J Math Chem (2012) 50:989–995
DOI 10.1007/s10910-011-9946-9

ORIGINAL PAPER

Global dynamics of the smallest chemical reaction system with Hopf bifurcation

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Received: 3 October 2011 / Accepted: 14 November 2011 / Published online: 24 November 2011

Abstract The global behavior of solutions is described for the smallest chemical reaction system that exhibits a Hopf bifurcation, discovered in [12]. This three-dimensional system is a competitive system and a monotone cyclic feedback system. The Poincaré–Bendixson theory extends to such systems [2,3,6,8] and a Bendixson criterion exists to rule out periodic orbits [4].

Keywords Competitive system · Uniform persistence · Monotone cyclic feedback system · Compact attractor · Periodic orbit · Bendixson criterion

1 Introduction and main results

In [12], Wilhelm and Heinrich discover the "smallest chemical reaction system" which may exhibit a Hopf bifurcation. Like the famous Lorenz system, it is a three dimensional system with only a single quadratic nonlinearity. The Hopf bifurcation is studied in detail in [13] using center manifold and normal form techniques which establish the existence of a stable periodic orbit very near the bifurcation point. However, as they point out, their analysis does not preclude that chaotic behavior may occur in this simple system. Sprott [10] has cataloged many other three dimensional systems with quadratic nonlinearities which can have chaotic dynamics. However, we will show that this particular chemical reaction system does not support chaos. We give a fairly complete analysis of the global dynamics of the system of ordinary differential equations studied in [13]. It is given by the following equations:

Hal L. Smith is supported by NSF Grant DMS-0918440.

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$$\begin{aligned} x' &= kx - k_2xy \\ y' &= k_5z - k_3y \\ z' &= k_4x - k_5z \end{aligned} \tag{1.1}$$

where $k_i > 0,\ 1 \le i \le 5$ and $k = k_1A - k_4$ where A is the concentration of "the outer reactant of the autocatalytic reaction". The k_i are rate constants and k need not be positive; see [12]. Variables x, y, z denote concentrations and therefore are nonnegative.

The scaling $\bar{x} = x/a,\ \bar{y} = y/b,\ \bar{z} = z/c$ and the choice $k_2b = 1,\ k_5c = k_3b,\ k_4a = k_5c$ leads to the system:

$$\begin{aligned} x' &= kx - xy \\ y' &= k_3(z - y) \\ z' &= k_5(x - z) \end{aligned} \tag{1.2}$$

where we have dropped the bar over variables for simplicity. Our focus is on the dynamics exhibited by (1.2) in the nonnegative octant $\mathbb{R}^3_+$.

System (1.2) is a competitive system because the signed undirected incidence graph of its Jacobian matrix has a single loop with two positive feedbacks and one negative one:

$$x \xrightarrow{+} z \xrightarrow{+} y \xrightarrow{-} x$$

See [3,8]; the change of variables $z \to -z$ gives the system the canonical form with all off-diagonal entries of the Jacobian being non-positive. Since it is three dimensional, the celebrated Poincaré–Bendixon theorem extends to its solutions by a result of Hirsch [2,3,8]: A compact omega or alpha limit set that contains no equilibrium is a periodic orbit. In fact, system (1.2) is also a monotone cyclic feedback system [6], for which the Poincaré–Bendixon theorem also holds (regardless of the dimension of the system). The recent paper [11] proposes an alternative smallest chemical reaction system supporting a Hopf bifurcation that is also a competitive quadratic system.

We note that 0 is the unique equilibrium of (1.2) if $k \le 0$; it is asymptotically stable if $k \le 0$ and unstable when $k > 0$. In the latter case, the stable manifold of 0 in $\mathbb{R}^3_+$ is $S = \{(x, y, x) \in \mathbb{R}^3_+ : x = 0\}$. If $k > 0$, there is an additional equilibrium $E = k(1, 1, 1)$ which is asymptotically stable if $k < k_3+k_5$ and unstable if $k > k_3+k_5$ with a pair of complex conjugate eigenvalues with positive real part and one negative eigenvalue.

Part (a) of the following result was proved in [13] using a linear Lyapunov function.

Theorem 1.1 *The following hold for* (1.2):

(a) *If* $k \le 0$*, every solution converges to* 0.
(b) *If* $0 < k < k_3 + k_5$*, then every solution except those on* S *converge to* E.
(c) *If* $k > k_3 + k_5$*, then every solution not starting on* S *or on the one-dimensional stable manifold of* E*, converges to a nontrivial periodic orbit. At least one*

periodic orbit is orbitally asymptotically stable and the number of periodic orbits is finite.

Moreover, if $k > 0$ *then any solution not starting in* S *satisfies*

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T u(s)ds = k, \quad u = x, y, z. \tag{1.3}$$

The main open problem concerning the dynamics of (1.2) is the number of periodic orbits in case (c). Numerical simulations suggest there is only one.

The geometry of the stable manifold of E is described in the following result. It is tangent at E to the eigenvector with sign pattern $(+, +, -)$ and has certain monotonicity properties due to the monotonicity of the time-reversed system.

Proposition 1.2 *Let* $k > k_3 + k_5$. *Then the stable manifold of* E *in* $\mathbb{R}^3_+$ *consists of* E *and two monotone solutions* $p_u(t) = (x_u(t), y_u(t), z_u(t))$, $t \in [0, \infty)$ *and* $p_l(t) = (x_l(t), y_l(t), z_l(t))$, $t \in [0, \infty)$.

p_u *satisfies* $p_u(0) = (x_u(0), 0, z_u(0))$ *with* $0 < x_u(0) < k < z_u(0)$, $p_u(\infty) = E$ *and* x_u, y_u *are strictly increasing while* z_u *is strictly decreasing. Therefore, the graph of* p_u *belongs to* $[0, k] \times [0, k] \times [k, \infty)$.

p_l *satisfies* $p_l(0) = (x_l(0), y_l(0), 0)$ *with* $x_l(0), y_l(0) > k$, $p_l(\infty) = E$ *and* x_l, y_l *are strictly decreasing while* z_l *is strictly increasing. Therefore, the graph of* p_l *belongs to* $[k, \infty) \times [k, \infty) \times [0, k]$.

As a consequence of Proposition 1.2, the unstable manifold of 0 connects 0 to a nontrivial periodic solution in case (c) of Theorem 1.1; it cannot be a heteroclinic orbit connecting 0 to E.

Theorem 1.3 *System* (1.2) *has a non-empty compact invariant set* A *that attracts all bounded subsets of* $\mathbb{R}^3_+$.

If $k \le 0$, *then* $A = \{0\}$.

If $k > 0$. *Then* $A \subset [0, M]^3$ *where* $M = \frac{k(k+k_5)(k+k_3)}{k_3 k_5}$.

Theorem 1.4 *If* $k > 0$, *then* (1.2) *is uniformly persistent, i.e.,* $\exists \eta > 0$ *such that:*

$$\min\{x(0), y(0), z(0)\} > 0 \Rightarrow \liminf_{t\to\infty} \min\{x(t), y(t), z(t)\} > \eta. \tag{1.4}$$

The attractor A *is the disjoint union* $A = \{0\} \cup C \cup A_1$ *where:*

(i) $\{0\}$ *attracts all bounded subsets of* S.
(ii) A_1 *is a compact invariant subset of the interior of* $\mathbb{R}^3_+$ *that attracts all compact subsets of* $\mathbb{R}^3_+$ *that do not intersect* S.
(iii) C *is the one-dimensional unstable manifold of* $\{0\}$ *which connects* 0 *to* A_1.

2 Proofs

Proof Proof of Theorem 1.3. Let $\phi(t, p)$ denote the solution of (1.2) which at $t = 0$ is at $p = (x(0), y(0), z(0))$. If $k \le 0$, then $x' \le 0$ and it is trivial to show that $A = \{0\}$.

Assume that $k > 0$. According to Theorem 2.33 in [9], we must show that (1.2) is point dissipative and for every bounded set B there exists $t_r \geq 0$ such that $\phi([t_r, \infty) \times B)$ is bounded.

We start by showing that it is point dissipative. If $x(0) = 0$, then $x(t) = 0$ for all t and there exists $\eta, \alpha > 0$ such that $y(t) + z(t) \leq \eta(y(0) + z(0))e^{-\alpha t}$. Assume that $x(0) > 0$. Then direct computation shows that

$$\begin{aligned} (y/x)' &\geq k_3(z/x) - (k + k_3)(y/x) \\ (z/x)' &\geq k_5 - (k + k_5)(z/x) \end{aligned} \tag{2.1}$$

It follows that $(z/x)_\infty \geq \frac{k_5}{k+k_5}$ and $(y/x)_\infty \geq \frac{k_3k_5}{(k+k_3)(k+k_5)}$ where $f_\infty = \liminf_{t\to\infty} f(t)$. Consequently, for every $\epsilon > 0$, there exists $t_0 > 0$ such that

$$x' = kx - x^2(y/x) \leq kx - m_\epsilon x^2, \quad t > t_0$$

where $m_\epsilon = \frac{k_3k_5}{(k+k_3)(k+k_5)} - \epsilon$. Hence, $x^\infty = \limsup_{t\to\infty} x(t) \leq k/m_\epsilon$ and, since $\epsilon > 0$ is arbitrary, $x^\infty \leq M$. Using this estimate and the differential equation for z immediately yields $z^\infty \leq M$; using this last estimate and the differential equation for y yields $y^\infty \leq M$. Thus, we have shown that all points are attracted to the bounded set $[0, M]^3$ and (1.2) is point dissipative.

Now we identify a family of positively invariant bounded sets. Let $0 < \sigma \leq \frac{k_5}{k+k_5}$, $0 < \rho \leq \frac{k_3\sigma}{k+k_3}$, and $K \geq k/\rho$. Define

$$B_{(\sigma,\rho,K)} = \{(x, y, x) \in [0, K]^3 : x = 0 \text{ or } z/x \geq \sigma \text{ and } \ y/x \geq \rho\}$$

We claim that $B_{(\sigma,\rho,K)}$ is positively invariant. Indeed, integrating the second inequality (2.1) leads to

$$(z/x)(t) \geq \frac{k_5}{k + k_5}(1 - e^{-(k+k_5)t}) + e^{-(k+k_5)t}(z/x)(0) \geq \sigma \tag{2.2}$$

for any solution starting in $B_{(\sigma,\rho,K)}$ with $x(0) \neq 0$. Similarly, using that $(z/x)(t) \geq \sigma$ in the first inequality (2.1) leads to

$$(y/x)(t) \geq \frac{k_3\sigma}{k + k_3}(1 - e^{-(k+k_3)t}) + e^{-(k+k_3)t}(y/x)(0) \geq \rho.$$

As $x' = kx - x^2(y/x) \leq x(k - \rho x) \leq 0$ when $x = K$, $z' = k_5(x - z) \leq 0$ when $z = K$ and $0 \leq x \leq K$, and $y' = k_3(z - y) \leq 0$ when $y = K$ and $0 \leq z \leq K$, the positive invariance of $B_{(\sigma,\rho,K)}$ follows.

Finally, we show that $\forall L > 0$ there exists $0 < \sigma < \frac{k_5}{k+k_5}$, $0 < \rho < \frac{k_3\sigma}{k+k_3}$, and $K \geq k/\rho$ such that $\phi(2, [0, L]^3) \subset B_{(\sigma,\rho,K)}$. Since $B_{(\sigma,\rho,K)}$ is bounded and positively invariant, this proves that $\phi([2, \infty) \times [0, L]^3)$ is bounded. Hence, bounded sets have uniformly bounded orbits.

Let $(x(0), y(0), z(0)) \in [0, L]^3$ and $x(0) > 0$. Integrating the second of (2.1) gives

$$\frac{z(t)}{x(t)} \geq \frac{k_5}{k+k_5}(1-e^{-(k+k_5)}),\ t \geq 1.$$

Let σ be the right side of the above inequality and note that $\sigma < \frac{k_5}{k+k_5}$. Substituting this estimate into the first of (2.1) and integrating leads to

$$\frac{y(2)}{x(2)} \geq \frac{k_3\sigma}{k+k_3}(1-e^{-(k+k_3)})$$

Let ρ be the right hand side of the above inequality and note that $\rho < \frac{k_3\sigma}{k+k_3}$. Now we can choose $K > k/\rho$ so large that $x(2), y(2), z(2) \leq K$ holds for every point $(x(0), y(0), z(0)) \in [0, L]^3$. It follows that for every point $(x(0), y(0), z(0)) \in [0, L]^3$, we have $(x(2), y(2), z(2)) \in B_{(\sigma,\rho,K)}$. □

Proof Proof of Proposition 1.2. The time reversed system of (2.1) is a monotone dynamical system with respect to the partial order induced by the octant $K = \{(x, y, z): x, y \geq 0, z \leq 0\}$. So we make use of Theorem 2.8 in [7]. By irreducibility of the Jacobian matrix at E, there is an eigenvector $v \in K$ with nonzero components. Moreover, the unstable manifold of E for the time-reversed system consists of E and two strictly monotone trajectories $P_u \in E - K$ and $P_l \in E + K$ that are described in Theorem 2.8 in [7]. The monotone trajectory P_u must exit $\mathbb{R}^3_+$ through the $y = 0$ hyperplane because the derivative of y is negative and bounded away from zero. □

Proof Proof of Theorem 1.4. We employ Theorem 8.17 in [9], using the notation developed there. Let $p = (x, y, z) \in \mathbb{R}^3_+$ and $\rho(p) = \min\{x, y, z\}$. $X_0 = \{p \in \mathbb{R}^3_+ : \rho(\phi(t, p)) = 0,\ t \geq 0\}$ consists of the stable manifold S of 0. The requisite compactness assumption (H) of Theorem 8.17 follows from Theorem 1.3. $\Omega = \cup_{p\in X_0}\omega(p) = \{0\}$ where $\omega(p)$ denotes the omega limit set of p. $M \equiv \{0\}$ is obviously an acyclic covering of Ω and it is an isolated invariant set in $\mathbb{R}^3_+$ because 0 is a hyperbolic equilibrium (Hartman–Grobman Theorem). Finally, M is weakly ρ-repelling, meaning that there is no $p \in \mathbb{R}^3_+$ such that $\rho(p) > 0$ and $\phi(t, p) \to M$ as $t \to \infty$. This follows because the stable manifold of 0 is exactly the $x = 0$ facet S where $\rho = 0$. Consequently, we may apply Theorem 8.17 in [9] to conclude that ϕ is uniformly weakly ρ-persistent: $\exists\eta > 0$ such that $\rho(p) > 0 \Rightarrow \limsup_{t\to\infty}\rho(\phi(t, p)) > \eta$. We conclude uniform strong persistence, i.e., replacing limsup by liminf in the above implication, by invoking Theorem 4.5 in [9].

The partition of the attractor $A = \{0\} \cup C \cup A_1$ is a consequence of Theorem 5.7 in [9]. □

Proof Proof of Theorem 1.1. Part (a) was proved in [13]. Part (c) follows from Theorems 1.1 and 1.2 of [14] where we check that the determinant of the Jacobian at E is $-kk_3k_5 < 0$.

The final assertion uses the uniform persistence established in Theorem 1.4, which implies that the set $D = [\eta, M]^3$ is an absorbing set for positive solutions of (1.2). Since $\frac{1}{T}\int_0^T \frac{x'}{x}ds = \frac{1}{T}\ln(x(T)/x(0)) \to 0$ as $T \to \infty$ because x is bounded and bounded away from zero, we see from the differential equation that $\lim_{T\to\infty} \frac{1}{T}\int_0^T (k - y(s))ds = 0$. Indeed, this limit is uniform for all solutions starting in D because $|\ln(x(T)/x(0))|$ is uniformly bounded on D. Thus,

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T y(s)ds = k$$

uniformly for solutions in D. The other limits follow more easily and they too are uniform in D.

Part (b) is more technical. We use the geometric approach of ruling out periodic orbits developed in [4] which uses the second additive compound $Df(p)^{[2]}$ of the Jacobian matrix $Df(p)$, where $f(p)$ denotes the vector field (1.2):

$$Df(p)^{[2]} = \begin{pmatrix} k-y-k_3 & k_3 & 0 \\ 0 & k-y-k_5 & -x \\ -k_5 & 0 & -(k_3+k_5) \end{pmatrix}$$

See, e.g., formula for $Df(p)^{[2]}$ in appendix of [5]. As $k < k_3 + k_5$, we may find $\epsilon \in (0, 1/2)$ such that $k/(1-2\epsilon) < k_3 + k_5$. Consider the 3×3 matrix-valued function $p \to A(p)$ where $A(p)$ is a diagonal matrix with diagonal entries $(1-2\epsilon)/x,\ (1-\epsilon)/x,\ -1/k_5$. Using the notation of [4], we compute the matrix function $B(p) = A_f A^{-1} + ADf(p)^{[2]}A^{-1}$ where A_f is the directional derivative of A with respect to vector field f. We find that

$$B(p) = \begin{pmatrix} -k_3 & k_3\frac{1-2\epsilon}{1-\epsilon} & 0 \\ 0 & -k_5 & k_5(1-\epsilon) \\ \frac{x}{1-2\epsilon} & 0 & -(k_3+k_5) \end{pmatrix} \tag{2.3}$$

The Lozinskiǐ measure $\mu(B)$ relative to the norm $|p| = \max\{|x|, |y|, |z|\}$ is (see pg 41 of [1]):

$$\mu(B) = \max\left\{-\epsilon k_3/(1-\epsilon), -\epsilon k_5, \frac{x}{1-2\epsilon} - (k_3+k_5)\right\}$$

Now we use that $\lim_{T\to\infty} \frac{1}{T}\int_0^T x(s)ds = k$ is uniform for all orbits starting in the absorbing set B and that $k/(1-2\epsilon) < k_3 + k_5$ to conclude that

$$\bar{q}_2 = \limsup_{T\to\infty} \sup_{p\in D} \frac{1}{T}\int_0^T \mu(B(\phi(s,p)))ds < 0.$$

Theorem 3.1 of [4] implies that there can be no nontrivial periodic orbit of (1.2). By the Poincaré–Bendixson theorem for competitive three dimensional systems [2,3,8], E attracts all solutions not starting on S. $\square$

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