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ARTICLE *in* INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH · MARCH 2002

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Stabilization of Fronts in a Reaction−Diffusion System: Application of the Gershgorin Theorem

Yelena Smagina,* Olga Nekhamkina, and Moshe Sheintuch

Department of Chemical Engineering, Technion, Haifa, Israel 32000

A formal approach for control design aimed at stabilization of front and pulse patterns in parabolic quasilinear PDE systems using proportional weighted-average feedback regulators and inhomogeneous actuators is suggested and demonstrated. The method capitalizes on the structure of the Jacobian matrix of the system, presented by a finite Fourier series in eigenfunctions. The finite bandwidth of this matrix and the dissipative nature of the parabolic PDE allow for the construction of the finite feedback regulator by direct application of the Gershgorin stability theorem. Whereas this formalism was rigorously proven for polynomial source functions, we expect this approach to apply to other systems as well. The control obtained stabilizes the solutions in a wide range within the bistability domain. The results are compared with those of other control approaches.

1. Introduction

Inhomogeneous solutions that emerge in reaction−diffusion (RD) systems with bistable kinetics have been the subject of intensive investigation that has been summarized in several monographs[1,2] and review articles.[3] A single-variable RD system may admit moving fronts that typically travel out of the system, and an uncontrolled system will reach the homogeneous state. A two-variable system that qualitatively describes catalytic systems, i.e., one that accounts for a diffusing activator and a slow and immobilized inhibitor, will also admit travelling fronts. The construction of a controller that enables to stabilize certain desired solutions in such a system is currently the subject of intensive research.[4,5] The interest in such systems stems from various sources: Global control or coupling has been shown to induce stationary patterns and complex motions in many catalytic and in other RD systems.[6,7] Moving and stationary fronts may appear in catalytic fixed-bed reactors, which are described by reaction−diffusion−convection systems;[8−12] we return to this problem in the Conclusion section, where we analyze the implications of this study of RD systems on the control design of systems with convection. Moving patterns due to reaction−diffusion interaction appear in a plethora of physiological systems, most notably in cardiac systems. Moving fronts also appear in certain distillation problems.

We consider a new approach for the stabilization of front-like solutions in reaction−diffusion systems by a control that responds to spatially weighted-average deviations of the state variable from a set point. The proposed control strategy provides a computer-aided methodology for evaluating the form, the number of space-average sensors, and the regulator gain magnitude required for different system parameters. As a result, the regulator obtained stabilizes front solutions in a wide range of parameters within the bistability domain.

The method considered here is based on the Gershgorin theorem. As in most control design approaches, we lump the partial differential equations (PDEs) into an infinite-dimensional system of ordinary differential equations (ODEs) and apply linear stability analysis to this system. The ODE structure is such that the control affects the diagonal dominance in only selected rows of the dynamics matrix. The stability criterion based on the Gershgorin theorem is more suitable for designing such a control. The usual methods of control (e.g., modal control) will influence all eigenvalues of the dynamic matrix and will not preserve its symmetric structure. Unlike most approaches, we do not apply the usual truncation of the infinite system of ODEs, but rather we propose to use the special form of the first infinite diagonal block of the linearized dynamics matrix. It is a band matrix with the finite bandwidth defined in terms of the order of a steady-state approximation by a finite Fourier series. Because of the dissipative nature of parabolic PDEs, only several of the first rows of this block do not satisfy the stability criterion that follow from the Gershgorin theorem.[13,14] These properties of the linearized ODE system allow us to reduce the stability analysis of an infinite-dimensional system to that of a finite-dimensional system. In the last step, the simple linear feedback control structure is applied to shift some of the diagonal elements of the dynamics matrix to the left-hand-side of the complex plane. The feedback control thus obtained is used for the realization of a distributed control strategy as a weighted global control.

We consider a one-dimensional reaction−diffusion model that is described by the quasilinear parabolic PDEs

$$x_t - x_{zz} = f(x,y) + v \tag{1}$$

$$y_t = \epsilon g(x,y) \tag{2}$$

subject to the no-flux boundary conditions

$$x_z|_0 = x_z|_L = 0 \tag{3}$$

Equations 1 and 2 represent a prototype of a general two-component reaction−diffusion model (the FitzHugh−

* To whom correspondence should be addressed. E-mail: cermssy@tx.technion.ac.il. Fax: 04-8230476.

10.1021/ie001003n CCC: $22.00 © 2002 American Chemical Society
Published on Web 03/23/2002

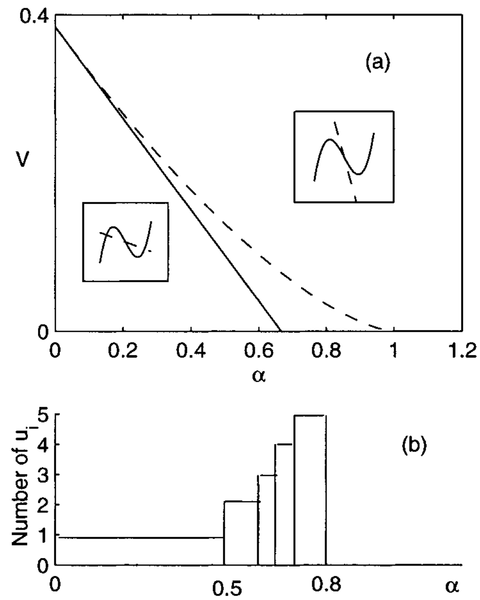

Figure 1. (a) Behavior of the uncontrolled system. The solid line (v_H) is the Hoph bifurcation for $\epsilon \to 0$, and the dotted line is the bistability boundary (v_{SN}). Insets show the x vs y phase plane. Moving fronts exist for $v < v_H$ with any ϵ and for $v_H < v < v_{SN}$ with sufficiently large ϵ; they do not exist for $v > v_{SN}$. (b) Number of sensors u_i required to stabilize a single front.

Nagumo model). We use the polynomial source functions

$$f(x,y) = -x^3 + x + y, \quad g(x,y) = -\alpha x - y \tag{4}$$

as they adequately simulate the bistable kinetics[7,1] and several analytical results are available.[2] In eqs 1 and 2, the variable $x = x(z,t)$ typically represents the activator, $y = y(z,t)$ is the slow variable (localized inhibitor), and $v = v(z,t)$ is an actuator (manipulated variable, control) that is introduced additively; α and ϵ are constants. The behavior of the uncontrollable system is mapped in Figure 1. $f(x,y) = 0$ (eq 4) is an S-shaped function, and the intersection with the linear function $g(x,y) = 0$ yields (with $v = 0$) two stable homogeneous solutions when $\alpha < {}^2/_3$ or an oscillatory solution surrounding a unique unstable state when $\alpha > 1$ and $\epsilon \to 0$. The system also admits three solutions for ${}^2/_3 < \alpha < 1$, but their stability depends on ϵ. For small ϵ, the inhibitor changes slowly, and the stability of eqs 1 and 2 can be approximated by eq 1 with frozen y.[7]

The activator described by the reaction−diffusion equation (eqs 1, 3, and 4; $y \equiv 0$) may admit inhomogeneous stationary solutions in an unbounded or sufficiently long system, but the front or pulse solution is stationary only for $v = 0$ and travels out of the system otherwise. The front velocity depends on v. The full system of equations (1−4) with $\alpha < {}^2/_3$ may also admit such a solution but an instability emerges when $\epsilon < \alpha$, and as $t \to \infty$ the system approaches one of the homogeneous stable solutions.

The aim of the paper is to stabilize a desirable stationary front or pulse steady state $x^s(z)$ by a distributed feedback control law of the form

$$v(z,t) = k\sum_{i=1}^{l}\psi_i(z)\, u_i(t) \tag{5}$$

where k is a constant gain coefficient of the regulator; $\psi_i(z)$ represents some fixed space-dependent functions (actuator distribution functions), while the time-dependent parts $u_i(t)$ (manipulated inputs, sensors) are expressed via the spatially weighted average of the activator deviation $x(z,t) - x^s(z)$ and l is the number of manipulated inputs $u_i(t)$. To simplify the application, we should design the system with the smallest l possible. It is necessary to find the form of $u_i(t)$, $\psi_i(z)$ (for assigned functions ψ_i, see Remark 3), and the minimum number of l, as well as the gain magnitude k.

We have recently analyzed the stability of one-dimensional patterns in reaction−diffusion systems of the type considered here (eqs 1−4) by analyzing the interactions between adjacent fronts and between fronts and the boundaries in bounded systems. We used approximate expressions for front velocities to study various control strategies in such a system.[16] An analysis of a single-variable model ($y \equiv 0$) showed that a single front or a pattern with n fronts is typically unstable as a result of the interactions between the fronts and between the fronts and the walls. Two simple control modes based on a single sensor and a single spatially homogeneous actuator were analyzed. Global control might or might not stabilize such a front whereas a point-sensor control will arrest this front. Both of these control actions cannot stabilize an n-front pattern, and that task calls for a distributed actuator. In a two-variable system we found that, for conditions that induce a stable moving front in an uncontrolled system (which corresponds to bistability in a lumped system, $\alpha < {}^2/_3$), global control is effective in arresting a single front only in short systems, whereas in long systems a pulse motion will emerge. Point-sensor control is effective for this task for any size of the system. Both approaches fail to stabilize an n-front pattern.

This paper presents a formal method for controller design using a novel approach. It verifies our previous approximate results and emphasizes the control problem in the range ${}^2/_3 < \alpha < 1$ that cannot be answered by a simple design based on a single actuator.

The paper is organized as follows: First, the structure of the lumped linearized infinite-dimensional system of ODEs is presented. Then, we reduce the general problem to that for the first component of a two-variable model and study the structure of the infinite-dimensional dynamics matrix obtained. The main theorem about the finiteness of the bandwidth of this matrix is proved and the inequalities of regulator gains are derived. Then, we study the possibilities of a global control strategy and apply it to several situations.

2. Analysis and Control Design

Following the linearization of eqs 1−4 around the steady states $x^s = x^s(z)$, $y^s = y^s(z)$, the steady solution of eqs 1−4 for $v = 0$, yields

$$\bar{x}_t - \bar{x}_{zz} = (-3\bar{x}^2 + 1)|_{x=x^s}\bar{x} + \bar{y} + v \tag{6}$$

$$\bar{y}_t = -\epsilon\alpha\bar{x} - \epsilon\bar{y} \tag{7}$$

where $\bar{x} = \bar{x}(z,t) = x(z,t) - x^s$ and $\bar{y} = \bar{y}(z,t) = y(z,t) - y^s$ are the deviations. We will use the conventional Galerkin approach for lumping eqs 6 and 7 by expanding the deviations $\bar{x}(z,t)$ and $\bar{y}(z,t)$ as

$$\bar{x}(z,t) = \sum_i a_i(t)\,\phi_i(z), \quad \bar{y}(z,t) = \sum_i b_i(t)\,\phi_i(z) \tag{8}$$

and propose that the control v also be expanded in the analogous but finite series

$$v(z,t) = \sum_{i=1}^{l} u_i(t)\, \phi_i(z) \tag{9}$$

where the orthonormal basis functions $\phi_i(z)$ are the eigenfunctions of the problem

$$\phi_{izz}(z) = -\lambda_i \phi_i(z), \quad \phi_{iz}(z)|_{z=0,L} = 0 \tag{10}$$

with the eigenvalues λ_i defined by

$$\lambda_i = \pi^2 (i-1)^2/L^2 \tag{11}$$

and $\phi_i(z)$

$$\phi_i(z) = \begin{cases} 1/\sqrt{L},\ i = 1 \\ \dfrac{\sqrt{2}}{\sqrt{L}} \cos \pi(i-1)\dfrac{z}{L},\ i = 2, 3, ... \end{cases} \tag{12}$$

Substituting eqs 8 and 9 into eqs 6 and 7 and integrating with weight eigenfunctions $\phi_j(z)$ results in the spectral representation of the linearized system (eqs 6 and 7) in the usual vector−matrix form

$$\begin{bmatrix} \dot{a} \\ \dot{b} \end{bmatrix} = \begin{bmatrix} -\Lambda + J & I \\ -\epsilon\alpha I & -\epsilon I \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} + \begin{bmatrix} I_l \\ 0 \end{bmatrix} u \tag{13}$$

where $a(t) = a = (a_1, a_2, ...)^{\mathrm{T}}$ and $b(t) = b = (b_1, b_2, ...)^{\mathrm{T}}$ are infinite-dimensional vectors; $u(t) = u = (u_1, u_2, ..., u_l)^{\mathrm{T}}$ is an l vector; I_l is an $l \times l$ unity matrix; and $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, ...)$, $I = \mathrm{diag}(1, 1, ...)$, $J = [J_{im}]$, i, $m = 1,2, ...$, are infinite-dimensional matrices with

$$J_{im} = \langle (-3x^{s^2} + 1)\phi_m, \phi_i \rangle, \quad i, m = 1, 2, ... \tag{14}$$

We assume that the measured output of system 13 is formed by the first l components of the infinite vector a

$$w = [a_1, a_2, ..., a_l]^{\mathrm{T}} = [I_l, 0]a$$

Let us control system 13 with the output w. The problem can then be stated as follows:

Problem 1. For the linearized system of ODEs 13, it is necessary to find the proportional finite-dimensional output feedback control

$$u = K_1 w = K_1 [a_1, a_2, ..., a_l]^{\mathrm{T}} \tag{15}$$

with the minimal size of the $l \times l$ gain matrix K_1 such that the closed-loop system

$$\begin{bmatrix} \dot{a} \\ \dot{b} \end{bmatrix} = \begin{bmatrix} -\Lambda + J + K & I \\ -\epsilon\alpha I & -\epsilon I \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} \tag{16}$$

be asymptotically stable. In eq 16, the infinite-dimensional matrix K has the form

$$K = \begin{bmatrix} K_1 & 0 \\ 0 & 0 \end{bmatrix} \tag{17}$$

We now turn to the reduction of the problem size. First, we define the stability of the open-loop dynamics matrix in eq 13 with $\epsilon > 0$ and $\alpha > 0$ in terms of the block

$$D = -\Lambda + J$$

Assertion 1. If the eigenvalues of the matrix D are real negative numbers, then the eigenvalues of the dynamics matrix in eq 13 have negative real parts (see Appendix for proof).

Note that the matrix D is symmetric and possesses only real eigenvalues.[13]

Therefore, if all eigenvalues of $D + K$ are negative, then the same conditions apply for the real parts of eigenvalues of the original matrix (eq 16). Problem 1 is reduced to the following:

Problem 2. For the linear infinite ODE system

$$\dot{a} = (-\Lambda + J)a + \begin{bmatrix} I_l \\ 0 \end{bmatrix} u, \quad w = [a_1, a_2, ..., a_l]^{\mathrm{T}} \tag{18}$$

with infinite-dimensional state vector a and finite-dimensional l vectors u and w, it is necessary to find the output finite-dimensional feedback control $u = K_1 w$ such that the closed-loop system $\dot{a} = (-\Lambda + J + K)a$, with K from eq 17, be asymptotic stable.

Let the inhomogeneous stationary solution $x^s(z)$ of the ODE

$$-x_{zz}{}^{s} = -x^{s3} + (1-\alpha)x^s, \quad x_z{}^{s}|_{0,L} = 0$$

be represented as the N-truncated Fourier series

$$x^s(z) = \sum_{i=1}^{N} \bar{a}_i \phi_i(z) \tag{19}$$

with some constant numbers $\bar{a}_i$ and $\phi_i(z)$ from eq 12. Because the function $x^s(z)$ is continuous and $\phi_i(z)$, $i = 1, 2, ...$, is a complete orthonormal set of functions, the Fourier series in eq 19 uniformly converges to the function $x^s(z)$. N is the number of terms required to approximate the steady solution with the desired accuracy.

Consider the relation between N and the structure of the matrix $D = -\Lambda + J$. To this end, we define a band matrix L with elements L_{im} as a matrix having $L_{im} = 0$ for $|i - m| > (\rho - 1)/2$ and $L_{im} \neq 0$ for $|i - m| \leq (\rho - 1)/2$,[17] where ρ is defined as the bandwidth of the matrix.

Theorem. The infinite-dimensional matrix J, with elements J_{im}, is a symmetric band matrix with a finite bandwidth ρ such that

$$\rho = 2(2N - 2) + 1 \tag{20}$$

(see Appendix for proof).

Now, we need to evaluate the diagonal elements of D.

Assertion 2. For $m > N$, the diagonal elements J_{mm}, $m = 1, 2, ...$, of the matrix J are equal to

$$-\frac{3}{L}\sum_{i=1}^{N} \bar{a}_i{}^2 + 1$$

where $\bar{a}_i$ is defined in eq 19 (see Appendix for proof).

It is evident from assertion 2 that the diagonal elements of J may change only in the range $1 \leq m \leq N$ and that, for $m > N$, these terms are constant numbers. Taking into account the structure of the matrix $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, ...)$: $\lambda_1 = 0$; $\lambda_i > 0$, $i = 2, 3, ...$; $\lambda_1 < \lambda_2 < ...$, we conclude that, for some $s \geq m > N$, the diagonal elements d_{ss} of the matrix $D = -\Lambda + J$ are negative real numbers with increasing absolute magnitudes in order of increasing s.

For further analysis, we apply the following sufficient criterion for stability, which results from the Gershgorin theorem.[13,14]

Stability Criterion. If, for an $n \times n$ matrix $G = \{g_{ij}\}$, i, $j = 1, 2, ..., n$, with real elements, the following inequalities hold

$$g_{ii} < -\sum_{j=1, j\neq i}^{n} |g_{ij}|, \quad i = 1, ..., n \tag{21}$$

then all of its eigenvalues are negative (or have negative real parts).

By virtue of the fact that the stability criterion was introduced only for finite-dimensional matrices, it cannot directly be used for infinite-dimensional matrices of a general structure.[18] On the other hand, according to the theorem above, the infinite-dimensional matrix $D = -\Lambda + J$ has a finite number of nonzero elements in every row. Moreover, in view of assertion 2 and the dissipative property of the elements $\lambda_1, \lambda_2, ...$ (see the above analysis), only a finite number μ of the first rows of the matrix D do not satisfy the stability criterion (for $i > \mu$, we have

$$-\lambda_i + J_{ii} < -\sum_{j=1, j\neq i}^{j^*} |J_{ij}|, \quad j^* = 2N-2, 2N-1, ...$$

Hence, it is enough to apply the stability criterion to the finite-dimensional $\mu \times \rho$ submatrix of the matrix D, where ρ is the bandwidth of D.

If we choose a gain matrix K in the form of eq 17 with $l = \mu$, where the $\mu \times \mu$ submatrix K_1

$$K_1 = \mathrm{diag}(k_1, k_2, ..., k_\mu) \tag{22}$$

has elements k_i that satisfy the inequalities

$$-\lambda_i + J_{ii} + k_i < -\sum_{j=1, j\neq i}^{j^*} |J_{ij}|, \quad i = 1, ..., \mu; \\ j^* = 2N-2, 2N-1, ..., 2N-2+\mu-1, \tag{23}$$

then the closed-loop system with the dynamics matrix $D + K$ will be stable. The appropriate k_i should be calculated from these inequalities.

We turn now to problem 1. Using eq 22, we can find the finite-dimensional feedback control (eq 15) with $l = \mu$ in the form

$$u = K_1[a_1, a_2, ..., a_\mu]^{\mathrm{T}} = \mathrm{diag}(k_1, k_2, ..., k_\mu) \\ [a_1, a_2, ..., a_\mu]^{\mathrm{T}} \tag{24}$$

where $u = u(t)$ is a $\mu \times 1$ column vector.

For $k_1 = k_2 = \cdots = k_\mu = k < 0$ with

$$k = \min(k_i), \quad i = 1, ..., \mu \tag{25}$$

the control in eq 24 becomes

$$u = k[a_1, a_2, ..., a_\mu]^{\mathrm{T}} \tag{26}$$

Remark 1. The infinite-dimensional control

$$u = ka \tag{27}$$

with the gain matrix $K = kI$, where I is a unity infinite-dimensional matrix, shifts all diagonal elements of the matrix $D + K$ to the left-hand part of the complex plane and simultaneously stabilizes its first rows. In this case, the feedback control law for the original system of PDEs (eqs 1–4) is defined as

$$v(z,t) = k[x(z,t) - x^s(z)] \tag{28}$$

This control can be used only when the state variable $x(z,t)$ is continuously measured.

Remark 2. Because the stability criterion is a sufficient one then the estimation based on "unstable" rows of D is an upper bound; sometimes control eq 26 with a smaller $\vartheta < \mu$ may be sufficient for stabilization (see next section).

Now, it is necessary to find the appropriate form of a distributed control that realizes control eq 26 in the original PDE system (eqs 1–4). It is easy to write this control as a global control with space-average sensors. The variables $a_i(t)$, $i = 1, 2, ...$, of the lumped system are expressed in terms of the state $\bar{x}(z,t)$ as[19]

$$a_i(t) = \int_0^L \bar{x}(z,t)\, \phi_i(z)\, \mathrm{d}z = \langle \bar{x}, \phi_i \rangle \tag{29}$$

Therefore, a finite-dimensional control u (eq 26) that shifts μ critical diagonal elements of the matrix D can be represented by a spatially weighted average of $\bar{x}(z,t)$ as

$$u = k[\langle \bar{x}, \phi_1 \rangle, \langle \bar{x}, \phi_2 \rangle, ..., \langle \bar{x}, \phi_\mu \rangle]^{\mathrm{T}} \tag{30}$$

Then, the distributed control $v(z,t)$ (eq 9) is a finite sum with μ terms as well

$$v(z,t) = k\sum_{i=1}^{\mu} u_i \phi_i = k\sum_{i=1}^{\mu}\{\int_0^L [x(z,t) - x^s(z)]\phi_i\, \mathrm{d}z\}\phi_i = \\ k\sum_{i=1}^{\mu} \langle \bar{x}, \phi_i \rangle \phi_i \tag{31}$$

The control in eq 31 is identical to the distributed feedback control in eq 5 with fixed space-dependent structures $[\psi_i(z)]$ that take the form of the eigenfunctions ϕ_i.

It is important to keep in mind that the control defined by eq 31 shifts all first μ diagonal elements of the matrix D. By virtue of the sufficiency of the Gershgorin criterion, it is sometimes enough to use the control defined by eq 26, which affects only a smaller number of rows $\vartheta < \mu$ of the dynamic matrix D (see remark 2). The value ϑ and the assigned row numbers $i_1, i_2, ..., i_\vartheta$ should be estimated by sequential simulation of the closed-loop lumped system with regulator 26 when $i = 1, 2, ..., \mu$. To shift the concrete diagonal elements of the matrix D only in the selected rows, we should use the control

$$v(z,t) = k\sum_i \langle \bar{x}, \phi_i \rangle \phi_i, \quad i = i_1, i_2, ..., i_\vartheta \tag{32}$$

Remark 3. For most practical applications, the shape of the actuator distribution functions $\psi_i = \psi_i(z)$ in eq 5 cannot be chosen directly as a set of eigenfunctions ϕ_i

because of technical constraints.[20] Expanding the assigned smooth functions ψ_i in eigenfunctions ϕ_j according to $\psi_i = \sum_{j=1}^{q}\beta_{ij}\phi_j$ and substituting these sums into eq 5, we can represent $v(z,t)$ with $l = \mu$ as

$$v(z,t) = [\phi_1, \phi_2, ..., \phi_q]B[u_1,u_2,...,u_\mu]^{\mathrm{T}}$$

where the $q \times \mu$ matrix B has elements β_{ij}. As a result, we return to problems 1 and 2 with the blocks I_l and K_1 in the input matrices and in matrix K (eq 17) replaced by the matrices B and BK_1, respectively. Diagonal elements of the $\mu \times \mu$ matrix K_1 in eq 22 are calculated from the inequalities

$$-\lambda_i + J_{ii} + \beta_{ii}k_i < -\sum_{j=1,j\neq i}^{j^*} |J_{ij}| - \sum_{j=1,j\neq i}^{\mu} |\beta_{ij}k_j|,$$
$$i = 1, ..., \mu;$$
$$j^* = 2N - 2, 2N - 1, ..., 2N - 2 + \mu - 1$$

Note that the solvability of these inequalities depends on the structure of the matrix B. In practice, the functions $\psi_j(z)$ are usually some sine or cosine functions; hence, the matrix B contains only one nonzero element in every column.

In conclusion, we present a computer-aided algorithm for the suggested approach.

Step 1. Calculate the desired steady state x^s of eqs 1−4 and approximate it by the series in eq 19. Evaluate N, the number of terms in eq 19.

Step 2. Linearize and lump the system of eqs 1−4. Compute the matrix $D = -\Lambda + J$ with the bandwidth ρ defined in eq 20.

Step 3. Find the critical μ rows of D that do not satisfy the inequalities

$$-\lambda_i + J_{ii} < -\sum_{j=1,j\neq i}^{j^*} |J_{ij}|, \quad j^* = 2N - 2, 2N - 1, ...$$

and calculate the gain k from eqs 23 and 25.

Step 4. Estimate the concrete row numbers $i_1, i_2, ..., i_\vartheta$ and form the control in eq 32 for the original PDEs (eqs 1−4).

3. Applications

We now apply the proposed methodology to the control of stationary-front and stationary-pulse solutions. We initially analyze and design a feedback regulator for one set of parameters ($\epsilon = 0.1$, $\alpha = 0.45$, $L = 20$), and then we study the control possibility for a wide range of α, namely, $0.1 \leq \alpha \leq 0.8$. Recall that an uncontrolled system admits a stable moving front for $\alpha < {}^2/_3$, whereas, for $\alpha_*(\epsilon) < \alpha < 1$ (with $\alpha_* \to {}^2/_3$ as $\epsilon \to 0$), the system admits a travelling front solution whose stability depends on ϵ.

3.1. Stabilization of a Single Front or Pulse ($\alpha = 0.45$). Single Front. To choose the appropriate value of N in the sum in eq 19, we consider the analytical solution of the ODE $-x_{zz}{}^s = -x^{s3} + (1 - \alpha)x^s$, $x_z{}^s|_{0,L} = 0$, which is $x^s = \sqrt{1-\alpha}\tanh(z\sqrt{0.5(1-\alpha})$. It may be obtained by rescaling of the single-variable problem $-x_{zz}{}^s = -x^{s3} + x^s$, $x_z{}^s|_{0,L} = 0$, which has the well-known solution $x^s = \tanh(z\sqrt{0.5})^2$. In Figure 2a, this solution (bold line) is compared with approximate solutions for different values of N (dashed lines); the maximum error $e = \max\{\mathrm{abs}[x(z)_{\mathrm{a}} - x(z)]\}$ is also plotted in Figure 2b.

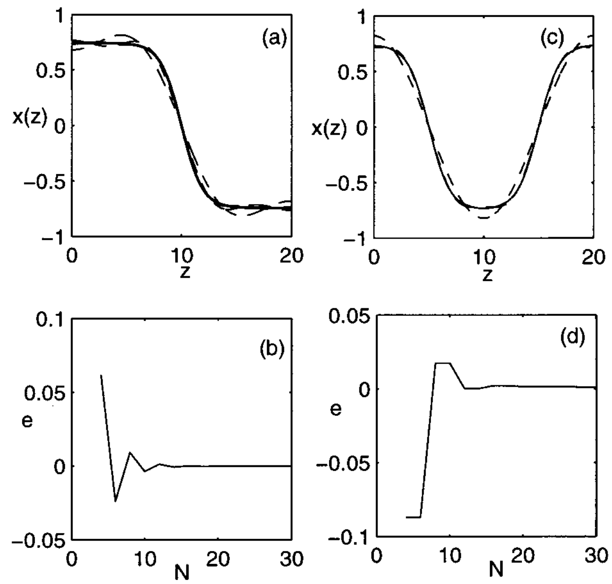

Figure 2. Comparison of analytical steady solutions (solid line) for a front and pulse (a, c) and their approximation by Fourier series with $N = 4$, 6 (dashed line), and 8 (for $N \geq 8$, the approximate and analytical solutions overlap). Also shown are the maximum error ($e = \max\{\mathrm{abs}[x(z)_{\mathrm{a}} - x(z)]\}$) between the analytical and approximate solutions (b, d) with increasing N ($\alpha = 0.45$, $\epsilon = 0.1$, $L = 20$; the analytical solution is that of the unbounded system with correction for the system length; see ref 16).

These plots suggest that $N = 8$ is sufficient for regulator synthesis, i.e., for a rough estimation of the gain coefficient k (see eq 25). Note that the study of the system behavior (linear stability analysis of the open-loop system) requires a higher-order approximation, namely, $N \geq 12$ ($e \leq 0.0014$).

Calculating the bandwidth ρ of the matrix D using eq 20, we obtain $\rho = 2(2N - 2) + 1 = 29$, and analyzing the first rows of D, we find that rows 1, 3, 5, and 7 do not satisfy the stability criterion (eq 21). The bounds on the gains k_i in these rows are −0.6090, −1.0145, −0.6825, and −0.1578, respectively. Evaluating the minimum k_i, we find from eq 25 that $k_{\min} = \min(k_i) = -1.0145$. The convergence of $k_{\min}$ with N is presented in Figure 3a.

We now study various control actions by plotting the unstable eigenvalues of the lumped system in eq 16 vs k. Figure 4a shows a plot of the two leading eigenvalues for the following control types

$$v = v_1(z,t) = k\langle\bar{x},\phi_1\rangle\phi_1 \tag{33}$$

$$v = v_3(z,t) = k\langle\bar{x},\phi_3\rangle\phi_3 \tag{34}$$

$$v = v_{1,3}(z,t) = k(\langle\bar{x},\phi_1\rangle\phi_1 + \langle\bar{x},\phi_3\rangle\phi_3) \tag{35}$$

Note that $v_1(z,t)$ affects the diagonal element d_{11} (dotted line), $v_3(z,t)$ affects the diagonal element d_{33} (dashed line), and $v_{1,3}(z,t)$ affects both diagonal elements d_{11} and d_{33} (solid line). The latter control, $v_{1,3}(z,t)$, with $k \leq -1$ results in a stable closed-loop lumped system. Such a system has a relatively wide margin of stability since the leading eigenvalue in the closed-loop system, −0.1049, is small ($k = -2$). Control $v_3(z,t)$, which affects only the third diagonal element, yields a stable solution for $k \leq -2$. However, in this case, the system has a small margin of stability for $-8 \leq k \leq -2$ (physically, this is expressed as large oscillations in the state response).

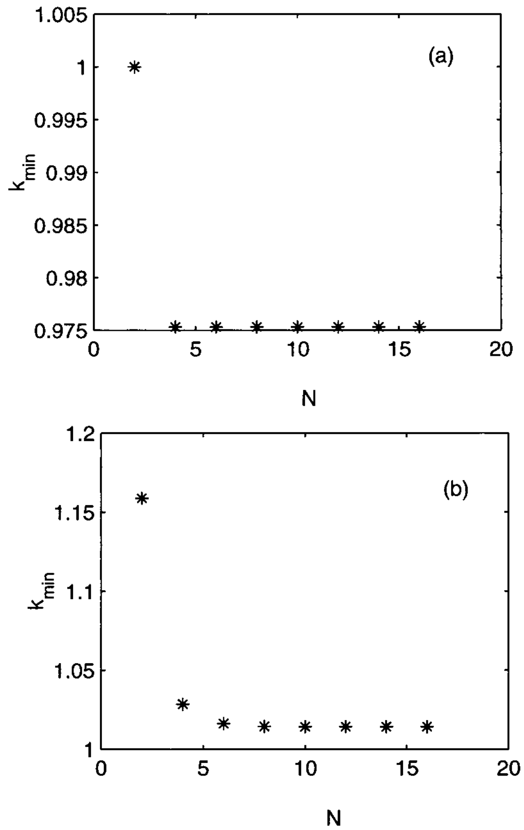

Figure 3. Convergence of the minimum gain (k_{min}) required to stabilize (a) a single front and (b) a stationary pulse with increasing N (terms in the sum in eq 19). The truncation order n of the lumped system (size of matrix D) is $n = 2N + 10$.

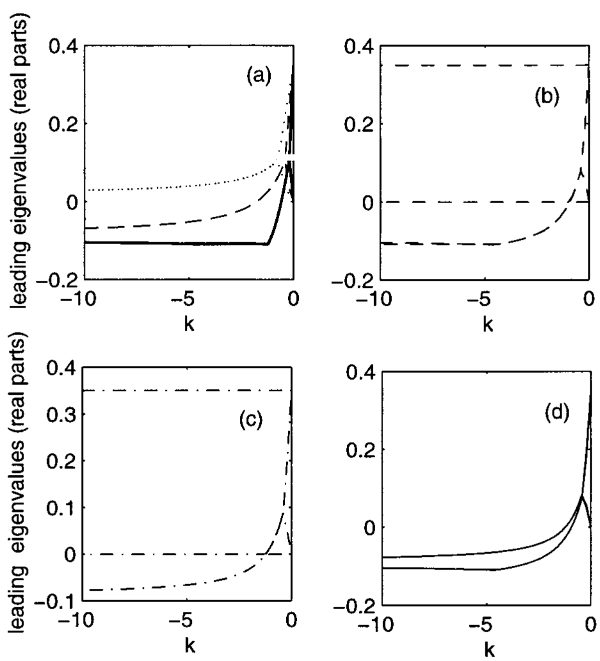

Figure 4. Comparison of various control actions showing the real parts of two leading eigenvalues of the closed-loop lumped system with control aimed at stabilizing (a) a front and (b–d) a pulse. For the front, we used the control v_1 (eq 33, dotted line), v_3 (eq 34, dashed line), and $v_{1,3}$ (eq 35, solid line), and for the pulse we used control actions (b) v_1, (c) v_2, and (d) $v_{1,2}$ (eq 36); $\alpha = 0.45$, $\epsilon = 0.1$, $L = 20$, $n = 16$ (32nd-order truncation of eq 13).

With increasing, $|k|$ the margin of stability is improved. Control $v_1(z,t)$ is unable to stabilize the system. The dynamics of the front position and the control behavior

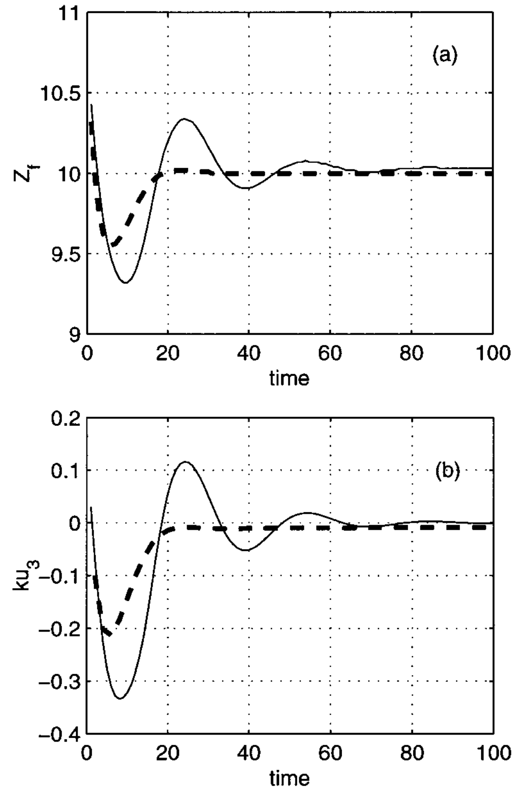

Figure 5. Dynamics of the closed-loop system response to an initial perturbation showing (a) the front position and (b) the control action $ku_3(t) = k\langle\bar{x},\phi_3\rangle$ for regulators v_3 (eq 34) with $k = -8$ (solid line) and $v_{1,3}$ (eq 35) with $k = -2$ (dashed line) aimed at stabilizing a single front. The parameters are as in Figure 4.

in the closed-loop system (Figure 5a,b) show that, whereas both the $v_3(z,t)$ and $v_{1,3}(z,t)$ regulators stabilize the front, the response with regulator $v_{1,3}$ (dashed line) is faster than that of regulator v_3 (solid line), which behaves like a stable focus.

Stationary Pulse. Repeating the same procedure for a stationary pulse, we find that $N = 8$ is sufficient to approximate the solution for synthesis purposes (see Figure 2c,d). The critical rows in matrix D are now 1, 2, 4, 5, and 6, and the limiting gain is $k_{min} = -0.9757$. The convergence of k_{min} with N is described in Figure 3b.

Applying the three control strategies

$$v = v_1(z,t) = k\langle\bar{x},\phi_1\rangle\phi_1, \quad v = v_2(z,t) = k\langle\bar{x},\phi_2\rangle\phi_2$$
$$v = v_{1,2}(z,t) = k(\langle\bar{x},\phi_1\rangle\phi_1 + \langle\bar{x},\phi_2\rangle\phi_2) \quad (36)$$

we find that controls $v_1(z,t)$ and $v_2(z,t)$ fail to stabilize the system (Figure 4b,c), whereas control $v_{1,2}(z,t)$, which simultaneously shifts the first and second diagonal elements of D, results in a stable closed-loop system (Figure 4d). The temporal behavior of the left front position in the closed-loop system and the time history of control $v_{1,2}(z,t)$ (eq 36) with $k = -4$ are presented in Figure 6a,b, respectively.

3.2. Estimation of the Number of Sensors u_i for Different α. The analysis above was repeated for α in the range $0.1 \le \alpha \le 0.8$, and the results are summarized in Tables 1–3. For a single front, matrix D has four critical rows (1, 3, 5, and 7) for α in the range $0.1 \le \alpha \le 0.45$. The number of critical rows grows to six for $0.5 \le \alpha \le 0.6$, and all seven first rows of matrix D are critical in the range $0.65 \le \alpha \le 0.8$. As expected, the number of

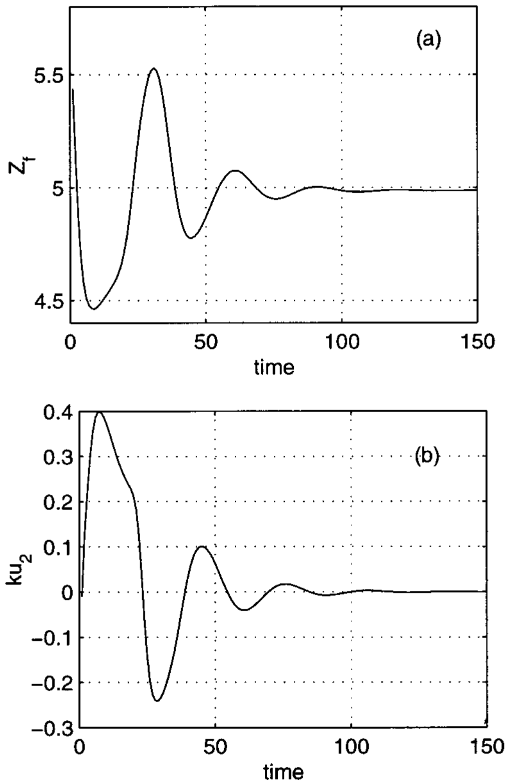

Figure 6. Dynamics of the closed-loop system response to an initial perturbation showing (a) the left front position and (b) the control action $ku_2(t) = k\langle\bar{x},\phi_2\rangle$ for regulator $v_{1,2}$ (eq 36) with $k = -4$ aimed at stabilizing a stationary pulse. The parameters are as in Figure 4.

Table 1. Number of Unstable Eigenvalues[a]

range of α	single front	stationary pulse
$\alpha = 0.1$	0 (2)	0 (1)
$0.15 \le \alpha \le 0.6$	1 (1)	2 (2)
$0.65 \le \alpha \le 0.7$	3 (1)	6 (2)
$\alpha = 0.75$	7 (1)	8 (2)
$\alpha = 0.8$	9 (1)	10 (2)
$\alpha = 0.85$	9 (1)	10 (2)

[a] Number of eigenvalues equal to zero in parentheses.

Table 2. Control Design for a Single Front

range of α	minimum number of sensors	controller form
$0.1 \le \alpha \le 0.4$	1	$v_1 = \langle\bar{x},\phi_1\rangle\phi_1$
$0.1 \le \alpha \le 0.5$	1	$v_3 = \langle\bar{x},\phi_3\rangle\phi_3$
$0.1 \le \alpha \le 0.6$	2	$v_{1,3} = \langle\bar{x},\phi_1\rangle\phi_1 + \langle(\bar{x},\phi_3\rangle\phi_3$
$0.1 \le \alpha \le 0.65$	3	$v_{1-3} = \sum_1^3 \langle\bar{x},\phi_i\rangle\phi_i$
$0.1 \le \alpha \le 0.7$	4	$v_{1-4} = \sum_1^4 \langle\bar{x},\phi_i\rangle\phi_i$
$0.1 \le \alpha \le 0.8$	5	$v_{1-5} = \sum_1^5 \langle\bar{x},\phi_i\rangle\phi_i$

unstable leading eigenvalues of the dynamics matrix in eq 13 increases as the parameter α increases (see Table 1).

A detailed analysis of the form and the minimal number of sensors u_i is summarized in Table 2. Evidently, a smaller number of sensors than predicted by critical rows is required.

Table 3. Control Design for a Stationary Pulse

range of α	minimum number of sensors	controller form
$0.1 \le \alpha \le 0.5$	2	$v_{1,2} = \sum_1^2 \langle\bar{x},\phi_i\rangle\phi_i$
$0.1 \le \alpha \le 0.6$	3	$v_{1,2,4} = \sum_1^2 \langle\bar{x},\phi_i\rangle\phi_i + \langle\bar{x},\phi_4\rangle\phi_4$
$0.1 \le \alpha \le 0.75$	5	$v_{1-5} = \sum_1^5 \langle\bar{x},\phi_i\rangle\phi_i$
$0.1 \le \alpha \le 0.8$	6	$v_{1-6} = \sum_1^6 \langle\bar{x},\phi_i\rangle\phi_i$

Similar results were obtained for a pulse solution. Matrix D has five critical rows for $0.1 \le \alpha \le 0.5$. The number of critical rows and the number of unstable eigenvalues grow with increasing of α (see Table 1). The results of an analysis of the form and the minimal number of weighted-average sensors are summarized in Table 3.

4. Conclusion

A formal approach for control design aimed at the stabilization of front and pulse patterns in parabolic quasilinear PDE systems using proportional weighted-average feedback regulators and inhomogeneous actuators has been suggested and demonstrated. The method capitalizes on the structure of the Jacobian matrix of the system, expanded in a finite Fourier series in eigenfunctions. The finite bandwidth of this matrix and the dissipative nature of the parabolic PDE allows to construct a finite feedback regulator by direct application of the Gershgorin stability theorem. Whereas this formalism was rigorously proven for polynomial source functions, we expect this approach to apply for other systems as well.

Although the case of polynomial source function is convenient, a realistic problem should use general source function; for example, a common term leading to bistability is the exponential Arrhenius term. In such a case, we need first to approximate the source term by some polynomial series (e.g., Taylor series) and then use the above formal methodology for evaluating the bandwidth of the lumped linearized dynamic matrix.

Mixed boundary conditions (rather than the no-flux) complicate the problem because, in this case, the eigenfunctions in eq 12 are the sum of sine and cosine terms. Hence, the N-truncated Fourier series of the steady solution in eq 19 will have a more complex form, and analytical evaluation of the finite bandwidth of the dynamic matrix becomes more complicated. A study of this case in the context of reaction−convection−diffusion system will be the subject of our future research.

We now comment on the possible implementation of such control design strategy and the extension of these results to other models, notably to reaction−convection−diffusion problems. In constructing distributed control in a catalytic reactor, one usually relies on temperature measurements for sensing and on heat supply for control. One would like to use the simplest possible sensors with measurements at certain points or of certain average properties. Sensing a spatially averaged temperature is relatively simple with resistors, in which the resistance is usually linear with the temperature. The same approach can be used to measure certain weighted averages if the resistor spatial features obey the desired weight function. In controlling the heat supply, one should design the system in a similar fashion or use supply modules that cover the system and can be operated individually.

Stationary fronts may appear in catalytic fixed-bed reactors that are described by reaction–convection–diffusion systems.[3] Fronts can result from a bistable source function, as in RD systems, and in that case the added convection "pushes" the front downstream. In typical fixed-bed reactors, the source function is not bistable, but fronts may emerge from the interaction of reaction and convection.[8–10] We have studied control design for stationary fronts for both classes of systems. In a recent work,[12] we studied the stabilization of a stationary pattern in a simple homogeneous model of a cross-flow catalytic reactor with realistic *Pe* values (ratio of convection to diffusion terms) and subject to realistic boundary conditions. Such a system admits bistability even without convection because of the interaction of nonlinear kinetics (due to exothermic activated reaction) with heat loss due to cooling and with a mass-generation source, either by a preceding reaction or by mass supply through the membrane wall.[21] Linear stability analysis combined with the Galerkin method was used for state feedback control of the distributed parameter system. The capabilities of global control and point-sensor control for stabilizing the front solution were studied by the manipulation of various reactor parameters including fluid flow and feed conditions. In another work,[22] we considered front stabilization in an adiabatic fixed-bed reactor, in which a first order Arrhenius reaction occurs: control was achieved via manipulation either of a certain parameter or of the flow rate or feed conditions. Using approximate models that reduce the full model to a system similar to that studied here, yet with convection, we were able to test the various suggested actuators and compare them with the performance of the full model under the same conditions.

Acknowledgment

This work was supported by the Israel Science Foundation and by the U.S.–Israel Binational Science Foundation. Y.S. and O.N. are partially supported by the Center for Absorption in Science, Ministry of Immigrant Absorption, State of Israel. M.S. is a member of the Minerva Center of Nonlinear Dynamics and of Technion's Institute of Catalysis Science of Technology.

Nomenclature

$a = a(t)$ = infinite-dimensional state vector of linearized lumped system
$b = b(t)$ = infinite-dimensional state vector of linearized lumped system
$B = \beta_{ij} = q \times \mu$ matrix of coefficients of expansion of ψ_i in eigenfunctions ϕ_i
$D = -\Lambda + J$ = infinite-dimensional matrix
$G = n \times n$ matrix
$f(x,y)$ = source function
$g(x,y)$ = source function
$I = \mathrm{diag}(1, 1, ...)$ = infinite-dimensional unity matrix
$I_l = l \times l$ unity matrix
J = infinite-dimensional Jacobian matrix
K = infinite-dimensional gain matrix
$K_l = l \times l$ gain matrix
$k = \min(k_i)$ = feedback gain coefficient
k_i = elements of the gain matrix K_l
L = reactor length
m = integer (index)
N = number of terms in the Fourier series in eq 19
n = order of truncation of the matrix D
Pe = Peclet number
t = time
$u = u(t) = l \times 1$ input vector of linearized lumped system
u_i = manipulated inputs, spatially averaged sensors
$v = v(z,t)$ = control (actuator)
$v_i = v_i(z,t)$ = control affected at diagonal element d_{ii} of D
$v_{i,j} = v_{i,j}(z,t)$ = control affected at diagonal elements d_{ii} and d_{jj} of D
$v_{i-j} = v_{i-j}(z,t)$ = control affected at diagonal elements d_{ii}, $d_{i+1,i+1}$, ..., d_{jj} of D
$w = w(t) = l \times 1$ output vector of linearized lumped system
$x = x(z,t)$ = state variable (activator)
$x^s = x^s(z)$ = steady state
$\bar{x} = x - x^s$ = deviation of x
$y = y(z,t)$ = state variable (inhibitor)
$y^s = y^s(z)$ = steady state
$\bar{y} = y - y^s$ = deviation of y
z = space variable
α = constant parameter
γ_i^* = eigenvalues of the matrix D
ϵ = constant parameter
ϑ = low bound on the number of critical rows of D
$\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, ...)$ = infinite-dimensional diagonal matrix
λ_i = eigenvalues of the linear operator
μ = upper bound on the number of critical rows of D (they do not satisfy the stability criterion)
ρ = bandwidth of the matrices J and D
$\phi_i = \phi_i(z)$ = eigenfunctions of the linear operator
$\langle \cdot,\varphi_i \rangle$ = integral with weight function φ_i
$\psi_i = \psi_i(z)$ = actuator distribution functions

Appendix

Proof of Assertion 1. Using a similarity transformation that does not change the determinant, we obtain for $s \neq -\epsilon$

$$\det\begin{bmatrix} sI - D & -I \\ \epsilon\alpha I & (s+\epsilon)I \end{bmatrix} = \det\begin{bmatrix} \left(s + \dfrac{\epsilon\alpha}{s+\epsilon}\right)I - D & 0 \\ \epsilon\alpha I & (s+\epsilon)I \end{bmatrix}$$

Because $\epsilon > 0$, the matrix in the last determinant has eigenvalues with negative real parts when the eigenvalues of the symmetric matrix D, (which coincide with real numbers $\gamma_i^* = s + \epsilon\alpha/(s + \epsilon)$, are negative. Hence, it is necessary to show that, if $\gamma_i^* < 0$ is an eigenvalue of the matrix D, then the appropriate value of s (where s is an eigenvalue of the dynamics matrix in eq 13) has a negative real part. Calculating the roots of the equation $s + \epsilon\alpha/(s + \epsilon) = \gamma_i^*$, we obtain

$$s_{1,2} = -0.5(\epsilon - \gamma_i^*) \pm \sqrt{0.25(\epsilon - \gamma_i^*)^2 - \epsilon(\alpha - \gamma_i^*)}$$

It is evident that, for $\epsilon > 0$, $\alpha > 0$, and $\gamma_i^* < 0$, the roots s_1 and s_2 have negative real parts. This concludes the proof of assertion 1.

Proof of the Theorem. The element J_{im}, i, $m = 1, 2, ...,$ of the infinite matrix J is calculated according to

$$J_{im} = \int_0^L (-3x^{s2} + 1)\phi_i\phi_m \, dz \qquad (A1)$$

where $\phi_m = \phi_m(z)$ and $\phi_i = \phi_i(z)$ are orthonormal basic eigenfunctions defined by eq 12 and the steady state $x^s = x^s(z)$ satisfies eq 19.

Note that the matrix J is symmetric, as $\phi_m\phi_i = \phi_i\phi_m$.

We evaluate the maximum number M of nonzero off-diagonal elements of J. Consider the first row of J when $\phi_i = \phi_1 = 1/\sqrt{L}$. The off-diagonal elements of the first row are calculated as

$$J_{1,m}|_{m>1} = \frac{1}{\sqrt{L}}\int_0^L (-3x^{s2} + 1)\phi_m \, dz = \frac{1}{\sqrt{L}}\int_0^L [-3(\sum_{i=1}^N \bar{a}_i\phi_i)^2 + 1]\phi_m \, dz = -\frac{3}{\sqrt{L}}\int_0^L (\sum_{i=1}^N \bar{a}_i\phi_i)^2\phi_m \, dz \qquad (A2)$$

Because

$$(\sum_{i=1}^N \bar{a}_i\phi_i)^2 = \sum_{i=1}^N \bar{a}_i^2\phi_i^2 + 2\sum_{i=1}^N\sum_{j=i+1}^N \bar{a}_i\bar{a}_j\phi_i\phi_j \qquad (A3)$$

then

$$J_{1,m}|_{m>1} = \frac{-3}{\sqrt{L}}[\int_0^L (\sum_{i=1}^N \bar{a}_i^2\phi_i^2)\phi_m \, dz + 2\int_0^L (\sum_{i=1}^N\sum_{j=i+1}^N \bar{a}_i\bar{a}_j\phi_i\phi_j)\phi_m \, dz] \qquad (A4)$$

Using eq 12, we evaluate $\phi_i^2(z)$ as

$$\phi_i^2(z) = \frac{1}{L}\left(1 + \frac{\sqrt{L}}{\sqrt{2}}\phi_{2i-1}\right), \quad i = 2, 3, ... \qquad (A5)$$

and calculate

$$\int_0^L (\sum_{i=1}^N \bar{a}_i^2\phi_i^2)\phi_m \, dz = \frac{1}{L}\int_0^L \sum_{i=1}^N \bar{a}_i^2\left(1 + \frac{\sqrt{L}\phi_{2i-1}}{\sqrt{2}}\right)\phi_m \, dz = \frac{1}{\sqrt{2L}}\int_0^L \sum_{i=1}^N \bar{a}_i^2\phi_{2i-1}\phi_m \, dz$$

The last term in the above expression does not vanish for $2i - 1 = m$, $i = 1, 2, ..., N$, $m = 1, 2, ...,$ and the maximum value of m is reached at $m = 2N - 1$. Therefore, the first term of eq A1 gives nonzero off-diagonal elements in the range

$$1 < m \le 2N - 1 \qquad (A6)$$

of the first row.

Consider the second term in eq A4. Because

$$\phi_i\phi_j|_{i>j} = \frac{\sqrt{2}}{2\sqrt{L}}(\phi_{i+j-1} + \phi_{i-j+1}), \quad i, j = 2, 3, ... \qquad (A7)$$

the second term of eq A4 also gives nonzero off-diagonal elements in the range described by eq A6. Therefore, the maximum value M of nonzero off-diagonal elements of the first row is defined from eq A6 as

$$M = 2N - 2 \qquad (A8)$$

Then, we find the $(k+1)$st row of the matrix J when $\phi_i = \phi_{k+1} = \sqrt{2}/\sqrt{L} \cos k\pi z/L$, $k = 1, 2, ...$ The off-diagonal elements of this row are calculated as

$$J_{k+1,m}|_{m>k+1} = \int_0^L (-3x^{s2} + 1)\phi_{k+1}\phi_m \, dz = -3\int_0^L (\sum_{i=1}^N \bar{a}_i\phi_i)^2\phi_{k+1}\phi_m \, dz \qquad (A9)$$

Substituting formulas eqs A7 and A3 into eq A9, we obtain

$$J_{k+1,m|m>k+1} = -\frac{3\sqrt{2}}{\sqrt{L}}[\int_0^L (\sum_{i=1}^N \bar{a}_i^2\phi_i^2)(\phi_{m-k} + \phi_{m+k}) \, dz + 2\int_0^L (\sum_{i=1}^N\sum_{j=i+1}^N \bar{a}_i\bar{a}_j\phi_i\phi_j)(\phi_{m-k} + \phi_{m+k}) \, dz] \qquad (A10)$$

The first term in eq A10 can be simplified by applying the formula

$$\phi_i^2(\phi_{m-k} + \phi_{m+k}) = \frac{1}{L}\left(1 + \frac{\sqrt{L}}{\sqrt{2}}\phi_{2i-1}\right)(\phi_{m-k} + \phi_{m+k})$$

Then, we have

$$\int_0^L (\sum_{i=1}^N \bar{a}_i^2\phi_i^2)(\phi_{m-k} + \phi_{m+k}) \, dz = \int_0^L \sum_{i=1}^N \bar{a}_i^2\frac{1}{L}\left(1 + \frac{\sqrt{L}\phi_{2i-1}}{\sqrt{2}}\right)(\phi_{m-k} + \phi_{m+k}) \, dz = \int_0^L \sum_{i=1}^N \bar{a}_i^2\frac{\phi_{2i-1}}{\sqrt{2L}}(\phi_{m-k} + \phi_{m+k}) \, dz$$

It is evident that the above expression does not vanish for $2i - 1 = m - k$ and $2i - 1 = m + k$. The maximum value of m is reached at $m = 2N - 1 + k$. Therefore, the first term in eq A10 gives nonzero off-diagonal elements in the range

$$k + 1 < m \le 2N + k - 1 \qquad (A11)$$

Consider the second term in eq A10. Because

$$\phi_i\phi_j(\phi_{m-k} + \phi_{m+k}) = \frac{\sqrt{2}}{2\sqrt{i}}(\phi_{i+j-1} + \phi_{i-j+1})(\phi_{m-k} + \phi_{m+k}) = \frac{\sqrt{2}}{2\sqrt{i}}(\phi_{i+j-1}\phi_{m-k} + \phi_{i+j-1}\phi_{m+k} + \phi_{i-j+1}\phi_{m-k} + \phi_{i-j+1}\phi_{m+k})$$

this term gives nonzero off-diagonal elements when $2N - 1 \geq m - k$ and $2N - 1 \geq m + k$. We find the following ranges for m: $k + 1 < m \leq 2N + k - 1$ and $k + 1 < m \leq 2N - k - 1$ and choose the maximum range that coincides with eq A11.

In the final stage, we find the maximum number M of nonzero off-diagonal elements of the $(k + 1)$st row: $M = 2N - 2$. This formula coincides with eq A8. Calculating the bandwidth of matrix J yields $\rho = 2M + 1$. This completes the proof.

Proof of Assertion 2. Because

$$J_{mm} = \int_0^L (-3x^{s2} + 1)\phi_m^{\ 2}\, dz \tag{A12}$$

using eq A3, we have

$$J_{mm} = -3\int_0^L \Big(\sum_{i=1}^{N} \bar{a}_i^{\ 2}\phi_i^{\ 2}\Big)\phi_m^{\ 2}\, dz - 6\int_0^L \Big(\sum_{i=1}^{N}\sum_{j=i+1}^{N} \bar{a}_i\bar{a}_j\phi_i\phi_j\Big)\phi_m^{\ 2}\, dz + \int_0^L \phi_m^{\ 2}\, dz \tag{A13}$$

From eqs A5 and A7 and the orthonormal property of ϕ_i, we can rewrite the above expression as

$$\begin{aligned} J_{mm} &= -3\int_0^L \left[\sum_{i=1}^{N} \bar{a}_i^{\ 2}\frac{1}{L}\left(1 + \frac{\sqrt{L}\phi_{2i-1}}{\sqrt{2}}\right)\right]\phi_m^{\ 2}\, dz - \frac{3\sqrt{2}}{\sqrt{L}}\int_0^L \Big[\sum_{i=1}^{N}\sum_{j=i+1}^{N} \bar{a}_i\bar{a}_j(\phi_{i+j-1} + \phi_{i-j+1})\phi_m^{\ 2}\Big]\, dz + 1 = \\ &1 - \frac{3}{L}\sum_{i=1}^{N}\bar{a}_i^{\ 2}\int_0^L \phi_m^{\ 2}\, dz - 3\int_0^L \left(\sum_{i=1}^{N}\bar{a}_i^{\ 2}\frac{\phi_{2i-1}}{\sqrt{2L}}\right)\phi_m^{\ 2}\, dz - \frac{3\sqrt{2}}{\sqrt{L}}\int_0^L \Big(\sum_{i=1}^{N}\sum_{j=i+1}^{N} \bar{a}_i\bar{a}_j(\phi_{i+j-1} + \phi_{i-j+1})\phi_m^{\ 2}\Big)\, dz = \\ &1 - \frac{3}{L}\sum_{i=1}^{N}\bar{a}_i^{\ 2} + \delta(m) \end{aligned}$$

where we use $\delta(m)$ to denote the last two terms in the above sum. Because $\phi_m^{\ 2}(z) = 1/L(1 + \sqrt{L}/\sqrt{2}\phi_{2m-1})$, all parts of $\delta(m)$ become zero for $m > N$. Therefore

$$J_{mm} = 1 - \frac{3}{L}\sum_{i=1}^{N} \bar{a}_i^{\ 2} \quad \text{for } m > N$$

and the assertion is proved.

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Received for review November 27, 2000
Revised manuscript received December 27, 2001
Accepted January 24, 2002

IE001003N