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Invariant sets and attractors for Hanusse-type chemical systems with diffusions

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Dedicated to Professor Adrian Petruşel at his 54th anniversary, with thanks for his friendship and hospitality

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ABSTRACT

We are concerned with Hanusse-type chemical models with diffusions. We show that some bounded invariant sets $\subset \mathbb{R}^N$ found for the ODE Hanusse-type models (corresponding to the case when diffusions are neglected) can be used to define invariant sets $\subset L^\infty(\Omega)^N$ with respect to the corresponding Hanusse-type PDE models (involving diffusions), where $\Omega \subset \mathbb{R}^n$, $n \leq 3$, denotes the reaction domain. Simulations for both the ODE and PDE Hanusse-type models are performed for suitable coefficients of the polynomials representing the reaction terms, showing that the attractors for the ODE model are also attractors, in fact the only attractors, for the PDE model.

1. Introduction

Consider the differential equation in $\mathbb{R}^N$

$$u'(t) = f(u(t)), \quad t \in \mathbb{R}, \tag{1.1}$$

where $f : \mathbb{R}^N \to \mathbb{R}^N$ is assumed to be a locally Lipschitz function. Thus, from the general existence theory, we know that for any $u_0 \in \mathbb{R}^N$ there exists a unique solution $u = u(t)$ of Eq. (1.1) that satisfies the initial condition

$$u(0) = u_0, \tag{1.2}$$

being defined on an open interval containing $t_0 = 0$ (i.e., u is a local solution of the Cauchy problem (1.1), (1.2)).

Definition 1. A subset $D \subset \mathbb{R}^N$ is said to be *positively invariant* with respect to Eq. (1.1) if for all $u_0 \in D$ the trajectory of the solution of problem (1.1), (1.2) remains in D as long as the solution exists in the future: $u(t) \in D$ for all $t > 0$, $t \in D(u)$ (the domain of u).

Let us recall the well-known Brezis–Nagumo theorem (see [1] and [2, p. 25]):

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Theorem 1. *A closed set $D \subset \mathbb{R}^N$ is positively invariant with respect to Eq. (1.1) if and only if the following tangency condition is satisfied*

$$\lim_{h\downarrow 0} \frac{1}{h} d(z + hf(z), D) = 0, \quad \forall z \in D, \tag{1.3}$$

where $d(x, D) := \min_{y\in D} \|x - y\|$, with $\|\cdot\|$ a norm of $\mathbb{R}^N$, say the Euclidean norm.

Remark 1. In fact Theorem 1 is valid in any general real Banach space X, under the condition that $f : X \to X$ is a locally Lipschitz function (obviously, if X is finite dimensional, then this condition is equivalent to the Lipschitz continuity of f on every bounded subset of X).

Remark 2. If $D \subset \mathbb{R}^N$ is a compact set satisfying condition (1.3), then for every $u_0 \in D$ there exists a unique solution u of problem (1.1), (1.2) defined on $[0, +\infty)$, with $u(t) \in D$ for all $t \in [0, +\infty)$. Indeed, the trajectory of the unique local solution u of problem (1.1), (1.2) remains in the compact set D (cf. Theorem 1) and so the solution exists on the whole positive half-line: $D(u) = [0, +\infty)$.

In [3] the Hanusse mathematical model [4] was revisited and additional similar models have been proposed to describe chemical reactions involving more species (see also Section 3). In fact, all these models (systems of ODEs whose right-hand sides are some polynomial functions of degree 2 of the unknown variables (concentrations)) can be regarded as differential equations in $\mathbb{R}^N$, $N \geq 3$, of the form (1.1). For certain coefficients of these differential systems, some positively invariant sets of the form

$$D = \left[a_1, \bar{a}_1\right] \times [a_2, \bar{a}_2] \times \cdots \times [a_N, \bar{a}_N] \subset \mathbb{R}^N, \quad 0 < a_i < \bar{a}_i < \infty \ (i = \overline{1, N}), \tag{1.4}$$

have been identified, based on the tangency condition (1.3). Indeed, for such coefficients the following inequalities were established in [3] for all $1 \leq i \leq N$

$$\begin{aligned} &f_i(x_1, \ldots, x_{i-1}, a_i, x_{i+1}, \ldots, x_N) > 0, \qquad f_i(x_1, \ldots, x_{i-1}, \bar{a}_i, x_{i+1}, \ldots, x_N) < 0, \\ &\forall x_j \in [a_j, \bar{a}_j],\ j = \overline{1, N},\ j \neq i, \end{aligned} \tag{1.5}$$

which lead to (1.3) (see, e.g., [5, Lemma 4.1, p.72]). Based on the invariance of the D's (following from Theorem 1), a closed trajectory (periodic solution) was supposed to exist for each of such ODE models. This was indeed the case, even more, the existence of an attractive closed curve (attractor) was established by numerical simulations in [3] for each of the Hanusse-type models investigated there, for suitable sets of coefficients.

In this paper we consider the same Hanusse-type models, but this time we also take into account the diffusions of species inside the reaction domain $\Omega \subset \mathbb{R}^n$, $n \leq 3$. So we have PDE systems of the form

$$\frac{\partial u_i}{\partial t} = \alpha_i \Delta u_i + f_i(u), \quad t \geq 0,\ x \in \Omega,\ i = \overline{1, N}, \tag{1.6}$$

where $u_i = u_i(t, x)$ denote the variable concentrations of the corresponding intermediate species, $\Delta := \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}$, and α_i are positive constants (diffusion coefficients). We associate with (1.6) the following natural boundary conditions

$$\frac{\partial u_i}{\partial \nu} = 0, \quad t \geq 0,\ x \in \partial\Omega,\ i = \overline{1, N}, \tag{1.7}$$

where $\frac{\partial u_i}{\partial \nu}$ denotes the outward normal derivative of u_i, and initial conditions

$$u_i(0, x) = u_i^0(x), \quad x \in \Omega,\ i = \overline{1, N}. \tag{1.8}$$

In the next section of this paper we show that the D invariant sets $\subset \mathbb{R}^N$ with respect to system (1.6) without diffusions can be used to define invariant sets $\subset L^\infty(\Omega)^N$ with respect to system (1.6) with diffusions. The last section of the paper (Section 3) is devoted to simulations for both the ODE and PDE Hanusse-type models for different values of the data (i.e., different suitable values of the coefficients involved in the polynomial reaction terms as well as different values of the α_i's), which will show that the attractive closed orbits (attractors) of the ODE Hanusse-type systems are also attractors for the PDE Hanusse-type systems. In fact there are no other attractors of these PDE systems. According to the usual terminology (see [6]), a Hanusse-type model may become self-organized (i.e., its trajectory gets closer and closer to a limit cycle as t goes to infinity) for suitable coefficients of the polynomials f_i. Note that the existence of these attractors is based only on numerical simulations (we only show rigorously the existence of bounded, positively invariant sets). It is well-known that the existence of periodic solutions (in particular the existence of attractive closed orbits) in the case $N \geq 3$ is an open problem even for ODE systems so performing simulations is currently the only possibility to investigate the temporal behavior of these models.

Besides the Hanusse-type models investigated in this paper, there have also been reported other self-organized chemical models, including the Brusselator (see [7]) and the Oregonator which is the simplest model of the Belousov–Zhabotinsky

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