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Global dynamics and robustness of reversible autocatalytic reaction–diffusion systems

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ABSTRACT

Global asymptotic dynamics of a representative cubic-autocatalytic reaction–diffusion system, the reversible Selkov equations, are investigated. This system features two pairs of oppositely signed nonlinear terms so that the asymptotic dissipative condition is not satisfied, which causes substantial difficulties in an attempt to attest that the longtime dynamics are asymptotically dissipative. An L^2 to H^1 global attractor of finite fractal dimension is shown to exist for the semiflow of the weak solutions of the reversible Selkov equations with the Dirichlet boundary condition on a bounded domain of dimension $n \leq 3$. A new method of rescaling and grouping estimation is used to prove the absorbing property and the asymptotical compactness. Importantly, the upper semicontinuity (robustness) in the H^1 product space of the global attractors for the family of solution semiflows with respect to the reverse reaction rate as it tends to zero is proved through a new approach of transformative decomposition to overcome the barrier of the perturbed singularity between the reversible and non-reversible systems by showing the uniform dissipativity and the uniformly bounded evolution of the union of global attractors under the bundle of reversible and non-reversible semiflows.

1. Introduction

In this work, we shall study global dynamics and robustness of a class of reversible autocatalytic reaction–diffusion systems represented by the reversible Selkov equations,

$$\frac{\partial u}{\partial t} = d_1 \Delta u + \rho - au + u^2 v - Gu^3, \quad t > 0,\ x \in \Omega, \tag{1.1}$$

$$\frac{\partial v}{\partial t} = d_2 \Delta v + \beta - bv - u^2 v + Gu^3, \quad t > 0,\ x \in \Omega, \tag{1.2}$$

where $d_1, d_2, \rho, \beta, a, b$, and G are positive constants, $\Omega \subset \mathbb{R}^n$ ($n \leq 3$) is a bounded domain that has a locally Lipschitz continuous boundary, with the homogeneous Dirichlet boundary condition

$$u(t, x) = 0, \qquad v(t, x) = 0, \quad t > 0,\ x \in \partial\Omega, \tag{1.3}$$

and an initial condition

$$u(0, x) = u_0(x), \qquad v(0, x) = v_0(x), \quad x \in \Omega. \tag{1.4}$$

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We do *not* assume that the initial data u_0 and v_0, nor $u(t,x)$ and $v(t,x)$, are nonnegative functions. We do *not* impose any other conditions on any of these positive parameters.

The original system of non-reversible Selkov equations [1], like the other cubic-autocatalytic reaction–diffusion systems such as the Brusselator equations [2,3], Gray–Scott equations [4–6], and Schnackenberg equations [7], was a system of ODEs proposed by Selkov [8–10] as a simplified model of a fundamental biochemical process called *glycolysis*, by which living cells obtain energy through breaking down sugar. This is a prototype of cubic-autocatalytic chemical and biochemical reactions that include the famous chlorite–iodide–malonic acid (CIMA) reaction and many enzyme and kinase reactions in biochemistry and physiology [8,9,11,12], such as the phosphofructokinase reaction in the process of glycolysis involving the macro-molecules ATP, ADP and AMP.

The reversible cubic-autocatalytic Selkov equations can be derived from the following prototypical reactions:

$$\mathrm{A} \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} \mathrm{S}, \qquad \mathrm{S} + 2\mathrm{P} \underset{k_{-2}}{\overset{k_2}{\rightleftarrows}} 3\mathrm{P}, \qquad \mathrm{P} \underset{k_{-3}}{\overset{k_3}{\rightleftarrows}} \mathrm{B}. \tag{1.5}$$

These reactions involve *non-zero reverse reaction rates* which, however, are usually assumed zero or neglected in most of the published research articles. Here A and B are respectively the reactant and the product whose concentrations $A = [\mathrm{A}]$ and $B = [\mathrm{B}]$ are assumed to be constants, and the concentrations $P = [\mathrm{P}]$ and $S = [\mathrm{S}]$ of the intermediate substrates P and S are unknown functions of (t,x). Here k_i's are rate constants of respective reactions. The law of mass actions in kinetics of chemical reactions and Fick's law of diffusion yield the following reversible Selkov equations:

$$\frac{\partial P}{\partial \tau} = D_1 \Delta P + k_{-3} B - k_3 P + k_2 S P^2 - k_{-2} P^3, \tag{1.6}$$

$$\frac{\partial S}{\partial \tau} = D_2 \Delta S + k_1 A - k_{-1} S - k_2 S P^2 + k_{-2} P^3, \tag{1.7}$$

where τ is time, D_1 and D_2 are the diffusive constants.

By nondimensionalization and redefining the parameters and the two unknowns, this reaction–diffusion system is reduced to the dimensionless form (1.1) and (1.2) of the reversible Selkov equations. Since the reaction $S + 2P \rightleftarrows 3P$ is the main reaction, the nondimensionalized reverse rate constant $G > 0$ is the key parameter in this system. When $G = 0$ which means the main reaction in (1.5) is non-reversible, (1.1) and (1.2) are then reduced to the diffusive Selkov equations whose global asymptotic dynamics have been studied in the author's paper [1].

Numerical simulations [13–15], experimental works [16–18,11], and mathematical analysis [19–29] have found that the Selkov equations (with $G = 0$) and the similar non-reversible Brusselator equations and Gray–Scott equations exhibit complex and interesting spatial–temporal patterns and dynamics [30–32], such as self-excitation, self-oscillations, self-replicating spikes, and bifurcations in space dimension $n \leq 2$.

Recently, in [3,6,1,7] the existence of a global attractor with finite fractal dimensionality in the L^2 space for the Brusselator equations, Gray–Scott equations, Selkov equations, and Schnackenberg equations in bounded domains of space dimension $n \leq 3$ was proved by the author. However, the methods of conducting *a priori* estimation in proving the absorbing property and in proving the asymptotical compactness for non-reversible equations do not work for the reversible Selkov equations (and the other non-reversible cubic-autocatalytic reaction–diffusion systems) in this paper.

The difficulty in studying this representative reversible Selkov equations lies in the additional pair of cubic terms $\pm Gu^3$ in (1.1) and (1.2), which takes into account the reversibility of the key cubic-autocatalytic chemical or biochemical reactions. As far as the authors are aware of, no results have been reported concerning global temporal–spatial patterns or dynamics of the reversible Selkov equations especially on 3D (three-dimensional) domains either by numerical simulations or through mathematical analysis.

The basic theory of global dynamics and applications can be found in [33–35] and many references therein. For a single reaction–diffusion equation, the asymptotic dissipation is attested by either imposing or checking the asymptotic sign condition on the nonlinear function $f(u)$, i.e.

$$\limsup_{|s|\to\infty} f(s)s \leq C$$

where $C \geq 0$ is some constant. However, for many reaction–diffusion systems consisting of two or more equations arising from chemical and biochemical kinetics, or from the activator–inhibitor equations such as Gierer–Meinhardt equations, the corresponding asymptotically sign condition *in vector version* as above is inherently not satisfied. This is the case for the reversible Selkov equations here. Only for few partially dissipative reaction–diffusion systems, such as FitzHugh–Nagumo equations, results on the existence of local attractors [34,35] and a global attractor [36] are known to exist. Another approach of constructing positively invariant regions can only be used to study local attractors and with restrictions to the solutions.

In this paper, for the *reversible* Selkov equations (1.1)–(1.2), we take a new approach of rescaling and grouping estimation to conduct estimates and to show the existence of an L^2 to H^1 global attractor. Moreover, we shall prove that the family of global attractors parametrized by the key reverse reaction rate $G \geq 0$ is upper-semicontinuous at $G = 0$, which reveals the robustness of the global asymptotic dynamics for such a class of singularly perturbed reversible reaction–diffusion systems. To the best knowledge of the author, these are novel results in the front of global dynamics of reversible autocatalytic reaction–diffusion systems.