On positivity of solutions of semi-linear convection-diffusion-reaction systems, with applications in ecology and environmental engineering

Messoud A. Efendiev¹, Hermann J. Eberl²

¹⁾Zentrum Mathematik (M12), Technische Universität München, Germany ²⁾Dept. Mathematics and Statistics, University of Guelph, Canada

Abstract

We present a necessary and sufficient condition for the positive invariance of the positive cone under general semi-linear convection-diffusion-reaction systems with constant coefficients, comprising Fickian diffusion as well as cross-diffusion. This criterion turns out to be a generalization of an invariance criterion for ordinary differential equations and also includes previously known sufficient criteria under weaker conditions. As an illustration of the main result we discuss a river quality model, a model of anaerobic waste digestion, and a predator-prey model.

Keywords: positive invariance, convection-diffusion-reaction, Streeter-Phelps model, anaerobic digestion, cross-diffusion (MSC: 35B05, 35K57, 92B99)

1 Introduction

The solutions of convection-diffusion-reaction systems arising in biology, ecology, or engineering often represent quantities such as population sizes or concentrations of nutrients, pollutants and other chemicals. Positivity is a natural and paramount property that these solutions need to possess. Models that do not guarantee it loose their validity and break down for small values of the solutions. In many instances, understanding that a particular model does not preserve positivity but allows under certain circumstances solutions to become negative, can lead to a better understanding of the model and its limitations. Therefore, one of the first steps in analyzing a biological or ecological model by mathematical techniques is traditionally to verify that solutions that originate from a positive initial state remain non-negative for all time. In other words, one shows that the positive cone is positively invariant under for the model under consideration. We will formulate and prove a theorem that provides the modeler with an easy to use tool to tackle this question. In this first version it is restricted to semi-linear convection-diffusion-reaction systems with constant coefficients. This class of equations is big enough, though, to comprise important and interesting applications in the engineering and biological sciences, as well as in other application areas, such as financial mathematics and modeling of social dynamics. We will demonstrate the application of this positivity criterion with three examples that are drawn from environmental engineering and ecology. While some sufficient conditions for positive invariance of diffusion-reaction equations are known in the literature, e.g. in [8], we present here a criterion that is also necessary. The proof is elementary and the criterion is easy to evaluate.

2 Main result

We consider the semi-linear convection-diffusion-reaction system

$$\partial_t u = a\Delta u - \gamma \cdot D u + f(u),$$

$$u|_{t=0} = u_0, \quad u|_{\partial\Omega} = 0,$$
(1)

where the dependent variable $u = (u^1, \ldots, u^k)$ is a vector-valued function of $t \in \mathbb{R}$ and $x \in \Omega \subset \mathbb{R}^n$, a is a $(k \times k)$ -matrix with constant coefficients such that $a + a^* > 0$, and $f \in C^1(\mathbb{R}^k, \mathbb{R}^k)$. Here $\gamma \cdot D u = \sum_{i=1}^n \gamma_i \partial_{x_i} u$, with γ_i a $(k \times k)$ -matrix with constant coefficients and Δ is the Laplacian, applied to the components of u. We assume that solutions u to (1) with initial data $u(0, \cdot) = u_0$ exist under appropriate compatibility conditions. (Note: if $f \in C^1$ then there exists $\delta_{u_0} > 0$, such that a solution of (1) exists in $[0, \delta_{u_0}]$).

We establish a criterion for positive invariance of the positive cone $K^+ = \{u^1 \ge 0, \dots, u^k \ge 0\}$, that is if u is a solution originating from initial data u_0 then

$$u_0 \in K^+ \Longrightarrow u(t) \in K^+.$$

Theorem 2.1. Let $a, \gamma_i, i = 1, ..., n$, be $(k \times k)$ -matrices with constant coefficients, such that $a + a^* > 0$ and $f \in C^1(\mathbb{R}^k, \mathbb{R}^k)$. Let $u_0 \in L^2(\Omega, \mathbb{R}^k)$ and the compatibility conditions on the data of (1) hold. Then in order to preserve the non-negative cone for (1) necessary and sufficient conditions are that the matrices a and $\gamma_i, i = 1, ..., n$ are diagonal and $f_i(u^1, ..., 0, ..., u^k) \ge 0$ for $u^1 \ge 0, ..., u^k \ge 0$.

Proof. Necessity. We assume that $u_0 \in K^+$ implies that $u(t) \in K^+$. Then for any pair $u_0, v \in K^+$ such that

$$(u_0,v)_{L^2} := \sum_{i=1}^k \int_{\Omega} u_0^i(x) v^i(x) \, dx = 0$$

we have

$$\left(\left.\frac{\partial u}{\partial t}\right|_{t=0}, v\right)_{L^2} = \lim_{\substack{t \to 0 \\ t > 0}} \left(\frac{u(t) - u_0}{t}, v\right)_{L^2} = \lim_{\substack{t \to 0 \\ t > 0}} \frac{u(t)}{t} \ge 0$$
(2)

where we used that $u(t) \in K^+$ due to necessity. On the other hand

$$\left(\frac{\partial u}{\partial t}\Big|_{t=0}, v\right)_{L^2} = \left(a\Delta u_0 - \gamma \operatorname{D} u_0 + f(u_0), v\right) \ge 0$$
(3)

for all $v \in K^+$, because u(t) is a solution of (1). Since $v \in K^+$ in (3) is arbitrary, we have

$$(a\Delta u_0 - \gamma D u_0 + f(u_0), v) \ge 0$$
(4)

for all pairs u_0, v with $(u_0, v)_{L^2} = 0$. Choosing in particular $u_0 = \left(0, \dots, \tilde{u}, \dots, 0\right)$ and $v_0 = \left(0, \dots, \tilde{v}, \dots, 0\right)$, with $\tilde{u} \ge 0$, $\tilde{v} \ge 0$, $i \ne j$, we obtain from (4) $\left(\left(a_{ij}\Delta \tilde{u}, \tilde{v}\right) - \sum_{\ell=1}^{n} \left(\gamma_{\ell}^{ij} \partial_{x_{\ell}} \tilde{u}, \tilde{v}\right) + f_j(0, \dots, \tilde{u}, \dots, 0), \tilde{v}\right)_{r,0} \ge 0$ (5)

From (5) it follows that, for almost all $x \in \Omega$ we have

$$a_{ij}\Delta \tilde{u} - \sum_{\ell=1}^{n} \gamma_{\ell}^{ij} \partial_{x_{\ell}} \tilde{u} + f_j(0, \dots, \tilde{u}, \dots, 0) \ge 0$$
(6)

for $i \neq j$. Note that (6) is a differential inequality for the scalar function \tilde{u} . Since (6) is a pointwise estimate, we obtain

$$a_{ij} = 0, \quad \gamma_{\ell}^{ij} = 0, \quad f_j(0, \dots, \tilde{u}_i, \dots, 0) \ge 0,$$
 (7)

for $i \neq j$, $\ell = 1, ..., n$. Our next goal is to show that (7) implies $f_i(u^1, ..., 0, ..., u^k) \ge 0$ for $u^j \ge 0, j = 1, ..., k$. Indeed, taking $a = \text{diag}(a_1, ..., a_k), \gamma_{\ell}^{ij} = \text{diag}(\gamma_{\ell}^1, ..., \gamma_{\ell}^k), \ell = 1, ..., n$, into account, for a pair $u_0 = (u^1, ..., 0, ..., u^k)$ and $v = (0, ..., \tilde{v}, ..., 0)$ from (4) we obtain that

$$f_i(u^1,\ldots,\underbrace{0}_i,\ldots,u^k) \ge 0, \tag{8}$$

for $u^j \ge 0$, j = 1, ..., k. This proves the necessity part of Theorem 2.1.

Sufficient. We assume that $a = \text{diag}(a^1, \ldots, a^k)$, $\gamma_{\ell} = \text{diag}(\gamma_{\ell}^1, \ldots, \gamma_{\ell}^k)$, $\ell = 1, \ldots, n$, and $f_i(u^1, \ldots, 0, \ldots, u^k) \ge 0$ for $u^j \ge 0$, $j = 1, \ldots, k$. We need to prove that if $u_0 \in K^+$, it follows that $u(t) \in K^+$.

To this end, we introduce the functions $u_+ = \max(u, 0)$ and $u_- = -\min(u, 0)$ and use that from $u \in H^1(\Omega)$ it follows that $u_+, u_- \in H^1(\Omega)$ and $(u_+, u_-)_{L^2} = (\nabla u_+, u_-) = (\nabla u_+, \nabla u_-) = 0$. Hence, it suffices to show that, if $u_-(0, x) = 0$ it follows that $u_-(t, x) = 0$, as long as a solution exists. Let $L_0 u := a \Delta u - \sum_{\ell} \gamma_{\ell} \partial_{x_{\ell}} u$. Then, since $u = u_+ - u_-$, we have

$$(L_0u, u_-)_{L^2} = -(L_0u_-, u_-)_{L^2} + (L_0u_+, u_-)_{L^2} = -(L_0u_-, u_-)_{L^2}.$$
(9)

Hence

$$(\partial_t u, u_-) = (f(u), u_-) - (L_0 u_-, u_-).$$
 (10)

Note that, $(\partial_t u, u_-)_{L^2} = (\partial_t u_+, u_-)_{L^2} - (\partial_t u_-, u_-)_{L^2} = -\frac{1}{2} \partial_t ||u_-||^2$ due to $(\partial_t u_+, u_-) = 0$. where we denote by $|| \cdot ||$ the corresponding norm in $L^2(\Omega, \mathbb{R}^k)$. Thus, we have

$$-\frac{1}{2}\partial_t \|u_-\|^2 = -(L_0 u_-, u_-)_{L^2} + (f(u), u_-)_{L^2}.$$
(11)

First, let us estimate the term (L_0u_-, u_-) in (11). Note that

$$(a\Delta u_{-}, u_{-})_{L^{2}} = -\sum_{i=1}^{k} a^{i} \|\nabla u_{-}^{i}\|^{2}$$
(12)

and

$$\left| \left(\gamma_{\ell}^{i} \frac{\partial u_{-}^{i}}{\partial x_{\ell}}, u_{-}^{i} \right)_{L^{2}} \right| \leq \varepsilon \left\| \nabla u_{-}^{i} \right\|^{2} + C_{\varepsilon} \left\| u_{-}^{i} \right\|^{2}.$$

$$(13)$$

Therefore from (11),(12) we obtain

$$\frac{1}{2}\frac{\partial}{\partial t}\|u_{-}\|^{2} + \sum_{i=1}^{k} a^{i} \|\nabla u_{-}^{i}\|^{2} = \sum_{i=1...k,\ell=1...n} \gamma_{\ell}^{i} (\nabla u_{-}^{i}, u_{-}^{i})_{L^{2}} - (f(u), u_{-})_{L^{2}}$$
(14)

and as a result of (13) and (14) we have

$$\partial_t \|u_-\|^2 \leq C_{\varepsilon} \|u_-\|^2 - (f(u), u_-)_{L^2}.$$
(15)

Next we estimate the last term in (15). Note that

$$(f(u), u_{-})_{L^{2}} = \sum_{i=1}^{k} \int_{\Omega} f_{i}(u^{1}, \dots, u^{k}) u_{-}^{i} dx.$$
 (16)

On the other hand, due to $f \in C^1(\mathbb{R}^k, \mathbb{R}^k)$ it follows that

$$f_i(u^1, \dots, u^k) = f_i(u^1, \dots, 0, \dots, u^k) + u^i F_i(u^1, \dots, u^k),$$
(17)

with $|F_i(u^1,\ldots,u^k)| \leq M$. We obtain

$$f_i(u^1,\ldots,u^k)u^i_-=f_i(u^1,\ldots,\underset{i}{0},\ldots,u^k)u^i_-+F_i(u^1,\ldots,u^k)$$

and

$$\int_{\Omega} f_i(u^1, \dots, u^k) u_-^i dx = \int_{\Omega} f_i(u^1, \dots, 0, \dots, u^k) u_-^i dx + \int_{\Omega} u_-^i u^i F_i(u^1, \dots, u^k) dx.$$
(18)

The last term in (18) admits the following estimate

$$\left| \int_{\Omega} u_{-}^{i} u^{i} F_{i}(u^{1}, \dots, u^{k}) \, dx \right| \leq \int_{\Omega} |u_{-}^{i}| |u^{i}| F_{i}(u^{1}, \dots, u^{k}) \, dx \leq M \int_{\Omega} (u_{-}^{i} + u^{i}) \, |u_{-}^{i}| \, dx = M \int_{\Omega} (u_{-}^{i})^{2} \, dx$$
(19)

Then

$$-(f(u), u_{-})_{L^{2}} = -\sum_{i} \int_{\Omega} f_{i}(u^{1}, \dots, 0, \dots, u^{k}) u_{-}^{i} dx - \sum_{i} \int_{\Omega} u_{-}^{i} u^{i} F_{i}\left(u^{1}, \dots, u^{k}\right) dx$$

$$\leq M \|u_{-}\|^{2} - \left(f_{i}(u^{1}, \dots, 0, \dots, u^{k}), u_{-}^{i}\right)_{L^{2}}.$$
(20)

Let us assume now for a moment that $f_i(u^1, \ldots, 0, \ldots, u^k) \ge 0$ (in fact, this is true only for $u^1 \ge 0, \ldots, u^k \ge 0$ and we don't have any reason to assume this a priori). Then with the help of (20) the estimate (15) becomes

$$\partial_t \|u_-\|^2 \leqslant M' \|u_-\|^2. \tag{21}$$

Taking into account $u_{-}(0) = 0$ we obtain $u_{-}(t) \equiv 0$, which in turn implies $u \in K^+$.

It remains to improve the arguments for $f_i(u^1, \ldots, 0, \ldots, u^k) \ge 0$. To this end, we use the following trick: Let us consider the representation of $f_i(u^1, \ldots, u^k)$, i.e.

$$f_i\left(u^1,\ldots,u^k\right)=f_i\left(u^1,\ldots,0,\ldots,u^k\right)+u^iF_i\left(u^1,\ldots,u^k\right),$$

define

$$\tilde{f}_i\left(u^1,\ldots,u^k\right) = f_i\left(|u^1|,\ldots,0,\ldots,|u^k|\right) + u^i F_i\left(u^1,\ldots,u^k\right)$$

and consider the equation

$$\frac{\partial u}{\partial t} = a\Delta u - \gamma \cdot \mathbf{D} u + \tilde{f}(u),$$

$$u\big|_{t=0} = u_0(x), \quad u\big|_{\partial\Omega} = 0.$$
(22)

For this equation we know that, if $u_0 \in K^+$ it follows that $u(t) \in K^+$. But for such $u(t) \in K^+$ we have

$$\begin{aligned} \frac{\partial u}{\partial t} &= a\Delta u - \gamma \cdot \mathbf{D} \, u + f(u), \\ u\big|_{t=0} &= u_0(x), \quad u\big|_{\partial\Omega} = 0, \end{aligned}$$
(23)

which implies that from $u_0 \in K^+$, it follows that $u(t) \in K^+$. This proves Theorem 2.1. **Remark 2.2.** Our criterion Theorem 2.1 applied to the linear case

$$\begin{pmatrix} f_1 (u^1, \ldots, u^k) \\ \vdots \\ f_k (u^1, \ldots, u^k) \end{pmatrix} = \begin{pmatrix} b_{11} \cdots b_{1k} \\ \vdots & \ddots & \vdots \\ b_{k1} \cdots & b_{kk} \end{pmatrix} \begin{pmatrix} u^1 \\ \vdots \\ u^k \end{pmatrix}$$

leads to the condition that the matrix $b = (b)_{ij}$ needs to be essentially positive, i.e. $b_{ij} \ge 0$, $i \ne j$.

Remark 2.3. In many classical applications in engineering and ecology one encounters positive diagonal matrices a (pure Fickian diffusion) and diagonal convection matrices γ_i . The criterion Theorem 2.1 is then equivalent to the tangent condition for positive invariance under ordinary differential equations, cf [10]. In other words, if the positive cone K^+ is positively invariant for the spatially homogeneous case, as described by the ordinary differential equation

$$u_t = f(u),$$

then it is also positively invariant if Fickian diffusion and a convective drift term is added. Positive invariance, however, does not carry over from the ODE case to the PDE case if cross-diffusion terms appear in the diffusion matrix a.

Remark 2.4. The "sufficient part" of Theorem 2.1 includes the invariance theorems of [8] restricted to constant coefficient systems, but the conditions required for Theorem 2.1 are weaker and quicker to verify for a particular system.

Remark 2.5. From a mathematical modeling perspective, positivity is one of the most important and natural properties that solutions of convection-diffusion-reactions systems should have, and one would obviously expect that general results like the one stated here exist in the literature and are easy to find. As it turns out, this is not the case [6, 12]; indeed it appears that most related results are indeed folklore theorems.

3 Applications

3.1 Extended Streeter-Phelps Theory

The Streeter-Phelps model describes self-purification of a river and is formulated in terms of the biological oxygen demand BOD and the dissolved oxygen concentration [5]. The first is a wa-

ter quality parameter in which several organic pollution sources are lumped. In essence, BOD measures how much oxygen is required by the (aerobic) bacteria to degrade the pollutants. The disslved oxygen concentration is a measure for the healthyness of the river. Under perfect conditions, BOD vanishes and the oxygen is at saturation level. In the original Streeter-Phelps model, the processes considered are transport of dissolved substrates by convection, decay of BOD due to microbial activity as a first order reaction, and re-aeration, that is external transfer of oxygen, proportionally to the oxygen deficit (*i.e.* the difference between the saturation concentration of oxygen and the actual value). Thus, the original Streeter-Phelps model is a linear first order equation and, therefore, analytically solvable [5]. Over the years several extensions of this model have been suggested, in particular including diffusion as a second transport mechanism and nonlinear reaction terms for BOD decay. An extended Streeter-Phelps model reads

$$b_t + vb_x = D_b b_{xx} - F(b) \tag{24}$$

$$c_t + vc_x = D_c c_{xx} - F(b) + k(c_{\infty} - c)$$
 (25)

where v is the (constant) flow velocity in the river, $D_{b,c}$ the diffusion coefficients, and k the reaeration rate. F(b) describes the decay of BOD due to microbial activity. Due to monotonicity considerations, it must hold $F(b) \ge 0$, F(0) = 0 and $F'(b) \ge 0$ (assuming that the reaction terms are smooth). The classical (linear) Streeter Phelps model has the first order reaction $F(b) = \bar{k}b$. Other models in the literature are the second order reaction model $F(b) = \tilde{k}b^2$ [7, 11] or the Monod term model $F(b) = \frac{b}{\gamma_2 + b}(\gamma_1 - \gamma_3 b)$ [2, 7]. While we can always assume a homogeneous Neumann condition at the downstream boundary, we have either non-homogeneous Dirichlet, non-homogeneous Neumann, or Robin boundary conditions upstream, depending on the physical situation. In order to apply our criterion it is sufficient to consider the right hand side of (24, 25), of Remark 2.3. The positivity of b is guaranteed by the definition of F. More interesting is the behavior of c. For c = 0 the right hand side of (25) becomes $kc_{\infty} - F(b)$. Hence, whether or not c remains positive depends on the parameters of re-aeration as well as on the parameters describing the decay of BOD and the initial data for b. Of course, negative values for the concentration of dissolved oxygen are unphysical. In this situation the Streeter-Phelps model breaks down. The river falls under an aerobic regime, which means that all oxygen consuming organisms will leave, die off or fall dormant, including the ones responsible for (24). Instead, anaerobic organisms take over and (24) but must be replaced by a different model. Environmentally, this is the worst case scenario. The decrease of oxygen following a pollution fall-out is known as the oxygen sag. In the long term c will approach the saturation concentration c_{∞} .

3.2 Anaerobic digestion of solid waste

The underlying model includes two processes, (i) hydrolysis, i.e. degradation of waste constituting poymers, and (ii) methanogenesis, i.e. production of methane by methanogenic bacteria. Both process rates are controlled by volatile fatty acids (VFA). In particular, high VFA concentrations slow down the process. The model is formulated in terms of the independent variables waste

density W, concentration of VFA S and concentration of methanogenic biomass B. In order to allow for spatio-temporal effects, such as formation of methanogenic pockets, we consider the model formulated in [4], based on previous work by Vavilin and co-workers in [9]

$$W_t = D_W \Delta W - \gamma_W u \nabla W - k_1 F(S) W =: f_1(W, S, B)$$
(26)

$$S_t = D_S \Delta S - \gamma_S u \nabla S + k_2 F(S) W - k_3 G(S) B =: f_2(W, S, B)$$

$$(27)$$

$$B_t = D_B \Delta B - \gamma_B u \nabla B + (k_4 G(S) - k_5) B =: f_3(W, S, B)$$

$$(28)$$

All parameters $k_{1,...,5}$, $\gamma_{W,S,B}$, $D_{W,S,B}$ are positive. u describes the velocity of leachate flow. In the model (26,27,28) we omitted an equation for methane production that is included in [4, 9]. This equation decouples for the system presented here.

The smooth coefficient function F(S) describes the dependency of hydrolysis on S; we have F(0) = 1, F'(S) < 0 and $\lim_{S\to\infty} F(S) = 0$. The smooth coefficient function G(S) describes the dependency of methanogenesis on S; G is a positive single-bump function with G(0) = 0, $\lim_{S\to\infty} G(S) = 0$ and exactly one local maximum \hat{S} , for which $k_4G(\hat{S}) - k_5 > 0$. This last condition implies the existence of exactly two values $S_2 > S_1 > 0$ such that $k_4G(S_i) = k_5$, where S_1 is very small in practical situations. Further conditions on F and G apply, which, however, are not of relevance for our current purpose, see [4] for more details. The term $-k_5B$ describes cell death of methanogenic biomass. Model (26, 27, 28) is completed by a set of appropriate boundary conditions.

It is easy to verify that non-negative initial data imply non-negative solutions using Th. 2.1, since

$$f_1(0, S, B) = 0, \quad f_2(W, 0, B) = k_2 W > 0, \quad f_3(W, S, 0) = 0$$

Although the solutions of (26, 27, 28) are bounded [4], there is no positive invariant interval $[0, \overline{W}] \times [0, \overline{S}] \times [0, \overline{B}] \in \mathbb{R}^3$, which implies that the bounds of the solution are established by the initial data. In order to show this we assume that the opposite is true and introduce the new variables

$$w := \bar{W} - W, \quad s := \bar{S} - S, \quad b := \bar{B} - B$$
 (29)

and study the positive cone $w \ge 0, s \ge 0, b \ge 0$. Then model (26, 27, 28) is transformed into

$$w_t = D_W \Delta w + \gamma_W u \nabla W + k_1 (\bar{W} - w) F(\bar{S} - s) := g_1(w, s, b)$$

$$(30)$$

$$s_t = D_S \Delta s + \gamma_S u \nabla S - k_2 (\bar{W} - w) F(\bar{S} - s) + k_3 G(\bar{S} - s) (\bar{B} -) = g_2(w, s, b)$$
(31)

$$b_t = D_B \Delta b + \gamma_B u \nabla B - (k_4 G(\bar{S} - s) - k_5)(\bar{B} - b) =: g_3(w, s, b)$$
(32)

Applying criterion Th. 2.1 to (30, 31, 32) gives

$$g_1(0,s,b) = k_1 \bar{W} F(\bar{S}-s) > 0$$
(33)

$$g_2(w,0,b) = -k_2(W-w)F(S) + k_3G(S)(B-b)$$
(34)

$$g_3(w,s,0) = -(k_4G(\bar{S}-s)-k_5)\bar{B}$$
(35)

This implies $g_2(w, 0, b) < 0$ for all pairs w, b such that b is close enough to \overline{B} and w close enough to 0. Moreover, we have $g_3(w, s, 0) > 0$ guaranteed only for very small $\overline{S} < S_1$, in which case cell death of methanogenic biomass prevails over methanogenesis. For $\overline{S} > S_1$, we have $g_3(w, s, 0) < 0$ for $S_1 < \overline{S} - s < S_2$.

3.3 Cross-diffusion in ecological models

In ecological models cross-diffusion describes populations moving in response to the spatial distribution of another population or resource. Examples are populations moving into regions with higher food availability, in the direction of a chemo-attractant or away from a chemo-repellent, predators moving toward regions with more prey, prey moving away from predators, etc. A general model for the dual-species case is

$$\frac{\partial u}{\partial t} = f(u,v) + D_{11} \frac{\partial^2 u}{\partial x^2} + \frac{\partial}{\partial x} \left(D_{12}(u) \frac{\partial v}{\partial x} \right)$$
(36)

$$\frac{\partial v}{\partial t} = g(u,v) + D_{22} \frac{\partial^2 v}{\partial x^2} + \frac{\partial}{\partial x} \left(D_{21}(v) \frac{\partial u}{\partial x} \right)$$
(37)

where the density-dependent cross-diffusional coefficient $D_{12}(u) > 0$ describes a population u that moves away from regions with high density of v (e.g. prey in a predator-prey model), while $D_{12}(u) < 0$ describes a population moving toward a region with higher density of v (e.g. predators). In [1, 3] cross-diffusion coefficients of the saturation form

$$D_{12}(u) = d_{12} \frac{u}{\epsilon_1 + u},$$
(38)

are assumed to be $D_{12}(u) = d_{12}$. With a similar simplification for D_{21}) one obtains the linearized cross-diffusion model

$$\frac{\partial u}{\partial t} = f(u,v) + D_{11} \frac{\partial^2 u}{\partial x^2} + d_{12} \frac{\partial^2 v}{\partial x^2}$$
(39)

$$\frac{\partial v}{\partial t} = g(u,v) + D_{22} \frac{\partial^2 v}{\partial x^2} + d_{21} \frac{\partial^2 u}{\partial x^2}$$
(40)

which was studied in [1] with respect to stability and persistence. Our Theorem 2.1 with Remark 2.3 implies that this system does not preserve positivity, even if the reaction terms satisfy $f(0, \cdot) \ge 0$, $g(\cdot, 0) \ge 0$. Hence, there exist initial data such that u or v become negative. The reason for this breakdown of the model is in the simplification $D_{12}(u) = d_{12}u(\epsilon_1 + u)^{-1} \approx d_{12}$ (similar for v), which implicitly assumes $\epsilon_1 \ll u$. This does not hold anymore if u becomes small. For small densities $u \approx 0$ or $v \approx 0$ the non-linear cross-diffusion coefficients (38) are $D_{12}(u) \approx 0$, $D_{21}(v) \approx 0$ and the nonlinear cross-diffusion model (36, 37) behaves like the Fickian diffusion-reaction model, which preserves positivity.

4 Conclusion

The Theorem 2.1 is an easy to verify and easy to apply criterion for positive invariance of the positive cone for certain parabolic systems. While in its present form it is restricted to semilinear convection-diffusion-reaction equations with constant coefficients in the spatial operators, the examples have shown that this class is large enough to include many models that arise in various application areas. In particular the criterion was shown to be useful in describing and discussing the breakdown of certain model assumptions, and it was demonstrated how the criterion can be used to study the existence of positive invariant intervals. An extension to more general non-linear systems is possible and will be presented in a forthcoming paper.

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