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Nonnegativity and positiveness of solutions to mass action reaction–diffusion systems

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Abstract We show that solutions of a mass action chemical kinetics reaction–diffusion system are nonnegative. Conditions for components of the solution to be strictly positive or identically zero are given, based on an indexing procedure due to A. I. Volpert [Mat. Sb. (Russian) **88**, 578–588 (1972); Math. USSR Sb. (English) **17**, 571–582]. The results are illustrated with some examples.

Keywords Reaction-diffusion systems · Chemical kinetics · Positiveness

1 Introduction

The nonnegativity and strict positiveness of the solution of a mass action chemical kinetics system in the case of an ordinary differential equations system is studied in [1], Chap. 12. The solution represents the concentrations of the chemical substances involved in a chemical reaction. It is shown that a solution of a mass action kinetics system is positive if the initial condition is positive and nonnegative if the initial condition is nonnegative.

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If some of the initial values are zero, then an indexing procedure can be used to determine which components are positive for positive time and which, if any, are identically zero. We extend these results to a reaction-diffusion system with different diffusion coefficients, that has nonnegative initial condition and zero-flux boundary condition. The theorem which shows nonnegativity of the solution, Theorem 3 (see Appendix), is more general and applies to other models from biology, ecology, etc.

A chemical mechanism of n chemical substances A_k, $k = 1, \ldots, n$ and m elementary reactions with rate constants k_i, $i = 1, \ldots, m$ is

$$\sum_{k=1}^{n} \alpha_{ik} A_k \xrightarrow{k_i} \sum_{k=1}^{n} \beta_{ik} A_k, \quad i = 1, \ldots, m. \tag{1}$$

The constants α_{ik}, β_{ik} are nonnegative numbers, called stoichiometric coefficients that are integers in a fully detailed mechanism.

Let the concentrations of A_k be denoted by u_k, $k = 1, \ldots, n$. If the law of mass action is employed then the rate of the i-th reaction is

$$w_i(\mathbf{u}) = k_i u_1^{\alpha_{i1}} \ldots u_n^{\alpha_{in}}, \quad i = 1, \ldots, m. \tag{2}$$

We assume that $u_k^0 = 1$ for $u_k \geq 0$. Let $\gamma_{ik} = \beta_{ik} - \alpha_{ik}$, for $i = 1, \ldots, m$, $k = 1, \ldots, n$. Then a solution of the initial value problem

$$\frac{\mathrm{d}u_k}{\mathrm{d}t} = \sum_{i=1}^{m} \gamma_{ik} w_i(\mathbf{u}), \quad k = 1, \ldots, n \tag{3}$$

$$u_k(0) = u_k^0 \geq 0 \tag{4}$$

gives the time evolution of the concentrations u_k, $k = 1, \ldots, n$.

We will denote by $\mathbf{u}$ a vector in $\mathbb{R}^n$, i.e., $\mathbf{u} = (u_1, \ldots, u_n)$. If $u_k \geq 0$ for $k = 1, \ldots, n$, we write $\mathbf{u} \geq \mathbf{0}$. Similarly, if $u_k > 0$ for all k then $\mathbf{u} > \mathbf{0}$.

If the concentrations u_k, $k = 1, \ldots, n$ are spatially nonhomogeneous functions, the corresponding reaction-diffusion system with nonnegative initial condition and zero-flux boundary condition is

$$\frac{\partial u_k}{\partial t} = d_k \Delta u_k + \sum_{i=1}^{m} \gamma_{ik} w_i\ , \quad (\mathbf{x}, t) \in \Omega \times (0, T] \tag{5}$$

$$u_k(\mathbf{x}, 0) = u_k^0(\mathbf{x})\ , \quad \mathbf{x} \in \Omega \tag{6}$$

$$\frac{\partial u_k}{\partial \nu}(\mathbf{x}, t) = 0, \quad \mathbf{x} \in \partial\Omega, \quad 0 < t \leq T. \tag{7}$$

All diffusion coefficients d_k are assumed to be positive. The set Ω is a bounded open and connected subset of $\mathbb{R}^s$ with a C^2 smooth boundary $\partial\Omega$. Since the concentrations u_k are nonnegative functions we take an initial condition $u_k(\mathbf{x}, 0) \geq 0$ for all $k = 1, \ldots, n$ and $\mathbf{x} \in \Omega$. Most chemical reactions take place in vessels without inflow or outflow of material through the side boundary, justifying the zero-flux boundary condition. The vector $\boldsymbol{\nu}$ is the unit outer normal to $\partial\Omega$. Under some additional smoothness assumptions on the initial condition $\mathbf{u}(\mathbf{x}, 0)$ and the boundary $\partial\Omega$, standard theorems [2,3] guarantee the existence and uniqueness of a classical solution to (5)–(7) for some $T > 0$, i.e., $\mathbf{u}(\mathbf{x}, t)$ belongs to $C^2(\Omega \times (0, T])$, $C^1(\bar{\Omega} \times (0, T])$ and $C(\bar{\Omega} \times [0, T])$ spaces.

The question to be considered here is about the solution being nonnegative and under what conditions it is positive. In [4] A. Volpert determines, using the indexing procedure explained below, which components of the solution to the ODE system (3) are positive for all $t > 0$, even when some of the respective initial conditions (4) are zero. We use the same indexing procedure in Theorem 1 to determine which components of the solution $\mathbf{u}(\mathbf{x}, t)$ to the reaction-diffusion system (5) are positive for all $t > 0$. We note that a maximum principle argument applies directly if each of the initial functions $u_k(\mathbf{x}, 0)$ is positive at some $\mathbf{x} \in \Omega$. However, this is not the case with the model of (1), since the initial concentrations of some substances will be taken identically zero. In Theorem 2 it is shown which concentrations $u_k(\mathbf{x}, t)$ will remain zeroes if they are zeroes initially.

1.1 Indexing procedure

It is common to assume that the intermediate and product substances in (1) are not present initially, meaning that $u_k(\mathbf{x}, t) \equiv 0$ for some indices k [5]. Next we explain the indexing procedure of A. I. Volpert, [1, p. 615], that determines all substances A_k in (1) whose concentrations stay positive for $t > 0$.

Let $\mathcal{A}_0$ be a given set of chemical substances A_k, such that their corresponding initial concentrations $u_k(\mathbf{x}, 0)$ are nonnegative and not identically zero. We consider that if $A_k \notin \mathcal{A}_0$ then $u_k(\mathbf{x}, 0) \equiv 0$. We assign an index 0 to all substances from $\mathcal{A}_0$. An index 0 is assigned also to all reactions, such that all of their reactants, i.e., chemical substances to the left of $\rightarrow$ in (1) have an index 0. Further indexing is carried out by induction. Suppose we have assigned indices less than κ to chemical substances and reactions. Then the index κ is assigned to all product substances, i.e., chemical substances to the right of $\rightarrow$ in (1), not having an index for which the reaction has an index $\kappa - 1$. The index κ is assigned also to all reactions not having an index and for which all reactant substances have indices at most κ. Depending on the choice of $\mathcal{A}_0$, not all substances will receive an index. Those that do are called *reachable* from $\mathcal{A}_0$. Those that do not are called *nonreachable* from $\mathcal{A}_0$ and receive an index of $+\infty$. In Theorems 1 and 2, we show that reachable substances will have positive concentration for positive time and nonreachable substances will have identically zero concentration for all time, respectively. We demonstrate the indexing procedure with the following example, which is a model of cool flame reaction, [6, p. 299].

Example 1 The scheme of the reaction is as follows:

$$
\begin{aligned}
A_1 + A_2 &\xrightarrow{k_1} A_3 \\
A_3 + A_4 &\xrightarrow{k_2} A_2 + A_5 \\
2A_5 &\xrightarrow{k_3} A_3.
\end{aligned}
$$

Let the set of initial substances be $\mathcal{A}_0 = \{A_1, A_2, A_4\}$, which implies that $u_1(\mathbf{x}, 0)$, $u_2(\mathbf{x}, 0)$, $u_4(\mathbf{x}, 0)$ are nonnegative and not identically zero. The indexing procedure gives:

$$\begin{array}{ll} 0. & \overset{0}{A_1} + \overset{0}{A_2} \xrightarrow{k_1} \overset{1}{A_3} \\ 1. & \overset{1}{A_3} + \overset{0}{A_4} \xrightarrow{k_2} \overset{0}{A_2} + \overset{2}{A_5} \\ 2. & \quad 2\overset{2}{A_5} \xrightarrow{k_3} \overset{1}{A_3}. \end{array}$$

The numbers on the left are the indices of the reactions and the numbers over the A_k's are the indices of the chemical substances. If instead $\mathcal{A}_0 = \{A_2, A_4\}$ then A_1, A_3 and A_5 will be nonreachable and will receive an index of $+\infty$.

2 Results

We start by showing that nonnegative initial conditions in (6) imply nonnegative solutions of (5)–(7). The following proposition follows from Theorem 3 in the Appendix.

Proposition 1 *Suppose that in (5)–(7) the initial condition is* $\mathbf{u}(\mathbf{x}, 0) \geq \mathbf{0}$. *Then the solution* $\mathbf{u}(\mathbf{x}, t) \geq \mathbf{0}$ *for all* $(\mathbf{x}, t) \in \bar{\Omega} \times [0, T]$.

Proof We consider the reaction term $f_k = \sum_{i=1}^{m} \gamma_{ik} w_i$ in the k-th equation of the system (5). We have to show that f_k is of the type studied in Theorem 3. If $\gamma_{ik} = \beta_{ik} - \alpha_{ik} < 0$ or $0 \leq \beta_{ik} < \alpha_{ik}$ it follows that $\alpha_{ik} > 0$. This means that A_k participates as a reactant on the left side of the i-th reaction in (1). Therefore if $\gamma_{ik} < 0$ the corresponding rate function w_i contains a factor of u_k. Hence we can rewrite the reaction term of the k-th equation as follows

$$\sum_{i=1}^{m} \gamma_{ik} w_i = \sum_{\gamma_{ik}<0} \gamma_{ik} w_i + \sum_{\gamma_{ik}\geq 0} \gamma_{ik} w_i = a_k u_k + b_k, \tag{8}$$

where $a_k u_k$ is the sum of all $\gamma_{ik} w_i$ such that $\gamma_{ik} < 0$ and b_k is the sum of all those $\gamma_{ik} w_i$ such that $\gamma_{ik} \geq 0$. Now $b_k \geq 0$ and $a_k \leq 0$ if $\mathbf{u} \geq 0$. Therefore if $\mathbf{u} \geq 0$ and $u_k = 0$ it follows that $f_k(\mathbf{u}) = a_k u_k + b_k \geq 0$.

By Theorem 3, where we take $\alpha(\mathbf{x}, t) = g(\mathbf{x}, t) \equiv \mathbf{0}$ in the boundary condition (13) it follows that $\mathbf{u}(\mathbf{x}, t) \geq \mathbf{0}$ for all $(\mathbf{x}, t) \in \bar{\Omega} \times [0, T]$. □

The following proposition is similar to Theorem 1.4, [7, p. 29]. Here we show that if some initial condition $u_k(\mathbf{x}, 0)$ is positive for some $\mathbf{x} \in \Omega$ then the component $u_k(\mathbf{x}, t) > 0$ for all $\mathbf{x} \in \bar{\Omega}$ and $t > 0$.

Proposition 2 *Let* $\mathbf{u}(\mathbf{x}, t)$ *be a solution of (5)–(7), such that* $\mathbf{u}(\mathbf{x}, 0) \geq \mathbf{0}$ *and some* $u_k(\mathbf{x}, 0)$ *is not identically zero for* $\mathbf{x} \in \Omega$. *Then* $u_k(\mathbf{x}, t) > 0$ *for all* $(\mathbf{x}, t) \in \bar{\Omega} \times (0, T]$.

Proof By Proposition 1 it follows that $\mathbf{u}(\mathbf{x}, t) \geq \mathbf{0}$ for all $(\mathbf{x}, t) \in \bar{\Omega} \times [0, T]$. We consider the k-th equation from (5)

$$\frac{\partial u_k}{\partial t} - d_k \Delta u_k = a_k u_k + b_k, \tag{9}$$

where $a_k(\mathbf{u}) \leq 0$ and $b_k(\mathbf{u}) \geq 0$ for $\mathbf{u} \geq \mathbf{0}$ from (8). Now assume that $u_k(\mathbf{x}_0, t_0) = 0$ for some $\mathbf{x}_0 \in \Omega$ and $t_0 \in (0, T]$. It follows that $u_k(\mathbf{x}, t) = 0$ for all $\mathbf{x} \in \bar{\Omega}$, $t \leq t_0$ by a strong minimum principle [8]. Thus $u_k(\mathbf{x}, 0) \equiv 0$, which contradicts $u_k(\mathbf{x}, 0)$ not identically zero. Using $u_k(\mathbf{x}, t) > 0$ for $(\mathbf{x}, t) \in \Omega \times (0, T]$, assume that for some $(\mathbf{x}_0, t_0) \in \partial\Omega \times (0, T]$, $u_k(\mathbf{x}_0, t_0) = 0$. It follows that $\frac{\partial u_k}{\partial \boldsymbol{\nu}} < 0$ at $(\mathbf{x}_0, t_0)$ by a strong minimum principle [8]. This is a contradiction with the zero-flux boundary condition. Thus $u_k(\mathbf{x}, t) > 0$ for $(\mathbf{x}, t) \in \bar{\Omega} \times (0, T]$. □

Using the indexing procedure we can obtain an even stronger result for the system (5). We will show in the next theorem that if every A_k in (1) receives a finite index then $\mathbf{u}(\mathbf{x}, t) > \mathbf{0}$ for all $(\mathbf{x}, t) \in \bar{\Omega} \times (0, T]$.

Theorem 1 *Let $\mathbf{u}(\mathbf{x}, t)$ be a solution of (5)–(7) in $\bar{\Omega} \times [0, T]$. Assume that $u_k(\mathbf{x}, 0) \geq 0$ is not identically zero for all corresponding $A_k \in \mathcal{A}_0$ and that if $A_k \notin \mathcal{A}_0$ then $u_k(\mathbf{x}, 0) \equiv 0$. Then $u_k(\mathbf{x}, t) > 0$ in $\bar{\Omega} \times (0, T]$ for all A_k that are reachable from $\mathcal{A}_0$.*

Proof Let A_k belong to $\mathcal{A}_0$, i.e., its index κ from the indexing procedure is zero. By Proposition 2, if $u_k(\mathbf{x}, 0) \geq 0$ is not identically zero then $u_k(\mathbf{x}, t) > 0$ in $\bar{\Omega} \times (0, T]$. Thus $u_k(\mathbf{x}, t) > 0$ in $\bar{\Omega} \times (0, T]$ for all $A_k \in \mathcal{A}_0$.

Further we proceed by induction on the index κ. Suppose it has been proved that $u_k(\mathbf{x}, t) > 0$ in $\bar{\Omega} \times (0, T]$ for all indices strictly less than κ. We consider the concentration u_k of the substance A_k with an index κ. For $\kappa > 0$, A_k is a product of some reaction with an index less or equal to $(\kappa - 1)$. Assume that this is the i-th reaction from (1). Since all of its reactants have indices from the indexing procedure less than κ it follows by the induction assumption that their respective concentrations are positive. Therefore at least one rate function w_i from the sum b_k in (8) is positive and $b_k(\mathbf{x}, t) = \sum_{\gamma_{ik}>0} \gamma_{ik} w_i > 0$ for $(\mathbf{x}, t) \in \Omega \times (0, T]$. Now consider (9) with $b_k > 0$ in $\Omega \times (0, T]$

$$\frac{\partial u_k}{\partial t} - d_k \Delta u_k - a_k u_k > 0. \tag{10}$$

Suppose that $u_k(\mathbf{x}_0, t_0) = 0$ for some $(\mathbf{x}_0, t_0) \in \Omega \times (0, T]$. By $\frac{\partial u_k}{\partial v} \leq$ and $\Delta u_k \geq 0$ at the point of local minimum $(\mathbf{x}_0, t_0) \in \Omega \times (0, T]$ and $d_k > 0$ we obtain a contradiction with (10).

Now suppose that the point $(\mathbf{x}_0, t_0) \in \partial\Omega \times (0, T]$ is such that $u_k(\mathbf{x}_0, t_0) = 0$. Using $u_k(\mathbf{x}, t) > 0$ in $(\mathbf{x}, t) \in \Omega \times (0, T]$, by a strong minimum principle [8] it follows that then $\frac{\partial u_k}{\partial \boldsymbol{\nu}} < 0$ at $(\mathbf{x}_0, t_0)$. This contradicts the zero-flux boundary condition.

Therefore $u_k(\mathbf{x}, t) > 0$ for all $(\mathbf{x}, t) \in \bar{\Omega} \times (0, T]$, where the corresponding A_k has an index κ. Thus $u_k(\mathbf{x}, t) > 0$ for all $(\mathbf{x}, t) \in \bar{\Omega} \times (0, T]$ and for all A_k that are reachable from $\mathcal{A}_0$. □

Example 1 (continued) By the law of mass action the rate functions are $w_1 = k_1u_1u_2$, $w_2 = k_2u_3u_4$ and $w_3 = k_3u_5^2$. Therefore the reaction-diffusion system is:

$$\frac{\partial u_1}{\partial t} = d_1\Delta u_1 - k_1u_1u_2$$
$$\frac{\partial u_2}{\partial t} = d_2\Delta u_2 - k_1u_1u_2 + k_2u_3u_4$$
$$\frac{\partial u_3}{\partial t} = d_3\Delta u_3 + k_1u_1u_2 - k_2u_3u_4 + +k_3u_5^2$$
$$\frac{\partial u_4}{\partial t} = d_4\Delta u_4 - k_2u_3u_4$$
$$\frac{\partial u_5}{\partial t} = d_5\Delta u_5 + k_2u_3u_4 - 2k_3u_5^2.$$

We assume zero-flux boundary condition. Let the initial condition be $\mathbf{u}(\mathbf{x}, 0) \geq \mathbf{0}$ and $u_k(\mathbf{x}, 0)$ not identically zero for $k = 1, 2, 4$ with $u_3(\mathbf{x}, 0) = u_5(\mathbf{x}, 0) = 0$ for all $\mathbf{X}$. By Theorem 1 it follows that $\mathbf{u}(\mathbf{x}, t) > \mathbf{0}$, for $(\mathbf{x}, t) \in \bar{\Omega} \times (0, T]$.

If at least one of the substances A_1, A_2 or A_3 is not present then the reaction from Example 1 can not proceed. For example if $u_1(\mathbf{x}, 0) \equiv 0$ then A_1, A_3 and A_5 are nonreachable from $\mathcal{A}_0 = \{A_2, A_4\}$ and their concentrations should remain zeroes. This leads us to the proof of the following theorem.

Theorem 2 *Let $\mathbf{u}(\mathbf{x}, t)$ be a solution of (5)–(7) in $\bar{\Omega} \times [0, T]$. Then $u_k(\mathbf{x}, t) \equiv 0$ in $\bar{\Omega} \times [0, T]$ for all A_k that are nonreachable from $\mathcal{A}_0$.*

Proof The first part of the proof is the same as in [1, p. 617]. We include it here for the convenience of the reader. Let N be the set of all indices of substances A_k nonreachable from $\mathcal{A}_0$. Next we show that in all of the differential equations for u_k with $k \in N$ from the system (5), each rate function w_i in the k-th equation has the form $w_i = \phi_i u_l$ for some $l \in N$, where $\phi_i = \phi_i(\mathbf{x}, t)$, (see Example 1). Let $k \in N$ then if $\alpha_{ik} > 0$ for some i, A_k is a reactant in the i-th reaction and $w_i = \phi_i u_k$ for $l = k$. If on the other hand $\beta_{ik} > 0$, $\alpha_{ik} = 0$, then in the i-th reaction at least one reactant A_l is nonreachable (otherwise A_k is reachable), so that $w_i = \phi_i u_l$ for some $l \neq k \in N$, with $\phi_i \geq 0$.

Now we consider the subsystem of equations from (5) with indices $k \in N$ and corresponding zero initial conditions and zero-flux boundary conditions. From the discussion in the previous paragraph it follows that the reaction term f_k for $k \in N$ can be written as $[f_k = \sum_{i=1}^{m} \gamma_{ik} w_i = h_{kk}u_k + \sum_{l \neq k} h_{kl}u_l]$, where $h_{kl} \geq 0$ for $l \neq k$. Therefore the uniqueness theorem for weakly-coupled parabolic systems [10, p. 191] applies to the subsystem with equation indices $k \in N$ of (5). The zero vector is a solution of this subsystem with zero initial and zero-flux boundary conditions. By uniqueness it follows that the zero is the only solution. □

3 Examples

Example 2 Consider the chemical reaction, called an elementary step:

$$A_1 + A_2 \xrightarrow{k} A_3.$$

The corresponding reaction-diffusion system is

$$\begin{aligned}\frac{\partial u_1}{\partial t} &= d_1 \Delta u_1 - k u_1 u_2\\ \frac{\partial u_2}{\partial t} &= d_2 \Delta u_2 - k u_1 u_2\\ \frac{\partial u_3}{\partial t} &= d_3 \Delta u_3 + k u_1 u_2\end{aligned}$$

with an initial condition $\mathbf{u}(\mathbf{x}, 0) \geq \mathbf{0}$, where $\mathbf{x} \in \Omega$ and a boundary condition $\frac{\partial \mathbf{u}}{\partial \nu} = \mathbf{0}$, where $(\mathbf{x}, t) \in \partial\Omega \times (0, T]$.

By Proposition 1, since $\mathbf{u}(\mathbf{x}, t) \geq \mathbf{0}$ for $\mathbf{x} \in \Omega$, it follows that $\mathbf{u}(\mathbf{x}, t) \geq \mathbf{0}$ for $(\mathbf{x}, t) \in \bar{\Omega} \times [0, T]$.

If $\mathcal{A}_0 = \{A_1, A_2\}$ the indexing procedure gives

$$0.\quad \overset{0}{A_1} + \overset{0}{A_2} \xrightarrow{k} \overset{1}{A_3}.$$

Therefore $\mathbf{u}(\mathbf{x}, t) > \mathbf{0}$ for $(\mathbf{x}, t) \in \bar{\Omega} \times (0, T]$ by Theorem 1. If $\mathcal{A}_0 = \{A_1\}$ or $\mathcal{A}_0 = \{A_2\}$, then by Theorem 2 it follows that $u_2(\mathbf{x}, t) \equiv 0$, $u_3(\mathbf{x}, t) \equiv 0$ or $u_1(\mathbf{x}, t) \equiv 0$, $u_3(\mathbf{x}, t) \equiv 0$, respectively.

Example 3 The following example, representing chlorination of ethylene is from [1, p. 616]. If the $\mathcal{A}_0 = \{A_1, A_3\}$ the reaction with the indexing is

$$\begin{array}{ll} 0. & \overset{0}{A_1} \xrightarrow{k_1} 2\overset{1}{A_2}\\ 1. & 2\overset{1}{A_2} \xrightarrow{k_2} \overset{0}{A_1}\\ 1. & \overset{1}{A_2} + \overset{0}{A_3} \xrightarrow{k_3} \overset{2}{A_4}\\ 2. & \overset{2}{A_4} + \overset{0}{A_1} \xrightarrow{k_4} \overset{3}{A_5} + \overset{1}{A_2}\\ 2. & \overset{2}{A_4} + \overset{1}{A_2} \xrightarrow{k_5} \overset{3}{A_5}\\ 2. & 2\overset{2}{A_4} \xrightarrow{k_6} \overset{3}{A_6}. \end{array}$$

The reaction-diffusion system takes the form

SYSTEM HERE,

with nonnegative initial condition $\mathbf{u}(\mathbf{x}, 0) \geq \mathbf{0}$, $\mathbf{x} \in \Omega$ and zero flux boundary condition $\frac{\partial \mathbf{u}}{\partial \boldsymbol{\nu}} = 0$, $(\mathbf{x}, t) \in \partial\Omega \times (0, T]$ takes the form:

$$\begin{aligned}
\frac{\partial u_1}{\partial t} &= d_1 \Delta u_1 - k_1 u_1 + k_2 u_2^2 - k_4 u_1 u_4 \\
\frac{\partial u_2}{\partial t} &= d_2 \Delta u_2 + 2k_1 u_1 - 2k_2 u_2^2 - k_3 u_2 u_3 + k_4 u_1 u_4 - k_5 u_2 u_4 \\
\frac{\partial u_3}{\partial t} &= d_3 \Delta u_3 - k_3 u_2 u_3 \\
\frac{\partial u_4}{\partial t} &= d_4 \Delta u_4 + k_3 u_2 u_3 - k_4 u_1 u_4 - k_5 u_2 u_4 - 2k_6 u_4^2 \\
\frac{\partial u_5}{\partial t} &= d_5 \Delta u_5 + k_4 u_1 u_4 + k_5 u_2 u_4 \\
\frac{\partial u_6}{\partial t} &= d_6 \Delta u_6 + k_6 u_4^2.
\end{aligned}$$

By Proposition 1, $\mathbf{u}(\mathbf{x}, 0) \geq \mathbf{0}$ for $\mathbf{x} \in \Omega$ implies that $\mathbf{u}(\mathbf{x}, t) \geq \mathbf{0}$ in $\bar{\Omega} \times [0, T]$. If we assume that $u_1(\mathbf{x}, 0) \geq 0$ and $u_3(\mathbf{x}, 0) \geq 0$ are not identically zero and all other $u_k(\mathbf{x}, 0) \equiv 0$, $k = 2, 4, 5, 6$ then by Theorem 1 it follows that $\mathbf{u}(\mathbf{x}, t) > \mathbf{0}$ in $\bar{\Omega} \times (0, T]$. If $\mathcal{A}_0 = \{A_3\}$ then only A_3 is reachable and $u_k(\mathbf{x}, t) \equiv 0$ for $k \neq 3$ by Theorem 2. If $\mathcal{A}_0 = \{A_1\}$ then only A_1 and A_2 are reachable and $u_k(\mathbf{x}, t) \equiv 0$ for $k = 3, 4, 5, 6$ by Theorem 2.

Appendix

Now we study the conditions for nonnegative solutions to the reaction-diffusion system

$$\frac{\partial \mathbf{u}(\mathbf{x}, t)}{\partial t} = D\Delta \mathbf{u}(\mathbf{x}, t) + \mathbf{f}(\mathbf{u}(\mathbf{x}, t)), \quad (\mathbf{x}, t) \in \Omega \times (0, T] \tag{11}$$

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{x} \in \Omega \tag{12}$$

$$\alpha(\mathbf{x}, t)\mathbf{u}(\mathbf{x}, t) + \frac{\partial \mathbf{u}}{\partial \nu}(\mathbf{x}, t) = \mathbf{g}(\mathbf{x}, t), \quad \mathbf{x} \in \partial\Omega, \quad 0 < t \leq T. \tag{13}$$

The diffusion matrix $D = diag(d_1, \ldots, d_n)$ is constant and diagonal and all of its diagonal elements are positive. The function $\mathbf{f}(\mathbf{u}) : \mathbb{R}^n \to \mathbb{R}^n$ is C^1 and its components $f_k(\mathbf{u})$ are such that $f_k(\mathbf{u}) \geq 0$ whenever $u_k = 0$ for $\mathbf{u} \geq \mathbf{0}$. The initial condition $\mathbf{u}_0(\mathbf{x})$ is a nonnegative continuous function on a bounded domain Ω. Let $\frac{\partial}{\partial \boldsymbol{\nu}}$ in (13) be the directional derivative in the direction of the outward pointing unit normal vector $\boldsymbol{\nu}$. The matrix $\alpha(\mathbf{x}, \mathbf{t})$ is diagonal and all of its diagonal elements $\alpha_i(\mathbf{x}, t)$ are nonnegative. All of the components $g_i(\mathbf{x}, t)$ of the vector function $\mathbf{g}$ are also nonnegative and bounded on the C^2 smooth boundary $\partial\Omega$. A classical solution $\mathbf{u}(\mathbf{x}, t)$ exists and is unique for some $T > 0$ under some additional smoothness assumptions [2,3], see Sect. 1.

In the next theorem we will consider the following problem where we have inequalities in (11) instead of equalities:

$$\frac{\partial \mathbf{u}(\mathbf{x},t)}{\partial t} - D\Delta u(\mathbf{x},t) - \mathbf{f}(\mathbf{u}(\mathbf{x},t)) \geq \mathbf{0}, \quad (\mathbf{x},t) \in \Omega \times (0,T] \tag{14}$$

$$\mathbf{u}(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}) \geq \mathbf{0}, \quad \mathbf{x} \in \Omega \tag{15}$$

$$\alpha(\mathbf{x},t)\mathbf{u}(\mathbf{x},t) + \frac{\partial \mathbf{u}}{\partial \nu}(\mathbf{x},t) = \mathbf{g}(x,t) \geq \mathbf{0} \quad \mathbf{x} \in \partial\Omega, \quad 0 < t \leq T. \tag{16}$$

Using inequalities is standard practice in the proof of maximum principle type results and the problem (11)–(13) is a special case of the problem (14)–(16).

The following theorem shows that nonnegative initial and boundary conditions imply nonnegative solutions to (11)–(13). It compares to results obtained in [3,9].

Theorem 3 *Assume that* $f_k(\mathbf{u}) \geq 0$ *in* (11), *whenever* $u_k = 0$ *and* $\mathbf{u} \geq \mathbf{0}$. *Then the solution* $\mathbf{u}(\mathbf{x},t)$ *of (14)–(16) satisfies* $\mathbf{u}(\mathbf{x},t) \geq \mathbf{0}$ *for all* $(\mathbf{x},t) \in \bar{\Omega} \times [0,T]$, *if* $\mathbf{u}_0(\mathbf{x},0) \geq \mathbf{0}$ *for all* $\mathbf{x} \in \Omega$ *and* $\mathbf{g}(\mathbf{x},t) \geq \mathbf{0}$ *for all* $(\mathbf{x},t) \in \partial\Omega \times (0,T]$.

Proof First we show that if there are strict inequalities in (14)–(16) for all $\mathbf{x}$ and t then $\mathbf{u}(\mathbf{x},t) > \mathbf{0}$ in $\bar{\Omega} \times [0,T]$. We argue by contradiction. Suppose that there is $t_0 > 0$ such that for some index k, $u_k(\mathbf{x}_0,t_0) = 0$ for some $\mathbf{x}_0 \in \bar{\Omega}$, where t_0 is the smallest such time. Therefore $\mathbf{u}(\mathbf{x},t) > 0$ for $\mathbf{x} \neq \mathbf{x}_0$, $\mathbf{x} \in \bar{\Omega}$ and $t \in [0,t_0]$.

Suppose that $\mathbf{x}_0 \in \Omega$. By $f_k(\mathbf{u}) \geq 0$, if $u_k = 0$ with $\mathbf{u} \geq \mathbf{0}$ we obtain the following inequality at the point $(\mathbf{x}_0,t_0)$

$$\frac{\partial u_k}{\partial t} - d_k \Delta u_k > f_k(\mathbf{u}(\mathbf{x}_0,t_0)) \geq 0.$$

Since $(\mathbf{x}_0,t_0) \in \Omega \times (0,T]$ is a point of local minimum for $u_k(\mathbf{x},t)$ in $\bar{\Omega} \times [0,t_0]$ and $d_k > 0$ we obtain a contradiction. Hence $\mathbf{x}_0 \notin \Omega$.

Clearly for $t_0 > 0$ and $\mathbf{x}_0 \in \partial\Omega$ it follows that at $(\mathbf{x}_0,t_0)$, the inequality $\alpha_k u_k + \frac{\partial u_k}{\partial \boldsymbol{\nu}} \leq 0$ is satisfied, giving a contradiction.

Therefore we have shown that $\mathbf{u}(\mathbf{x},t) > \mathbf{0}$ for all $(\mathbf{x},t) \in \bar{\Omega} \times [0,T]$, whenever all inequalities in (14)–(16) are strict.

To show that a solution $\mathbf{u}(\mathbf{x},t)$ to (14)–(16) is nonnegative we use a perturbation argument. First we show that the function

$$\mathbf{u}^{\epsilon}(\mathbf{x},t) = \mathbf{u}(\mathbf{x},t) + \bar{\boldsymbol{\epsilon}} e^{\sigma t} H(\mathbf{x})$$

satisfies (14)–(16) with strict inequalities. The vector $\bar{\boldsymbol{\epsilon}}$ belongs to $\mathbb{R}^n$ and each of its n components is equal to $\epsilon > 0$. The constant $\sigma > 0$ will be determined later. The function $H(\mathbf{x}) = e^{h(\mathbf{x})}$, where $h(\mathbf{x})$ is a $C^2(\bar{\Omega})$ smooth function, such that $\frac{\partial h}{\partial \boldsymbol{\nu}} \geq 1$ on $\partial\Omega$. The existence of a function, such as $h(\mathbf{x})$ is shown in Lemma D.7, [10, p. 294]. This kind of perturbation on $\mathbf{u}(\mathbf{x},t)$ is used for a more general parabolic system in [11, p. 131].

Let u_k^ϵ be the k-th entry in the vector $\mathbf{u}^\epsilon$ and we will show that it satisfies

$$\frac{\partial u_k^\epsilon(\mathbf{x},t)}{\partial t} > d_k \Delta u_k^\epsilon(\mathbf{x},t) + f_k(\mathbf{u}^\epsilon), \quad (\mathbf{x},t) \in \Omega \times (0,T] \tag{17}$$

$$u_k^\epsilon(\mathbf{x},0) > 0, \quad \mathbf{x} \in \Omega \tag{18}$$

$$\alpha_k u_k^\epsilon(\mathbf{x},t) + \frac{\partial u_k^\epsilon(\mathbf{x},t)}{\partial \boldsymbol{\nu}} > 0, \quad (\mathbf{x},t) \in \partial\Omega \times (0,T]. \tag{19}$$

The initial condition is strictly positive since

$$u_k^\epsilon(\mathbf{x},0) = u_k(\mathbf{x},0) + \epsilon H(\mathbf{x}) > 0.$$

The inequality (19) is satisfied by u_k^ϵ, since

$$\alpha_k u_k^\epsilon + \frac{\partial u_k^\epsilon}{\partial \boldsymbol{\nu}} = \alpha_k u_k + \frac{\partial u_k}{\partial \boldsymbol{\nu}} + \epsilon e^{\sigma t} H(\mathbf{x}) \left(\alpha_k + \frac{\partial h}{\partial \boldsymbol{\nu}} \right) > 0.$$

Since the function $\mathbf{f}(\mathbf{u})$ is Lipschitz on a compact set, containing a neighborhood of the range of the solution $\mathbf{u}$ it satisfies the inequality:

$$|f_k(\mathbf{u}) - f_k(\mathbf{u}^\epsilon)| \le \|\mathbf{f}(\mathbf{u}) - \mathbf{f}(\mathbf{u}^\epsilon)\| \le L\|\mathbf{u} - \mathbf{u}^\epsilon\| = L\sqrt{n}\epsilon e^{\sigma t} H(\mathbf{x}), \tag{20}$$

where $\| \ \|$ is the Euclidean norm in $\mathbb{R}^n$ and L is a positive constant. Using the Lipschitz condition (20) and the inequality (14) for u_k we obtain for $u_k^\epsilon(\mathbf{x},t)$:

$$\begin{aligned} \frac{\partial u_k^\epsilon}{\partial t} = \frac{\partial u_k}{\partial t} + \epsilon\sigma e^{\sigma t} H(\mathbf{x}) \ge \\ d_k \Delta u_k + f_k(\mathbf{u}) + \epsilon\sigma e^{\sigma t} H(\mathbf{x}) = \\ d_k \Delta u_k^\epsilon - \epsilon e^{\sigma t} d_k \Delta H(\mathbf{x}) + f_k(\mathbf{u}) + \epsilon\sigma e^{\sigma t} H(\mathbf{x}) \ge \\ d_k \Delta u_k^\epsilon - \epsilon e^{\sigma t} d_k \Delta H(\mathbf{x}) + f_k(u^\epsilon) - L\sqrt{n}\epsilon e^{\sigma t} H(\mathbf{x}) + \epsilon\sigma e^{\sigma t} H(\mathbf{x}) = \\ d_k \Delta u_k^\epsilon + f_k(\mathbf{u}^\epsilon) + \epsilon \left(\sigma - L\sqrt{n} - d_k \frac{\Delta H(\mathbf{x})}{H(\mathbf{x})} \right) e^{\sigma t} H(\mathbf{x}) > \\ d_k \Delta u_k^\epsilon + f_k(\mathbf{u}^\epsilon) \end{aligned}$$

The last inequality is satisfied upon choosing

$$\sigma > 2\, max \left\{ L\sqrt{n}\, , \ \max_{1 \le k \le n} d_k \frac{\max_{\mathbf{x} \in \bar{\Omega}} |\Delta H(\mathbf{x})|}{\min_{\mathbf{x} \in \bar{\Omega}} H(\mathbf{x})} \right\}.$$

We have obtained for $u_k^\epsilon(\mathbf{x},t)$ and for each $k = 1, \ldots, n$ the inequalities (17)–(19). By the first part $\mathbf{u}^\epsilon > \mathbf{0}$ for $(\mathbf{x},t) \in \overline{\Omega} \times [0,T]$ and any $\epsilon > 0$. Therefore it follows that for $\epsilon \to 0$ the limit gives $\mathbf{u}(x,t) \ge \mathbf{0}$ as a solution to (14)–(16). □

Remark If Dirichlet boundary condition is used instead (16) will be replaced by $\mathbf{u}(\mathbf{x}, t) = \mathbf{g}(\mathbf{x}, t) \geq 0$ for $(\mathbf{x}, t) \in \partial\Omega \times (0, T]$. The previous theorem can be proved by using a simpler perturbation $\mathbf{u}^{\epsilon}(\mathbf{x}, t) = \mathbf{u}(\mathbf{x}, t) + \bar{\boldsymbol{\epsilon}} e^{\sigma t}$, where $\bar{\boldsymbol{\epsilon}} = (\epsilon, \ldots, \epsilon)^T$ and $\sigma > 0$.

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