GLOBAL QUALITATIVE DYNAMICS OF THE BRUSSELATOR SYSTEM

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Abstract. We study the dynamics of the Brusselator model by describing the global flow of this differential system in the Poincaré disc, and we prove that its unique equilibrium point is a global attractor.

1. Introduction and statement of the results

We consider the differential system

$$\begin{aligned} \dot{x} &= a + x^2y - (b+c)x, \\ \dot{y} &= bx - x^2y, \end{aligned} \tag{1}$$

called the *Brusselator model* where x and y are the dimensionless concentration of some species and the parameters a, b, c are all positive. Such differential system appears in several branches of the sciences, mainly in chemistry because it exhibits kinetics of model trimolecular irreversible reactions (see [3, 4] for details). The first integrals of system (1) in function of its parameters were studied in [5].

We will determine the qualitative behavior of all the solutions of system (1), by describing its phase portraits in the Poincaré disc in function of its parameters. See the appendix for the definitions and the basic results that we use, and in particular for the definition of the Poincaré disc.

We say that two vector fields on the Poincaré disc are topologically equivalent if there exists a homeomorphism of the Poincaré disc which sends orbits to orbits preserving or reversing their orientation.

Our main result is the following one.

Theorem 1. *The global phase portrait of system* (1) *in the Poincaré disc is topologically equivalent to the one described in Figure 1. Note that its unique finite singular point is a global attractor.*

The proof of Theorem 1 is given in section 2, the more delicate step in this proof is to show the non–existence of periodic solutions. We have also

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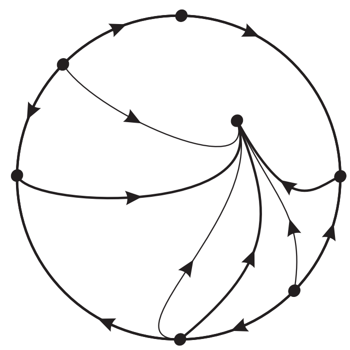

FIGURE 1. This phase portrait in the Poincaré disc has 16 separatrices and 3 canonical regions.

included an appendix with all the definitions and basic results related with the Poincaré compactification.

2. Proof of Theorem 1

By the change of coordinates and reparametrization of time of the form

$$x \to aX/b, \quad y \to b^2Y/a, \quad t \to \tau/a,$$

we can write system (1) as

$$\begin{aligned} \dot{x} &= \\ \dot{y} &= x - x^2 y, \end{aligned} \tag{2}$$

where $k = c/b > 0$. The dot denotes derivative with respect to the new variable τ and we have renamed the new variables (X, Y) as (x, y).

2.1. **The finite singular points.** The unique finite singular point is $(1/k, k)$. The Jacobian matrix M of system (2) at this singular point is

$$M = \begin{pmatrix} 1-k & 1/k^2 \\ -1 & -1/k^2 \end{pmatrix}.$$

The eigenvalues of M are

$$\frac{-1 + k^2 - k^3 \pm \sqrt{(1 - k^2 + k^3)^2 - 4k^3}}{2k^2}.$$

We study the zeroes of $1 - k^2 + k^3 = 0$ and we get two complex solutions and the following real one

$$\bar{k} = \frac{1}{3} - \frac{1}{3}\Big(\frac{2}{25 - 3\sqrt{69}}\Big)^{1/3} - \frac{1}{3}\Big(\frac{1}{2}(25 - 3\sqrt{69})\Big)^{1/3} < 0.$$

Since we are interested for the values of $k > 0$, and then we have that $-1 + k^2 - k^3 < 0$, the equilibrium point is always stable. Moreover, the determinant of M is $1/k > 0$, and so the finite singular point is either a hyperbolic node or a hyperbolic focus. We compute the zeroes of $(1-k^2+k^3)^2-4k^3=0$, and we get four complex zeroes and two real ones, which are

$$k_1 = \frac{1}{3} - \frac{5}{3}\Big(\frac{2}{11+3\sqrt{69}}\Big)^{1/3} + \frac{1}{3}\Big(\frac{1}{2}(11+3\sqrt{69})\Big)^{1/3} = 0.5698.. > 0$$

and

$$k_2 = \frac{1}{3} + \frac{1}{3}\Big(\frac{47}{2} - \frac{3\sqrt{93}}{2}\Big)^{1/3} + \frac{1}{3}\Big(\frac{1}{2}(47+3\sqrt{93})\Big)^{1/3} = 2.1478.. > k_1.$$

So if $k \in (0, k_1] \cup [k_2, +\infty)$ the singular point $(1/k, k)$ is a hyperbolic stable node, and if $k \in (k_1, k_2)$ it is a hyperbolic stable focus.

Now we shall show that this system has no periodic solutions, the proof will use the Dulac–Bendixson criterion, i.e.:

Theorem 2. *If there exists a C^1 function $B(x, y)$ in a simply connected region R such that $\partial(BP)/\partial x + \partial(BQ)/\partial y$ has constant sign and is not zero in a simply connected domain R, then the C^1 differential system $\dot{x} = P(x, y)$, $\dot{y} = Q(x, y)$ does not have periodic orbits in R.*

For a proof of this criterion see Theorem 7.12 of [2].

Proposition 3. *The polynomial differential system* (2) *has no periodic solutions.*

Proof. First note that for $k > 0$ the singular point $(1/k, k)$ belongs to the positive quadrant $x > 0$ and $y > 0$. We have that

$$\dot{x}|_{\{x=1/(1+k),y>0\}} = \frac{y}{(1+k)^2} > 0 \quad \text{and} \quad \dot{y}|_{\{x>0,y=0\}} = x > 0. \tag{3}$$

If there exists a periodic solution, since it must surrounds the unique singular point $(1/k, k)$ (see for more details Theorem 1.31 of [2]), from (4) the periodic solution must be contained in the simply connected region

$$R = \{x > \frac{1}{1+k}, y > 0\}.$$

For any positive integer n consider the function

$$B(x, y) = \frac{1}{(x - 1/(1+k))^2}.$$

We apply the Dulac–Bendixson criterion to the differential system (2) in the region R with the function $B(x, y)$, note that $B(x, y) > 0$ in R. Then for $P(x, y) = 1-(1+k)x + x^2y$ and $Q(x, y) = x - x^2y$, we get that

$$\begin{aligned} g(x,y) = & \ \frac{\partial(BP)}{\partial x} + \frac{\partial(BQ)}{\partial y} \\ = & \ \frac{(k+1)^2\left(k^2x - k\left(x^3-2x+1\right) - x^3 + x^2 - 2xy + x - 1\right)}{((k+1)x-1)^3}. \end{aligned}$$

Note that in the region R the curve $g(x,y)=0$ is equivalent to the curve

$$f(x,y)=y-\frac{((k+1)x-1)\left(k+1-x^2\right)}{2x}=0, \tag{4}$$

defined for $x>\sqrt{k+1}$.

We claim that the curve $f(x,y)=0$ in the region R is transversal with respect to the flow of the differential system (2), i.e.

$$\left.\frac{\partial f}{\partial x}P+\frac{\partial f}{\partial y}Q\right|_{f=0}\neq 0 \quad \text{in } R.$$

Due to this claim a periodic orbit cannot intersect the curve $f(x,y)=0$ in the region R, therefore the function $g(x,y)$ does not vanish on a periodic orbit, and by the Dulac–Bendixson criterion the differential system (2) has no periodic solutions, as we want to prove.

Now we prove the claim. We have that

$$\left.\frac{\partial f}{\partial x}P+\frac{\partial f}{\partial y}Q\right|_{f=0}=-\frac{h(x)}{4x^2},$$

where

$$\begin{aligned} h(x)= \quad & 2(k+1)^2x^7-5(k+1)x^6+(-2k^3-6k^2-6k+1)x^5+8(k+1)^2x^4 \\ & -4(2k+3)x^3+(k^3+3k^2+3k+3)x^2-3(k+1)^2x+2(k+1). \end{aligned}$$

Using the Sturm sequence associated to the polynomial $h(x)$ it follows that the polynomial $h(x)$ has no real roots in the interval $(\sqrt{k+1},\infty)$. Consequently the claim is proved. See [9] for the definition and the properties of a Sturm sequence, we note that the algebraic manipulator mapple allows to compute the Sturm sequence associated to a polynomial. This completes the proof of the proposition. □

We have all the finite information. In the next subsection we study the infinite singular points.

2.2. **The infinite singular points.** On the local chart U_1 system (2) becomes

$$\begin{aligned} \dot u &= -u-u^2+v^2+(1+k)uv^2-uv^3, \\ \dot v &= v(-u+(1+k)v^2-v^3). \end{aligned}$$

The singular points (u,v) of this system on $v=0$ must satisfy $-u(1+u)=0$. So we have two infinite singular points in the local chart U_1: $q_1=(u,v)=(0,0)$ and $q_2=(u,v)=(-1,0)$. Computing the Jacobian matrix M_1 at the point q_1 we get

$$M_1=\begin{pmatrix}-1 & 0\\ 0 & 0\end{pmatrix}.$$

So, q_1 is semi-hyperbolic. Using Theorem 2.19 in [2] we get that it is a saddle. On the other hand, the Jacobian matrix M_2 at the point q_2 is

$$M_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

and so the point q_2 is a hyperbolic unstable node.

On the local chart U_2 system (2) becomes

$$\begin{aligned} \dot{u} &= u^2 + u^3 - (1+k)uv^2 + v^3 - u^2v^2, \\ \dot{v} &= uv(u - v^2). \end{aligned} \tag{5}$$

So the origin of U_2 is an equilibrium point whose linear part is identically zero, and by the Poincaré–Hopf Theorem (see for instance chapter 6 of [2]) its topological index must be 0.

We apply the blow-up techniques to study it, see for instance [1]. We first do a vertical blow-up. For this, we consider the new variables (u, w) where $w = v/u$. In these new variables system (5) writes

$$\begin{aligned} \dot{u} &= u^2(1 + u - u(1+k)w^2 - u^2w^2 + uw^3), \\ \dot{w} &= -uw(1 - (1+k)uw^2 + uw^3). \end{aligned}$$

We eliminate the common factor u by making a rescaling of time and we get

$$\begin{aligned} \dot{u} &= u(1 + u - u(1+k)w^2 - u^2w^2 + uw^3), \\ \dot{w} &= -w(1 - (1+k)uw^2 + uw^3). \end{aligned} \tag{6}$$

System (6) has a unique singular point on $u = 0$ which is $(u, w) = (0, 0)$. Computing the eigenvalues of the Jacobian matrix of system (6) at the origin we get that they are 1 and -1. Hence, the origin is a saddle. Going back through the changes of variables passing we do not have all the information for determining the local phase portrait at the origin of the local chart U_2. So we must do a horizontal blow-up. Hence, we consider the new variables (w, v) where $w = u/v$. In these new variables system (5) can be written as

$$\begin{aligned} \dot{w} &= v(v + w^2 - (1+k)wv), \\ \dot{v} &= wv^3(w - v). \end{aligned}$$

We eliminate the common factor v by making a rescaling of time and we get

$$\begin{aligned} \dot{w} &= v + w^2 - (1+k)wv, \\ \dot{v} &= wv^2(w - v). \end{aligned} \tag{7}$$

System (7) has a unique singular point on $v = 0$ which is the origin. Computing the eigenvalues of the Jacobian matrix at $(w, v) = (0, 0)$ we get that the origin is a nilpotent singular point. In order to determine its local behavior we need to do another blow-up. We thus consider another vertical

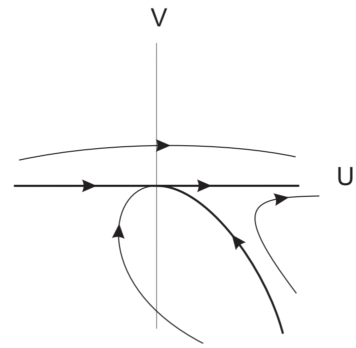

FIGURE 2. The local phase portrait at the origin of the local chart U_2.

blow-up of the form (w_1, v) where $w_1 = w/v$. In these new variables (7) writes

$$\dot{w}_1 = 1 - w_1 v(1+k) + w_1^2 v + w_1^2 v^3 - w_1^3 v^3,$$
$$\dot{v} = -w_1 v^4 (1 - w_1).$$

Note that this system has no singular points. Going back through the changes of variables from (w_1, v) until (u, v), and taking also into account the information on the horizontal blow-up we get that the origin of the local chart U_2 in the variables (u, v) is the degenerate saddle node of Figure 2.2.

2.3. **The phase portrait in the Poincaré disc.** Taking into account the local phase portraits at the finite and infinite singular points, together with the behavior of the vector field associated to system (2) on the axes of coordinates, and that in view of Proposition 3 system (2) has no limit cycles surrounding the finite singular point, the phase portrait in the Poincaré disc of system (2) is the one given in Figure 1. From this global phase portrait it follows that the equilibrium point $(1/k, k)$ is a global attractor. This concludes the proof of the theorem.

APPENDIX: BASIC RESULTS AND THE POINCARÉ DISC

In this section we present some basic results and notations which are necessary for stating and proving our results.

2.4. **Singular points of differential systems in $\mathbb{R}^2$.** Consider a differential system $\dot{x} = P(x, y)$, $\dot{y} = Q(x, y)$ in $\mathbb{R}^2$. A singular point or an equilibrium point of the differential system (2) is a point $(x_0, y_0) \in \mathbb{R}^2$ such that $P(x_0, y_0) = Q(x_0, y_0) = 0$.

We recall that a *hyperbolic singular point* is a singular point (x_0, y_0) such that the eigenvalues of the Jacobian matrix

$$\begin{pmatrix} \dfrac{\partial P}{\partial x}(x_0,y_0) & \dfrac{\partial P}{\partial y}(x_0,y_0) \\ \dfrac{\partial Q}{\partial x}(x_0,y_0) & \dfrac{\partial Q}{\partial y}(x_0,y_0) \end{pmatrix} \tag{8}$$

have nonzero real part. A *semi-hyperbolic singular point* is a singular point such that one of the eigenvalues of the matrix (8) is zero. A *nilpotent singular point* is a singular point such that the eigenvalues of the matrix (8) are both zero but the matrix is not identically zero. Finally, a *linearly zero singular point* is a singular point for which the matrix (8) is identically zero. For details on the local phase portraits of the hyperbolic, semi-hyperbolic and nilpotent singular points see [2]. On the other hand, the local phase portraits of the linearly zero singular points must be studied using the change of variables called blow-ups, see for instance [1].

2.5. **Poincaré compactification.** Let $p_i(x_1, x_2)$ be a real polynomial in the variables x_1, x_2, and let $X = (p_1, p_2)$ be a polynomial vector field of degree d in $\mathbb{R}^n$, being d the maximum of the degrees of the polynomials p_i for $i = 1, 2$ (see all the details in Chapter 5 of [2]).

The *Poincaré sphere* is defined as $\mathbb{S}^2 = \{y = (y_1, y_2, y_3) \in \mathbb{R}^3 : \sum_{i=1}^{3} y_i^2 = 1\}$ and its tangent space at the point $y \in \mathbb{S}^2$ is denoted by $T_y\mathbb{S}^2$. We identify the space $\mathbb{R}^2$ where is defined the polynomial vector field X with the tangent space $T_{(0,0,1)}\mathbb{S}^2$. We define the central projection $f : T_{(0,0,1)}\mathbb{S}^2 \longrightarrow \mathbb{S}^2$ as follows: to each point $q \in T_{(0,0,1)}\mathbb{S}^2$ the central projection f associates to q the two intersection points of the sphere $\mathbb{S}^2$ with the straight line which connects the points q with the origin of coordinates. Note that the infinity of $\mathbb{R}^2 \equiv T_{(0,0,1)}\mathbb{S}^2$ corresponds to the equator $\mathbb{S}^1 = \{y \in \mathbb{S}^2 : y_3 = 0\}$ of $\mathbb{S}^2$.

This central projection f provides two copies $Df \circ X$ of the polynomial vector field X in $\mathbb{S}^2$, one in the northern hemisphere and the other in the southern. Denote by X' the vector field defined by these two copies of X into the sphere $\mathbb{S}^2$ minus its equator $\mathbb{S}^1$. We can extend the vector field X' on $\mathbb{S}^2 \backslash \mathbb{S}^1$ to an analytic vector field $p(X)$ on $\mathbb{S}^2$ defining $p(X) = y_3^{d+1}\mathcal{X}'$. Let $\pi : \mathbb{R}^3 \longrightarrow \mathbb{R}^2$ the projection $\pi(y_1, y_2, y_3) = (y_1, y_2)$. Then the projection by π of the closed northern hemisphere of $\mathbb{S}^2$ is the *Poincaré disc* D. Note that the interior of D is diffeomorphic to $\mathbb{R}^2$ and its boundary $\mathbb{S}^1$ is the infinity of $\mathbb{R}^2$, and $\pi(p(X))$ is the extension of the polynomial vector field X to the Poincaré disc D.

For computing the analytic expression of $p(X)$ we consider the sphere $\mathbb{S}^2$ as a differentiable manifold. We consider $U_i = \{y \in \mathbb{S}^2 : y_i > 0\}$ and $V_i = \{y \in \mathbb{S}^2 : y_i < 0\}$ for $i = 1, \ldots, 3$. The corresponding coordinates maps are given by $F_i\colon U_i \to \mathbb{R}^2$ and $G_i\colon V_i \to \mathbb{R}^2$ by

$$F_i(y) = G_i(y) = \frac{1}{y_i}(y_{j_1}, y_{j_2})$$

with $1 \leq j_1 < j_2 \leq 3$ and $j_k \neq i$ for $k = 1, 2$. After a rescaling in the independent variable in the local chart (U_1, F_1) the expression of $p(X)$ is

$$z_2^d(-z_1 p_1 + p_2, -z_2 p_1),$$

where $p_i = p_i(1/z_2, z_1/z_2)$ for $i = 1, 2$.

In a similar manner we can deduce the expression of $p(X)$ in the local chart (U_2, F_2). This is

$$\begin{aligned} &z_2^d(-z_1 p_2 + p_1, -z_2 p_2), \\ &\quad p_i = p_i(z_1/z_2, 1/z_2), \text{ for } i = 1, 2. \end{aligned}$$

In the chart (V_i, G_i) the expression of $p(X)$ is the same than in the chart (U_i, F_i) multiplied by $(-1)^d$ for $i = 1, 2$.

2.6. **Topological equivalent polynomial vector fields.** We recall that two polynomial vector fields X and Y on $\mathbb{R}^2$ are *topologically equivalent* if there is a homeomorphism on the Poincaré disc D preserving the infinity $\mathbb{S}^1$ and carrying orbits of the flow of $\pi(p(X))$ into trajectories of the flow of $\pi(p(Y))$, either preserving or reversing the sense of all the orbits.

A *separatrix* of the Poincaré compactification $\pi(p(X))$ is a trajectory which is either an equilibrium point, or a limit cycle, or an orbit on the boundary of a hyperbolic sector at an equilibrium point, finite or infinity, or any orbit contained at the infinity $\mathbb{S}^1$. The closed set (see Neumann [7]) formed by all separatrices of $\pi(p(X))$ is denoted by Σ_X.

A *canonical region* of $\pi(p(X))$ is an open connected component of $D \setminus \Sigma_X$. The union of Σ_X plus one orbit chosen from each canonical region is the *separatrix configuration* of $\pi(p(X))$, denoted by Σ'_X. Two separatrix configurations Σ'_X and Σ'_Y are *equivalent* if there is a homeomorphism in B preserving the infinity $\mathbb{S}^1$ carrying orbits of Σ'_X into orbits of Σ'_Y, either preserving or reversing the sense of all orbits.

Markus [6], Neumann [7] and Peixoto [8] characterized the topologically equivalence between two Poincaré compactified vector fields by showing that two Poincaré compactified polynomial vector fields $\pi(p(X))$ and $\pi(p(Y))$ with finitely many separatrices are topologically equivalent if and only if their separatrix configurations Σ'_X and Σ'_Y are equivalent.

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