \delta'^{n+1}A \,+\, D'^n)\underline{G}^{n+1/2} \;=\; (I \,-\, \delta'^{n+1}B)\underline{G}^n, \\ (I \,+\, \delta'^{n+1}B)\underline{G}^{n+1} \;=\; (I \,-\, \delta'^{n+1}A \,-\, (D^{'})^n)\underline{G}^{n+1/2}. \end{cases}$$

The notation used is the same as in (10) and D^n and $(D^{'})^n$ are diagonal matrices whose diagonal elements are $\Delta t^{n+1}u_{ij}^n p_{ij}^n/2Y_H$ and $\Delta t^{n+1}u_{ij}^n q_{ij}^n/2Y_G$, respectively. Note that the stability result given in Theorem 2.3 is still valid for (17).

In [5] we showed that if the initial data for the continuous problem are nonnegative, then so, too, is (each component of) the solution. Also, nonnegativity of the solution and the conservation property (see below) were vital ingredients for the characterization of the longtime behavior. Unfortunately, nonnegativity of the initial data for the ADI scheme may not be preserved, and this causes problems when attempting to characterize the longtime behavior of the discrete problem. Note that we could guarantee that $\underline{u}^n$ and $\underline{v}^n$ remained nonnegative by truncating $f_{ij}^{n+1/2}$ at zero; however, this would destroy the discrete conservation property Theorem 3.2. We will show that nonnegativity of $\underline{u}^n$ and $\underline{v}^n$ will be preserved provided the time step is chosen sufficiently small. Since a suitable step size is not known a priori, we consider the following modification of the basic ADI scheme.

- Select an initial step size Δt^0 and nonnegative initial data G^0, H^0, u^0, and v^0.
- For $n = 0, 1, 2, \ldots$
  - let $\Delta t^{n+1} = \Delta t^n$.
  - Calculate $(G^{n+1}, H^{n+1}, u^{n+1}, v^{n+1})$ using the ADI scheme (16).
  - If (u^{n+1}, v^{n+1}) are nonnegative, continue. Otherwise, discard these updated values, reduce Δt^{n+1}, and repeat the previous step.

We show below that, for a fixed mesh size, Δt will remain bounded away from zero, and the nonnegativity of (u^n, v^n) will allow us to establish longtime behavior analogous to the continuous problem. Note that initial transients may cause the solution to change rapidly, causing the time step to initially be reduced to an undesirably small value that would not otherwise be necessary. Examination of the proofs below shows that they remain valid if Δt is arbitrarily increased at a finite number of times, so the step size can be adjusted upwards when the solution settles down.

3.1. Large time asymptotics. We begin by showing that if $\underline{f}^{n+1/2}$ is bounded independently of n, then there is a step size Δt that guarantees $\underline{u}^n$ and $\underline{v}^n$ will be nonnegative.

LEMMA 3.1. *Assume that there is a (lower) bound $\hat{f} \geq 0$ such that $f_{ij}^{n+1/2} \geq -\hat{f}$, for all ij, n, and let the initial data $\underline{u}^0$ and $\underline{v}^0$ be nonnegative. If $\Delta t^{n+1} \max(b_{max}, \hat{f}) < 1$, then*

$$u_{ij}^n \geq 0, \quad v_{ij}^n \geq 0, \quad \textit{for all } ij,\ n,$$

where $b_{max} = \max_{\alpha>0} b(\alpha) = \lim_{\alpha\to\infty} b(\alpha)$ is defined in section 1.

Proof. Rearranging the last two equations of (16) gives

$$\begin{cases} u_{ij}^{n+1} &=& \frac{(1+\Delta t^{n+1} f_{ij}^{n+1/2})u_{ij}^n + \Delta t^{n+1} b_{ij}^{n+1} v_{ij}^n}{1+\Delta t^{n+1} a_{ij}^{n+1}}, \\ v_{ij}^{n+1} &=& \Delta t^{n+1} a_{ij}^{n+1} u_{ij}^{n+1} + (1-\Delta t^{n+1} b_{ij}^{n+1}) v_{ij}^n. \end{cases}$$

By hypotheses $(1+\Delta t f_{ij}^{n+1/2})$ and $(1-\Delta t b_{ij}^{n+1})$ are nonnegative, so that (u^{n+1}, v^{n+1}) will be nonnegative provided (u^n, v^n) is likewise nonnegative. ∎

Remark. Note that $\underline{f}^{n+1/2}$ approximates f which is nonnegative, and since the ADI is a first-order consistent scheme, we expect $\hat{f} \leq O(\Delta t + h)$. In this case, the only real restriction on the time step is $\Delta t \leq 1/b_{max}$.

We next establish the discrete version of the conservation of mass.

THEOREM 3.2. *Let $U_{ij}^n = u_{ij}^n + v_{ij}^n$ be the total numerical cell density. Then for $n = 0, 1, 2, \ldots$*

$$\sum_{i,j=0}^{N} \gamma_i\gamma_j \left(\frac{Y_H H_{ij}^{n+1} + Y_G G_{ij}^{n+1}}{2} + U_{ij}^{n+1} \right) = \sum_{i,j=0}^{N} \gamma_i\gamma_j \left(\frac{Y_H H_{ij}^{n} + Y_G G_{ij}^{n}}{2} + U_{ij}^{n} \right).$$

(*Recall that $\gamma_i = 1$ if $1 \leq i \leq N-1$ and $\gamma_i = 1/2$ for $i = 0$ and $i = N$.*)

Proof. The (discrete) Neumann boundary conditions guarantee that

$$\sum_{i=0}^{N} \gamma_i (H_{i-1j}^n - 2H_{ij}^n + H_{i+1j}^n) = 0,$$
$$\sum_{j=0}^{N} \gamma_j (H_{ij-1}^n - 2H_{ij}^n + H_{ij+1}^n) = 0,$$

and similarly for G. Multiplying the first four equations of (16) by $\Delta t^{n+1}/2$ and summing over all indices gives

$$\begin{cases} \sum_{i,j=0}^N \gamma_i\gamma_j G_{ij}^{n+1} &=& \sum_{i,j=0}^N \gamma_i\gamma_j G_{ij}^{n} - \sum_{i,j=0}^N \gamma_i\gamma_j \Delta t^{n+1} \frac{u_{ij}^n q_{ij}^n}{Y_G} G_{ij}^{n+1/2}, \\ \sum_{i,j=0}^N \gamma_i\gamma_j H_{ij}^{n+1} &=& \sum_{i,j=0}^N \gamma_i\gamma_j H_{ij}^{n} - \sum_{i,j=0}^N \gamma_i\gamma_j \Delta t^{n+1} \frac{u_{ij}^n p_{ij}^n}{Y_H} H_{ij}^{n+1/2}. \end{cases}$$

These two equations show that

$$\sum_{i,j=0}^{N} \gamma_i\gamma_j (Y_G G_{ij}^{n+1} + Y_H H_{ij}^{n+1})/2$$
$$= \sum_{i,j=0}^{N} \gamma_i\gamma_j (Y_G G_{ij}^{n} + Y_H H_{ij}^{n})/2 - \sum_{i,j=0}^{N} \gamma_i\gamma_j \Delta t^{n+1} f_{ij}^{n+1/2} u_{ij}^n.$$

Summing the last two equations of (16) over all indices gives

$$\sum_{i,j=0}^{N} \gamma_i\gamma_j(u_{ij}^{n+1}+v_{ij}^{n+1}) = \sum_{i,j=0}^{N} \gamma_i\gamma_j(u_{ij}^{n}+v_{ij}^{n}) + \sum_{i,j=0}^{N} \gamma_i\gamma_j \Delta t^{n+1} f_{ij}^{n+1/2} u_{ij}^{n}.$$

Adding these two equations establishes the theorem. ∎

COROLLARY 3.3. *Let the initial data* $\underline{u}^0$ *and* $\underline{v}^0$ *be nonnegative. Then for* h *fixed and* $\Delta t^0/h^2 \le C_\delta$, $\{H_{ij}^n\}$, $\{G_{ij}^n\}$, $\{H_{ij}^{n+1/2}\}$, $\{G_{ij}^{n+1/2}\}$, $\{u_{ij}^n\}$, *and* $\{v_{ij}^n\}$ *are all bounded independently of* n. *The bounds depend only upon* Ω *and the initial data.*

Proof. Boundedness of $\{H_{ij}^n\}$ and $\{G_{ij}^n\}$ follows from Theorem 2.3. The conservation of mass (Theorem 3.2) and the nonnegativity of $\underline{u}^n$ and $\underline{v}^n$ then show that $\underline{u}^n$ and $\underline{v}^n$ are also bounded. For the half-step sequences we consider the first equation in (10)

$$\begin{aligned}\underline{H}^{n+1/2} &= (I+\delta^{n+1}A+D^n)^{-1}(I-\delta^{n+1}B)\underline{H}^n \\ &= (I+\delta^{n+1}A+D^n)^{-1}(I-\delta^{n+1}B)(I+\delta^{n+1}B)^{-1}(I+\delta^{n+1}B)\underline{H}^n.\end{aligned}$$

Now, apply Lemma 2.1 and Theorem 2.3 to obtain

$$\begin{aligned}\|\underline{H}^{n+1/2}\|_h &\le \|(I+\tilde{A}^n)^{-1}\|_h\, \|(I-\delta^{n+1}B)(I+\delta^{n+1}B)^{-1}\|_h\, \|(I+\delta^{n+1}B)\underline{H}^n\|_h \\ &\le \sigma((I+\tilde{A}^n)^{-1})\, \|(I+\delta^{n+1}B)\underline{H}^n\|_h \\ &\le \|(I+\delta^0 B)\underline{H}^0\|_h.\end{aligned}$$

A similar estimate holds for G so that $\{G_{ij}^{n+1/2}\}$ and $\{H_{ij}^{n+1/2}\}$ are also bounded. ∎

At this point we can show that for h fixed, the assumptions of Lemma 3.1 will be valid so that our procedure for selecting Δt will be successful in the sense that the step sizes are bounded away from zero.

COROLLARY 3.4. *The half-step values* $\{f_{ij}^{n+1/2}\}$ *are bounded uniformly in* n *by a constant of the form* C/h^2, *where* C *depends upon the domain* Ω, *the initial data, and* $C_\delta \equiv \Delta t^0/h^2$. *Therefore, the minimum time step required to guarantee nonnegativity of* $\underline{u}^n$ *and* $\underline{v}^n$ *is proportional to* h^2.

Proof. It is clear that a pointwise bound $\mathcal{B}$ on $\underline{G}^n$, $\underline{G}^{n+1/2}$, $\underline{H}^n$, and $\underline{H}^{n+1/2}$ implies a bound on $\underline{f}^{n+1/2}$ of size $\mathcal{B}^2$. The pointwise bounds on $\underline{G}^n$, etc. are derived from uniform bounds on their $\|.\|_h$ norms, and since $\max_{ij}|H_{ij}| \le \|\underline{H}\|_h/h$, it follows that $\mathcal{B} \simeq 1/h$. Lemma 3.1 now shows that $\underline{u}^n$ and $\underline{v}^n$ will be nonnegative with a time step size bounded away from zero. ∎

In [5] we have shown that the densities of nutrient and buffer, H and G, respectively, tend to constants and that the active cell density u vanishes as $t \to \infty$, so that a (steady state) pattern is formed by inactive cells v. We next establish the corresponding results for the discrete scheme. That is, $\underline{H}^n$ and $\underline{G}^n$ converge to constant vectors (i.e., each component has the same value); $\underline{u}^n$ vanishes as $n \to \infty$, and $b_{ij}^n v_{ij}^n \to 0$ for every index pair ij.

We begin with a lemma which lists some basic properties of the matrices A and B. In the sequel we will identify the components of a vector of nodal values by their position on the mesh. For example, we say that $\underline{w}$ is constant on rows if for each index i, $w_{ij} = w_{ik}$, $0 \le j, k, \le N$.

LEMMA 3.5. *Let A and B be the two matrices obtained by the second-order central difference operators $-\Delta_{xh}$ and $-\Delta_{yh}$, respectively, with zero flux boundary condition. Then*

(i) *A and B are both real, symmetric, and nonnegative definite with respect to the inner product $(.,.)_h$ (see (11)).*

(ii) *The smallest eigenvalue of A and B is zero. The eigenvectors of A corresponding to zero eigenvalues are constant on rows. The eigenvectors of B corresponding to the zero eigenvalues are constant on columns of the mesh.*

Proof. The lemma follows directly from the structure of A and B. Up to a permutation of the variables, A and B are block diagonal matrices of the form

$$A = \begin{pmatrix} A_0 & & & \\ & A_1 & & \\ & & \ddots & \\ & & & A_N \end{pmatrix}, \quad A_i = \begin{pmatrix} 2 & -2 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -2 & 2 \end{pmatrix}, \quad i = 0, 1, \ldots, N.$$

Each of the diagonal blocks is the natural discretization of the second derivative with Neumann boundary conditions in one dimension, and it is clear that each block has exactly one zero eigenvalue with corresponding constant eigenvector. □

THEOREM 3.6. *Let the initial data $\underline{u}^0$ and $\underline{v}^0$ be nonnegative; then the discrete concentrations $\underline{G}^n$ and $\underline{H}^n$ calculated by the ADI scheme (16) converge to constant vectors as $n \to \infty$, i.e.,*

$$\underline{H}^n \to \underline{H} \qquad \textit{and} \qquad \underline{G}^n \to \underline{G},$$

where $\underline{H}$ and $\underline{G}$ are constant vectors. Moreover, $\underline{u}^n \to 0$ and $b_{ij}^n v_{ij}^n \to 0$ as $n \to \infty$ for all ij.

Proof. Let $\underline{w}^n = (I + \delta^{n+1} B)\underline{H}^n$, and recall that

$$\underline{w}^{n+1} = (I - \tilde{A}^n)(I + \tilde{A}^n)^{-1}(I - \delta^{n+1} B)(I + \delta^{n+1} B)^{-1}\underline{w}^n,$$

where $\tilde{A}^n = \delta^{n+1} A + D^n$, D^n being a nonnegative diagonal matrix. Corollary 3.3 shows that $\{\underline{H}^n\}$ (and hence $\{\underline{w}^n\}$) and $\{D^n\}$ are bounded independently of n. We may then pass to a subsequence $\{n_k\}_{k=1}^{\infty}$ such that $\underline{w}^{n_k} \to \underline{w}$ and $\tilde{A}^{n_k} = \delta^{n_k+1} A + D^{n_k} \to \tilde{A} = \delta^{\infty} A + D$, where D is a nonnegative diagonal matrix, and δ^{∞} is the final value of δ^n and is determined by the minimum time step size Δt^{∞} required to guarantee that u^n and v^n remain nonnegative. Note that $\{\|\underline{w}^n\|_h\}$ is a nonincreasing sequence so that

$$\begin{aligned} \|\underline{w}\|_h &= \lim_{k\to\infty} \|\underline{w}^{n_{(k+1)}}\|_h \\ &\le \lim_{k\to\infty} \|\underline{w}^{n_k+1}\|_h \\ &\le \lim_{k\to\infty} \|(I - \tilde{A}^{n_k})(I + \tilde{A}^{n_k})^{-1}(I - \delta^{n+1} B)(I + \delta^{n+1} B)^{-1}\underline{w}^{n_k}\|_h \\ &\le \|(I - \tilde{A})(I + \tilde{A})^{-1}(I - \delta^{\infty} B)(I + \delta^{\infty} B)^{-1}\underline{w}\|_h. \end{aligned}$$

Observe that since $\|(I - \tilde{A})(I + \tilde{A})^{-1}\|_h \le 1$ it follows that

$$\|\underline{w}\|_h \le \|(I - \delta^{\infty} B)(I + \delta^{\infty} B)^{-1}\underline{w}\|_h.$$

If $\{(\underline{x}_i, \lambda_i)\}$ are the eigenvector/eigenvalues of $\delta^\infty B$, and we expand $\underline{w} = \sum w_i \underline{x}_i$ in terms of the eigenvectors, then

$$\|\underline{w}\|_h^2 = \sum_i w_i^2 \leq \sum_i \left(\frac{1-\lambda_i}{1+\lambda_i}\right)^2 w_i^2 = \|(I - \delta^\infty B)(I + \delta^\infty B)^{-1}\underline{w}\|_h^2.$$

Since $\lambda_i \geq 0$, it follows that the only possible nonzero coefficients w_i in the expansion for $\underline{w}$ are those corresponding to zero eigenvalues of $\delta^\infty B$. Since the eigenvectors corresponding to the zero eigenvalues are column constant by Lemma 3.5, it follows that $\underline{w}$ must be a column-constant vector. Then $\underline{H}^n \to \underline{H}$ with $\underline{H}$ being column constant. Similarly, $\underline{G}^n \to \underline{G}$ with $\underline{G}$ being column constant.

Since column-constant vectors are invariant under multiplications by $(I - \delta^\infty B)$, $(I+\delta^\infty B)^{-1}$, etc., $\|\underline{w}\|_h \leq \|(I-\tilde{A})(I+\tilde{A})^{-1}\underline{w}\|_h$. We may repeat the above argument to deduce that $\underline{w} = \sum w_i \mathbf{y}_i$, where $\mathbf{y}_i$ are the eigenvectors of $\tilde{A}$ corresponding to zero eigenvalues.

We claim that an eigenvector corresponding to a zero eigenvalue of $\tilde{A} = \delta^\infty A + D$ is constant on a row, and in this particular instance the entries in (the nonnegative diagonal matrix) D corresponding to this row are zero. To see this, recall that A is block diagonal with each block corresponding to a row in the mesh, and each block is nonnegative definite with a single zero eigenvalue with constant eigenvector. Moreover, adding a positive quantity to any diagonal of such a block renders that block positive definite, making all of the eigenvalues of that block strictly positive. Thus, in order for a zero eigenvalue to occur, the entries of D corresponding to a block must vanish.

Since $\underline{w} = \sum w_i \mathbf{y}_i$ where each $\mathbf{y}_i$ is row constant, it follows that $\underline{w}$ is constant on rows. However, $\underline{w}$ is also constant on columns, so it must be constant on all of the mesh. Also, if $\underline{w} \neq 0$, then each block of $\tilde{A}$ must have a zero eigenvalue implying $D = 0$. Note, too, that $\underline{H} = (I + \delta^\infty B)^{-1}\underline{w}$ so that $\underline{H}$ is also constant. Similarly, $\underline{G}$ is constant, and if $\underline{G} \neq 0$, then $D' = 0$.

At this point we can show that the whole sequence converged and that it was unnecessary to pass to a subsequence. Since $\{\|\underline{w}^n\|_h\}$ is a monotone decreasing sequence bounded below by zero, it converges to a limit ℓ, and in particular $\|\underline{w}\|_h = \ell$. As $\underline{w}$ is a constant vector, the constant must be $\pm\ell/\sqrt{|\Omega|}$. If $\ell = 0$, $\underline{w} = 0$ is clearly the limit of the sequence otherwise $\{\underline{w}^n\}$ is a sequence with (at most) two limit points $\underline{w}^+$, $\underline{w}^-$, both constant vectors. If $\ell \neq 0$, we can split $\{\underline{w}^n\}$ into two sequences, with each sequence converging to one of the limit points. We claim, however, that only one of the sequences is nontrivial. If not, we can find arbitrarily large indices n such that $\underline{w}^n$ is near $\underline{w}^+$ and $\underline{w}^{n+1}$ is near $\underline{w}^-$. Letting $\underline{e}^n = \underline{w}^n - \underline{w}^+$, and recalling that A and B annihilate constant vectors, it follows that

$$\underline{e}^{n+1} = (I - \tilde{A}^n)(I + \tilde{A}^n)^{-1}(I - \delta^{n+1}B)(I + \delta^{n+1}B)^{-1}\underline{e}^n + \underline{d}^n,$$

where $d_{ij}^n = -2\ell D_{ij}^n/[\sqrt{\Omega}(1 + D_{ij}^n)]$, where D_{ij}^n are the diagonal entries of D^n. Since $D^n \to 0$ it follows that $\underline{d}^n \to 0$. Taking the norm of both sides shows that $\|\underline{e}^{n+1}\|_h \leq \|\underline{e}^n\|_h + \|\underline{d}^n\|_h$. For n large, the right-hand side is arbitrarily small, showing $\underline{w}^{n+1}$ is also close to $\underline{w}^+$, contradicting $\ell \neq 0$.

We now show that $\underline{u}^n \to 0$. Denote by G^∞ and H^∞ the constant values of $\underline{G}$ and $\underline{H}$, respectively. We will consider three situations: one of G^∞ or H^∞ is negative; both are positive; and one is zero.

Beginning with the (unphysical) situation, suppose that one of G^∞ or H^∞ is negative. Then for n large, the quantities p_{ij}^n, q_{ij}^n, and b_{ij}^n and hence f_{ij}^n will all vanish, and $a_{ij}^n = a(0) > 0$. The equation for u_{ij}^n then becomes

$$u_{ij}^{n+1} = u_{ij}^n/(1 + \Delta t\, a(0))$$

so that $u_{ij}^n \to 0$. Next, when $\underline{H} > 0$ and $\underline{G} > 0$, it follows that $D = 0$ (and $D' = 0$). But the diagonal entries of D^n are of the form $u_{ij}^n p_{ij}^n / Y_H$, and since $p_{ij}^n \to V_0 G^\infty/(K_0 + G^\infty H^\infty) > 0$, it follows that $u_{ij}^n \to 0$.

We finally show that if either $\underline{H} = 0$ or $\underline{G} = 0$, then $\underline{u}^n$ converges to zero. Suppose for the sake of argument that $\underline{H} = 0$. Since $\underline{H}^{n+1/2} = (I + \tilde{A}^n)^{-1}(I - \delta^{n+1} B)\underline{H}^n$, it follows that $\underline{H}^{n+1/2} \to 0$ so that $f_{ij}^{n+1/2} \to 0$, $a_{ij}^n \to a(0) > 0$, and $b_{ij}^n = 0$ for every index pair ij and n sufficiently large. Thus, for any $0 < \epsilon < a(0)/2$ we may find n_0 sufficiently large to guarantee that $|f_{ij}^{n+1/2}| < \Delta t^\infty\, \epsilon / \Delta t^0$, $a_{ij}^n > 2\epsilon$, and $b_{ij}^n = 0$ when $n \geq n_0$ (Δt^∞ is the final time step size). The equation for u_{ij}^n then shows

$$u_{ij}^n = \left(\frac{1 + \Delta t^\infty f^{n-1/2}}{1 + \Delta t^\infty a_{ij}^n} \right) u_{ij}^{n-1} \leq \left(\frac{1 + \Delta t^\infty \epsilon}{1 + 2\Delta t^\infty \epsilon} \right) u_{ij}^{n-1} \leq \cdots \leq \left(\frac{1 + \Delta t^\infty \epsilon}{1 + 2\Delta t^\infty \epsilon} \right)^{n-n_0} u_{ij}^{n_0},$$

so $\underline{u}^n \to 0$.

The proof that $b_{ij}^{n+1} v_{ij}^n \to 0$ follows from the equation for u_{ij}^n

$$b_{ij}^{n+1} v_{ij}^n = (1/\Delta t + a_{ij}^n) u_{ij}^{n+1} - (1/\Delta t + f_{ij}^n) u_{ij}^n \to 0.$$

Since $\underline{b}^n$ depends continuously upon $\underline{G}^n$ and $\underline{H}^n$ which both converge, we may replace b_{ij}^{n+1} above by b_{ij}^n. ∎

3.2. Convergence. Below we show that, subject to two minor modifications, the ADI scheme (16) fits into the general framework of section 2 so that the numerical solutions converge to the solution of the continuous problem. It then follows that the large time asymptotic values obtained numerically will converge to the steady state solution of the continuous problem as the mesh is refined.

The ADI scheme (16) does not quite fit into the general framework of section 2. The first problem has to do with the fact that the nonlinear terms contain products of G and H, and multiplication is not globally Lipschitz on $\Re^2$. This issue was circumvented when analyzing the continuous problem by using the maximum principle to show that G and H were bounded, and multiplication is Lipschitz on bounded sets. Indeed, if the initial data is nonnegative, $0 \leq G(x,t) \leq \|G_0\|_{L^\infty(\Omega)}$ and $0 \leq H(x,t) \leq \|H_0\|_{L^\infty(\Omega)}$ for all $x \in \Omega$ and $t \geq 0$. Knowing these explicit bounds, we can modify (16) by computing a_{ij}^n, b_{ij}^n, p_{ij}^n, and q_{ij}^n with truncated values $\min(G^+, \|G_0\|_{L^\infty(\Omega)})$ and $\min(H^+, \|H_0\|_{L^\infty(\Omega)})$. The coefficients $\underline{a}$, $\underline{b}$, $\underline{p}$, and $\underline{q}$, are now bounded Lipschitz functions of $\underline{G}$ and $\underline{H}$, and the scheme is still consistent with the continuous problem.

The second obstruction to using the general results of section 2 has to do with the calculation of the term $f_{ij}^{n+1/2}$ in (16). Since the ADI scheme does not satisfy a maximum principle, $G_{ij}^{n+1/2}$ and $H_{ij}^{n+1/2}$ may not be uniformly bounded. It follows that the term $f_{ij}^{n+1/2}$ may not be bounded, unlike its continuous counterpart $f = V_0 GH/(K_0 + GH)$, which is bounded by the constant V_0 when G and H are nonnegative. This causes a problem when attempting to obtain a priori bounds on u. Again, we can circumvent this problem by working with the truncated value $\min(f_{ij}^{n+1/2}, V_0)$, and the scheme remains consistent. Note, however, that this modification destroys the exact conservation property given in Theorem 3.2. When the truncated value is used, the total mass may decrease so that the equality in Theorem 3.2 would be replaced by an inequality. Aside from this minor modification, the results on large time asymptotics remain unaltered.

We next establish stability and consistency for the equations governing the growth of the two cell types. We then show that the coupling of these equations to the diffusion equations can be viewed as reaction terms that fit into the framework of Corollary 2.7.

LEMMA 3.7 (stability). *Let a^{n+1}, b^{n+1}, $f^{n+1/2}$, $n = 0, 1, 2, \dots$ satisfy $a^{n+1} \geq 0$, $b^{n+1} \geq 0$, $f^{n+1/2} \leq B$, and let (u_0, v_0) be given with $u^0 \geq 0$ and $v^0 \geq 0$. Calculate (u^n, v^n), $n = 1, 2, \dots$ according to*

$$u^{n+1} + \Delta t^{n+1} a^{n+1} u^{n+1} = u^n + \Delta t^{n+1} b^{n+1} v^n + \Delta t^{n+1} f^{n+1/2} u^n,$$
$$v^{n+1} - \Delta t^{n+1} a^{n+1} u^{n+1} = v^n - \Delta t^{n+1} b^{n+1} v^n,$$

with time steps satisfying $1 + \Delta t^{n+1} f^{n+1/2} \geq 0$, and $1 - \Delta t^{n+1} b^{n+1} \geq 0$. Then

$$|u^n| + |v^n| \leq (|u^0| + |v^0|) \prod_{j=0}^{n-1} (1 + B\Delta t^{j+1}) \leq (|u^0| + |v^0|) e^{BT},$$

where $T = \sum_{j=1}^{n} \Delta t^j$.

Proof. As in Lemma 3.1 the restrictions on the time step guarantee that $u^n \geq 0$ and $v^n \geq 0$ for all n. Adding the equations for (u^{n+1}, v^{n+1}) gives

$$u^{n+1} + v^{n+1} = (1 + \Delta t^{n+1} f^{n+1/2}) u^n + v^n \leq (1 + B\Delta t^{n+1})(u^n + v^n),$$

from which the bound follows. ∎

LEMMA 3.8 (consistency). *Let $\tilde{a}$, $\tilde{b}$, $\tilde{f} : [0, \infty) \to [0, \infty)$ be continuous and bounded, and let $(\tilde{u}^0, \tilde{v}^0)$ be given. Denote by $(\tilde{u}, \tilde{v})$ the solution of*

$$\frac{d\tilde{u}}{dt} + \tilde{a}u = \tilde{b}\tilde{v} + \tilde{f}\tilde{u},$$
$$\frac{d\tilde{v}}{dt} - \tilde{a}u = -\tilde{b}\tilde{v}$$

with initial data $(\tilde{u}^0, \tilde{v}^0)$. Let $\tilde{u}^n$, $\tilde{v}^n$, $\tilde{a}^n$, and $\tilde{b}^n$ denote $\tilde{u}(t^n)$, $\tilde{v}(t^n)$, etc., and $f^{n+1/2}$ approximate $\tilde{f}(t^n)$ with error $O(\Delta t^{n+1})$. Then

$$\frac{1}{\Delta t^{n+1}} (\tilde{u}^{n+1} - \tilde{u}^n) + \tilde{a}^{n+1} \tilde{u}^{n+1} = \tilde{b}^{n+1} \tilde{v}^n + \tilde{f}^{n+1/2} \tilde{u}^n + \tilde{r}_1^{n+1},$$
$$\frac{1}{\Delta t^{n+1}} (\tilde{v}^{n+1} - \tilde{v}^n) - \tilde{a}^{n+1} \tilde{u}^{n+1} = -\tilde{b}^{n+1} \tilde{v}^n + \tilde{r}_2^{n+1},$$

where $\tilde{r}_i^{n+1} = O(\Delta t^{n+1})$, $i = 1, 2$, on bounded intervals $0 \leq t \leq T$.

This lemma follows from an elementary Taylor series argument.

LEMMA 3.9 (comparison). *Let $\{(u^n, v^n)\}_{n=0}^N$ be a solution of*

$$\frac{1}{\Delta t^{n+1}} (u^{n+1} - u^n) + a^{n+1} u^{n+1} = b^{n+1} v^n + f^{n+1/2} u^n + r_1^{n+1},$$
$$\frac{1}{\Delta t^{n+1}} (v^{n+1} - v^n) - a^{n+1} u^{n+1} = -b^{n+1} v^n + r_2^{n+1}$$

with (u^0, v^0) specified, and let $\{(\tilde{u}^n, \tilde{v}^n)\}_{n=0}^N$ be a solution with coefficients $\tilde{a}^n$, $\tilde{b}^n$, $\tilde{r}^n$, and $\tilde{f}^{n+1/2}$ and initial data $(\tilde{u}^0, \tilde{v}^0)$. Assume that the coefficients $\tilde{a}^n$, a^n, $\tilde{b}^n$, and b^n

are all nonnegative, and write $E_u^n = \tilde{u}^n - u^n$ *and* $E_v^n = \tilde{v}^n - v^n$. *Then for* $T > 0$ *fixed, and for all* n *satisfying* $\sum_{j=1}^n \Delta t^j \leq T$, *the errors* E_u *and* E_v *are bounded by*

$$|E_u^n| + |E_v^n|$$

$$\leq e^{BT} \left[|E_u^0| + |E_v^0| + C \sum_{j=1}^{n} \Delta t^j \left(|\tilde{a}^j - a^j| + |\tilde{b}^j - b^j| + |\tilde{f}^{j-1/2} - f^{j-1/2}| \right.\right.$$

$$\left.\left. + |\tilde{r}^j - r^j| \right) \right],$$

where $B = \max_{0 \leq j \leq N-1}(|\tilde{f}^{j+1/2}| + 2|\tilde{b}^{j+1}|)$, *and* C *depends upon* $\max_{1 \leq j \leq N} |\tilde{u}^j|$, *and* $\max_{1 \leq j \leq N}(|u^j| + |v^j|)$.

Proof. Subtracting the equation for (u^n, v^n) from that for $(\tilde{u}^n, \tilde{v}^n)$ gives

$$\begin{aligned}
(1 + \Delta t^n a^n) E_u^n &= (1 + \Delta t^n \tilde{f}^{n-1/2}) E_u^{n-1} \\
&\quad + \Delta t^n \left(u^{n-1}(\tilde{f}^{n-1/2} - f^{n-1/2}) - \tilde{u}^n(\tilde{a}^n - a^n) + \tilde{v}^{n-1}(\tilde{b}^n - b^n) \right. \\
&\quad \left. + b^n(\tilde{v}^{n-1} - v^{n-1}) + (\tilde{r}_1^n - r_1^n) \right),
\end{aligned}$$

$$\begin{aligned}
E_v^n - \Delta t^n a^n E_u^n &= (1 - \Delta t^n \tilde{b}^n) E_v^{n-1} \\
&\quad + \Delta t^n \left(\tilde{u}^n(\tilde{a}^n - a^n) - \tilde{v}^{n-1}(\tilde{b}^n - b^n) - b^n(\tilde{v}^{n-1} - v^{n-1}) + (\tilde{r}_2^n - r_2^n) \right).
\end{aligned}$$

Taking the inner product with $(s_1, s_2) = (\mathrm{sgn}_0(E_u^n), \mathrm{sgn}_0(E_v^n))$ ($\mathrm{sgn}_0(x) = 1$ if $x > 0$, -1 if $x < 0$, and zero if $x = 0$) we obtain

$$\begin{aligned}
&|E_u^n| + |E_v^n| + \Delta t^n a^n |E_u^n|(1 - s_1 s_2) \leq (1 + B\Delta t^n)(|E_u^{n-1}| + |E_v^{n-1}|) \\
&\quad + \Delta t^n C \left(|\tilde{u}^n| \, |\tilde{a}^n - a^n| + |v^{n-1}| \, |\tilde{b}^n - b^n| + |u^{n-1}| \, |\tilde{f}^{n-1/2} - f^{n-1/2}| + |\tilde{r}^n - r^n| \right).
\end{aligned}$$

Upon noting that the second term on the left is nonnegative, the discrete Gronwall inequality now yields the estimate. □

LEMMA 3.10 (convergence). *Assume that a solution* $(\tilde{G}, \tilde{H}, \tilde{u}, \tilde{v})$ *of* (15) *with nonnegative initial data has* $(\tilde{G}, \tilde{H})$ *of class* C^4 *and* $(\tilde{u}, \tilde{v})$ *of class* C^2. *Let* $\{(\underline{G}^n, \underline{H}^n, \underline{u}^n, \underline{v}^n)\}$ *denote the solution of* (16) *with the modification that* $\underline{a}^n$, $\underline{b}^n$, $\underline{p}^n$, *and* $\underline{q}^n$ *are computed with truncated values of* $\underline{G}$ *and* $\underline{H}$,

$$G \leftarrow \min(G^+, \|G_0\|_{L^\infty(\Omega)}), \qquad H \leftarrow \min(H^+, \|H_0\|_{L^\infty(\Omega)}),$$

and $\underline{f}^{n+1/2}$ *truncated above by a constant* V_0. *Assume that the initial data is nonnegative, and time steps are nonincreasing and chosen sufficiently small to guarantee that* (u^n, v^n) *remain nonnegative.*

Let $\underline{E}_G^n = \underline{\tilde{G}}^n - \underline{G}^n$, *etc. denote the pointwise error of the approximate solution, and assume that the errors in the initial data satisfy*

$$\|(I + \delta^1 B)\underline{E}_G^0\|_h \leq O(\Delta t^0 + h^{3/2}), \qquad \|(I + \delta^1 B)\underline{E}_H^0\|_h \leq O(\Delta t^0 + h^{3/2}),$$

and $\|\underline{E}_u^0\|_h$, $\|\underline{E}_v^0\|_h = O(\Delta t^0 + h^{3/2})$. *Then for* $T > 0$ *fixed and any* n *such that* $\sum_{j=1}^n \Delta t^j \leq T$, *the errors satisfy*

$$\|\underline{E}_G^n\|_h + \|\underline{E}_G^{n-1/2}\|_h + \|\underline{E}_H^n\|_h + \|\underline{E}_H^{n-1/2}\|_h + \|\underline{E}_u^n\|_h + \|\underline{E}_v^n\|_h \leq C(\Delta t^0 + h^{3/2}),$$

where $C = C(T)$ *is independent of the mesh parameters* Δt *and* h.

Proof. Define F_1^n and F_2^n by

$$F_{1ij}^n = \frac{u_{ij}^n p_{ij}^n}{Y_G}, \qquad F_{2ij}^n = \frac{u_{ij}^n q_{ij}^n}{Y_H}.$$

Recalling that $\underline{p}^n$ is bounded and $\underline{u}^n$ is bounded by Lemma (3.7), estimates of the form

$$|\tilde{F}_{1ij}^n - F_{ij}^n| \le \frac{1}{Y_G}\left(|\tilde{u}_{ij}^n - u_{ij}^n||\tilde{p}_{ij}^n| + |u_{ij}^n||\tilde{p}_{ij}^n - p_{ij}^n|\right)$$

show that $\underline{F}_1^n$ and $\underline{F}_2^n$ are Lipschitz functions of $\underline{u}^n$, $\underline{p}^n$, etc. By construction, $\underline{p}^n$ and $\underline{q}^n$ are Lipschitz functions of $\underline{G}^n$ and $\underline{H}^n$. Moreover, the coefficients $\underline{a}^n$ and $\underline{b}^n$ and $\underline{f}^{n-1/2}$ of the difference equations for $\underline{u}^n$ and $\underline{v}^n$ are Lipschitz functions of $\underline{G}^n$, $\underline{G}^{n-1/2}$, and $\underline{H}^n$, $\underline{H}^{n-1/2}$, so Lemma (3.9) shows that

$$|\underline{E}_u^n| + |\underline{E}_v^n| \le \left[|\underline{E}_u^0| + |\underline{E}_v^0| + C\sum_{j=1}^{n} \Delta t^j (|\underline{E}_G^j| + |\underline{E}_G^{j-1/2}| + |\underline{E}_H^j| + |\underline{E}_H^{j-1/2}|)\right] e^{CT}.$$

It follows that the reaction terms F_1 and F_2 are of the general form considered in Corollary 2.7, and the estimates for the errors in G and H follow immediately. The estimates for u and v then follow from the previous equation. ◻

4. Numerical experiments. Biologists have long observed (e.g., Hauser [10]) that concentric ring patterns can be formed in bacterial growth when a drop of nutrient is placed at the center of an agar pour plate. In this section, we model this problem using the ADI scheme given in the last section. We have computed with various parameter functions, and observed a range of behavior, but only one example is shown here due to limited space.

We choose the growth rate function $f(GH)$ according to Monod's law [15, 18]

$$f(GH) = \begin{cases} \frac{10\,GH}{5+GH}, & H \ge 0,\ G \ge 0, \\ 0 & \text{otherwise.} \end{cases}$$

Physically $G \ge 0$ and $H \ge 0$ so that $f(GH)$ is nonnegative and bounded. Parameter functions a and b are defined as follows:

$$a(GH) = \begin{cases} \frac{10}{1+18HG}, & H \ge 0,\ G \ge 0,\ HG \le 0.3, \\ p_a(HG), & H \ge 0,\ G \ge 0,\ 0.3 < HG \le 0.5, \\ 0 & \text{otherwise,} \end{cases}$$

$$b(GH) = \begin{cases} \frac{HG}{2+HG}, & H \ge 0,\ G \ge 0,\ HG \ge 1.2, \\ p_b(HG), & H \ge 0,\ G \ge 0,\ 1.0 \le HG < 1.2, \\ 0 & \text{otherwise.} \end{cases}$$

The intermediate functions p_a and p_b are cubic splines which are defined in such a way that $a(\cdot)$ and $b(\cdot)$ are first-order continuously differentiable. Constant parameters are chosen as

$$D_H = 0.025,\ D_G = 0.005,\ Y_H = 10,\ Y_G = 1.$$

The computation is done with a uniform step size $\Delta t = 0.003$. The square region is taken as $[-4, 4]^2$ with mesh size 120^2. Figures 3–6 give density plots of cell densities for two levels of torpor, u and v, and of two substrate concentrations, H and G. It is observed that distributions of H and G tend to uniform constants, all active cells eventually vanish, and ring pattern is formed by inactive cells. Figure 3, showing inactive cells, resembles patterns observed in biological experiments [7, 8, 10].

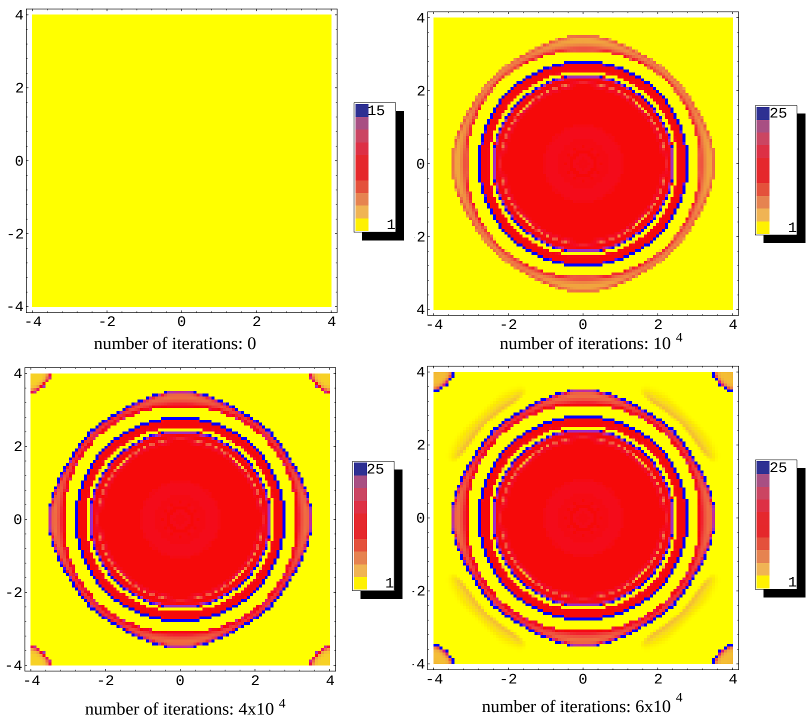

FIG. 3. *Density plots of inactive cells.*

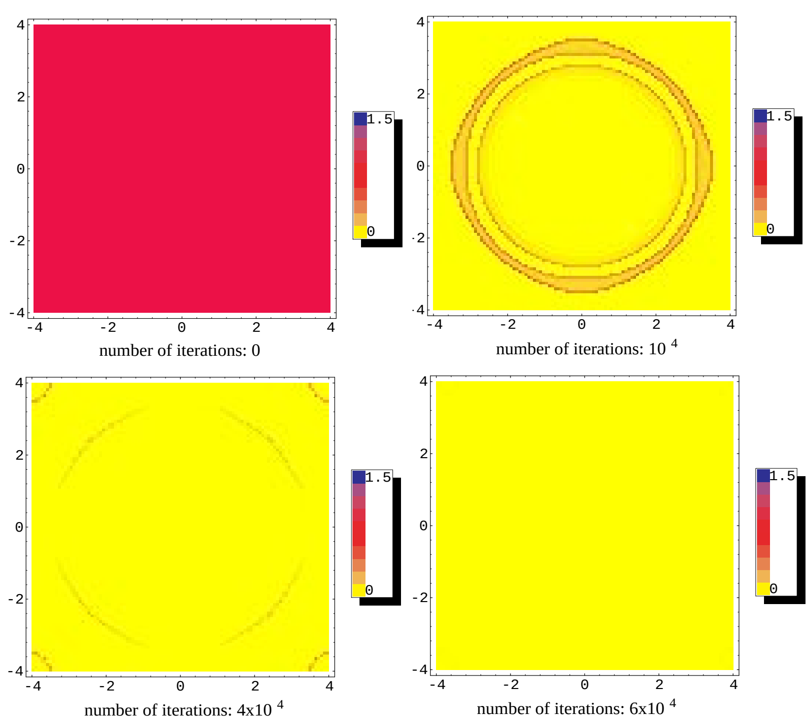

FIG. 4. *Density plots of active cells.*

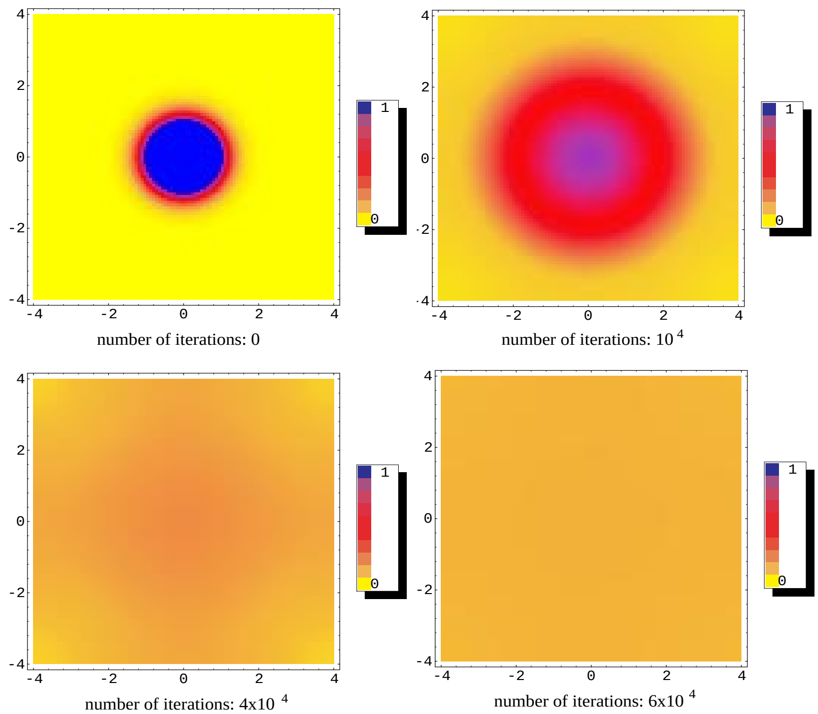

FIG. 5. *Density plots of nutrient.*

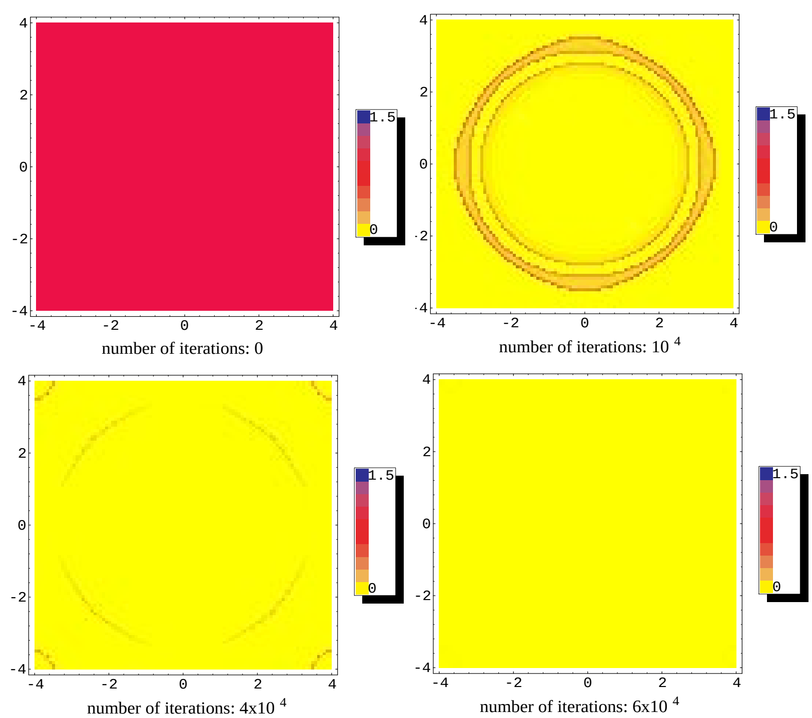

FIG. 6. *Density plots of buffer.*

5. Summary. In this paper, we consider a class of reaction-diffusion systems and the related hysteretic reaction-diffusion systems. Such systems have been used for computer simulation of accretion patterns in cell biology.

An ADI method is proposed for solving the systems. We have shown the following results:

- stability of the ADI method in the discrete norm $\|\cdot\|_h$;
- error estimates and convergence of the method for the reaction-diffusion systems with smooth nonlinear reaction functions;
- positivity of the cell density and the numerical conservation law;
- longtime behavior of the numerical solution; and
- computational results.

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