A chemical representation of a chaotic system with a unique stable equilibrium point

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Abstract: In this paper we present a chemical representation of a chaotic system with only one stable equilibrium point. The approach invokes cooperative catalysis and slow–fast reactions, primarily. The obtained chemical based chaotic dynamical system preserves the eigenvalues of the unique and stable equilibrium point along with the Lyapunov's dimension and exponents of the original one.

Keywords: Chaotic behaviour, Cooperative Autocatalysis, Hidden attractor, Unique stable equilibrium point.

1. INTRODUCTION

Wang and Chen (2012) presented the first chaotic dynamical system with a unique stable equilibrium point derived from a perturbation of the Sprott system, case E. The dynamical system equations are:

$$\frac{dx}{dt} = \dot{x} = yz + a$$
$$\frac{dy}{dt} = \dot{y} = x^2 - y \qquad (1)$$
$$\frac{dz}{dt} = \dot{z} = 1 - 4x$$

When $a = 0.006$, system (1) exhibits a chaotic behaviour despite the existence of a unique stable equilibrium point, $\mathbf{E} = [1/4, \ 1/16, \ -16a]$, with associated eigenvalues: $\lambda_1 = -0.96069$, $\lambda_{2,3} = -0.01966 \pm 0.50975\ i$.

The counterintuitive dynamical result reported by Wang and Chen (2012) was confirmed and extended by other researchers. For example, Molaile et al. (2013) derived 23 minimal chaotic three dimensional dynamical systems with a unique and stable equilibrium point. Later, Wei and Zhang (2014) reported hidden hyperchaotic attractors in a four-dimensional modified Lorenz–Stenflo system with three quadratic nonlinearities and only one stable equilibrium. The work of Kingni et al. (2014) went further: authors proposed a three-dimensional chaotic autonomous
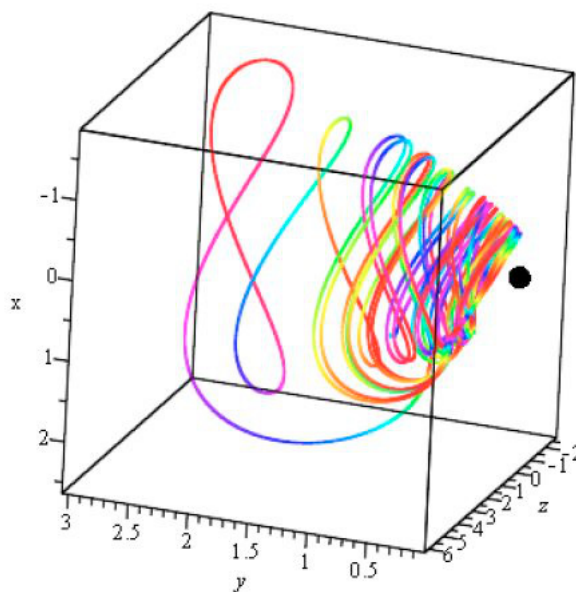

Fig. 1. Chaotic attractor of dynamical system (1) with $a = 0.006$. Black dot stands for the unique and stable equilibrium point, $\mathbf{E} = [1/4, \ 1/16, \ -0.096]$. Initial conditions: $[1, \ 1, \ 1]$.
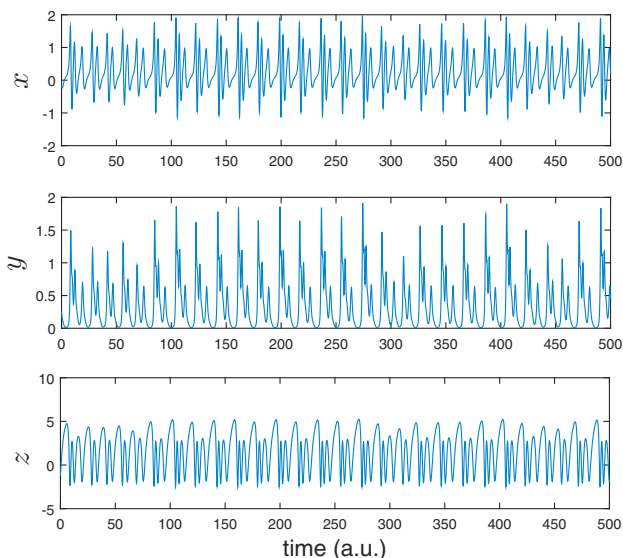
Fig. 2. Time series of dynamical system (1) with $a = 0.006$.

system with only one stable equilibrium whose physical existence was verified using the Orcard-PSpice software along with Routh-Hurwitz conditions that allow to choose linear controllers for chaotic synchronization. Moreover, Kingni et al. (2014) obtained necessary conditions for the commensurate fractional order version of the proposed system to remain chaotic; they also found that chaos is present in an order less than three. More recently, Moreno et al. (2015) used Monte-Carlo methods to find the simplest chaotic three dimensional system with quadratic nonlinearities and one stable equilibrium point.

However, none of the chaotic systems with one stable equilibrium point can be interpreted as a chemical derived dynamical system. This issue motivates the following question: is it possible to transform the system by Wang and Chen (2012) into a chemical representation such that the induced (possibly *mass action kinetic*) polynomial ODEs model a real chemical system? The mere existence of a possible reacting system (organic or inorganic) with a unique and stable equilibrium point with a hidden chaotic attractor seems paradigmatic for the (bio)chemical scientific community as it happened when the first nonlinear oscillations were reported by Zhabotinsky (Epstein and Pojman, 1998).

Some mathematical efforts focused in the transformation of chaotic systems into chemical ones have been reported. Toth and Hars (1986) shown for the Lorenz and Rossler chaotic systems that none of the proper or improper orthogonal transformations transform them into a (mass action) kinetic equation representing a possible chemistry. On the other hand, the approach proposed by Poland (1993) uses cooperative catalysis and slow reactions followed by rapid ones where the former type of reactions controls the contribution to the polynomial ODEs. With this approach, the negative cross–effect that prevents the chemical interpretation of most chaotic systems appears to be explained naturally. Therefore, as a first step towards the finding of a mass action kinetic system with one stable equilibrium point and chaotic dynamics,

we use the approach by Poland (1993) to obtain a chemical representation of the chaotic system founded by Wang and Chen (2012).

This contribution is organised as follows: In section 2 we briefly present the necessary mathematical background to derive a chemical system from a chaotic dynamical one in accordance with the work of Poland (1993). Section 3 shows the chemical based chaotic dynamical system obtained from (Wang and Chen, 2012) using the approach of Poland (1993). A discussion is given in section 4. Finally, some conclusions are drawn in section 5.

2. MATERIALS AND METHODS

In this section we present the ideas discussed by Poland (1993) that allow to obtain an equivalent set of multivariate polynomial ODEs (not necessarily *mass action* type) from a chaotic polynomial ODEs so that the obtained ODEs have a direct interpretation in terms of chemical reactions.

The "theoretical reaction building blocks" that may be used to derive the chemical version of the Wang &Chen system chaotic dynamical system are:

- Constant sources, that is, reactions of the type,

$$S \xrightarrow{k} X, \tag{2}$$

where S is a chemical species present in excess, hence a source. Thus, to account for the production of X, the term "k"(which encodes the constant concentration of S) need to appear at the right hand side of the ODEs.

- Cooperative catalysis:

$$C + X + Y \xrightarrow{k} X + Y + Z \tag{3}$$
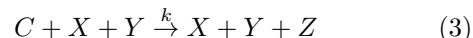
Let us note that the net reaction is $C \xrightarrow{k} Z$; chemical species X and Y collide each other along with C, acting as catalyst because there is not a net production of X and Y, only production of Z. In mathematical terms, the production of Z is expressed with the term"kxy"at the right hand side of the corresponding ODEs.

- Slow/Fast couples. In order to account for the net reaction $Y \rightarrow R$, where R stands for an external reservoir and Y must decrease at a rate that is independent of Y concentration, we need to invoke a two reaction scheme as follows:

$$D + X + Z \xrightarrow{k} D^* + X + Z \quad (slow) \tag{4}$$
$$D^* + Y \rightarrow D + R \quad (fast) \tag{5}$$
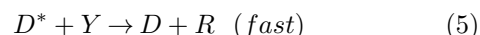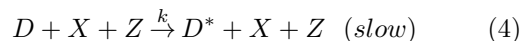
Because the first reaction is *slow*, it will dominate the dynamics of the consumption of Y. Thus, the concentration of Y will decrease at a rate of "$-kxz$".

- Sinks. It refers to reactions where a chemical species degrades itself. An example of this type of reaction is $X \xrightarrow{k} R$. The mathematical representation is "$-kx$".

Lumping the aforementioned type of reactions we can write the ODEs as:

$$\frac{d\mathbf{x}}{dt} = \mathbf{J}_S + \mathbf{N}_C \mathbf{J}_C + \mathbf{N}_R \mathbf{J}_R + \mathbf{N}_E \mathbf{J}_E \tag{6}$$

where $\mathbf{J}_S, \mathbf{J}_C, \mathbf{J}_R,$ and $\mathbf{J}_E$ represent the current vectors for constant sources, cooperative catalysis, slow/fast couples,

and sinks, respectively. Matrices $\mathbf{N}_C$, $\mathbf{N}_R$, and $\mathbf{N}_E$ are the appropriate stoichiometric matrices of the aforementioned type of reactions.

3. RESULTS

Using the theoretical background briefly presented in the last section, we derive a set of chemical reactions that induces an equivalent system of polynomial ODEs (Poland, 1993). As a first step it is necessary to shift the solutions of system (1) to the positive orthant. It can be seen from Fig. 2 that x and z have positive and negative values whereas y evolve in the positive orthant. Hence, we need to displace variables x and z only. To that end, we define the following:

$$\bar{x} = x + \Delta, \quad \bar{y} = y, \quad \bar{z} = z + \Delta \qquad (7)$$

where Δ is a positive scalar. Substitution of (7) into (1) lead to:

$$\frac{d(\bar{x} - \Delta)}{dt} = (\bar{y})(\bar{z} - \Delta) + a$$

$$\boxed{\frac{d\bar{x}}{dt} = \bar{y}\bar{z} - \Delta\bar{y} + a} \qquad (8)$$

$$\frac{d\bar{y}}{dt} = (\bar{x} - \Delta)^2 - \bar{y}$$

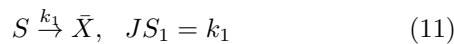$$\boxed{\frac{d\bar{y}}{dt} = \bar{x}^2 - 2\Delta\bar{x} + \Delta^2 - \bar{y}} \qquad (9)$$

$$\frac{d(\bar{z} - \Delta)}{dt} = 1 - 4(\bar{x} - \Delta)$$

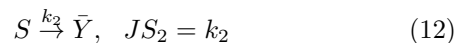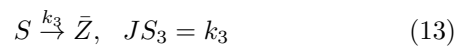$$\boxed{\frac{d\bar{z}}{dt} = -4\bar{x} + (1 + 4\Delta)} \qquad (10)$$

3.1 Sources terms

Let us first consider those source terms that appear in Eqs. (8)-(10) and their chemical representation. Thus, from Eq. (8), we have "$+a$":
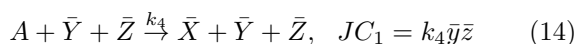
$$S \xrightarrow{k_1} \bar{X}, \quad JS_1 = k_1 \qquad (11)$$

From Eq. (9), we have "$+\Delta^2$":

$$S \xrightarrow{k_2} \bar{Y}, \quad JS_2 = k_2 \qquad (12)$$

And from Eq. (10), we have "$1 + 4\Delta$":

$$S \xrightarrow{k_3} \bar{Z}, \quad JS_3 = k_3 \qquad (13)$$

3.2 Cooperative catalysis

To account for the term "$\bar{y}\bar{z}$" we have the reaction:

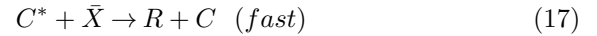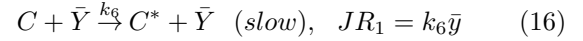$$A + \bar{Y} + \bar{Z} \xrightarrow{k_4} \bar{X} + \bar{Y} + \bar{Z}, \quad JC_1 = k_4\bar{y}\bar{z} \qquad (14)$$

with a net effect of $A \to \bar{X}$. From Eq. (9) we have the term "$\bar{x}^2$" which can be explained trough the next reaction:

$$B + 2\bar{X} \xrightarrow{k_5} \bar{Y} + 2\bar{X}, \quad JC_2 = k_5\bar{x}^2 \qquad (15)$$

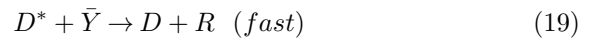The net effect of the above reaction in $B \to \bar{Y}$.

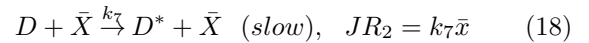### 3.3 Slow/fast couples

Equation (8) has the term "$-\Delta\bar{y}$", whose contribution can be explained with reactions:

$$C + \bar{Y} \xrightarrow{k_6} C^* + \bar{Y} \quad (slow), \quad JR_1 = k_6\bar{y} \qquad (16)$$
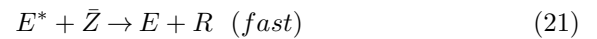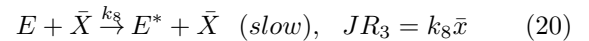
$$C^* + \bar{X} \to R + C \quad (fast) \qquad (17)$$

As a consequence of the above slow/fast reaction, we have the consumption of $\bar{X}$, that is $\bar{X} \to R$.

To account for the term "$-2\Delta\bar{x}$" in Eq. (9) we have the following reactions:

$$D + \bar{X} \xrightarrow{k_7} D^* + \bar{X} \quad (slow), \quad JR_2 = k_7\bar{x} \qquad (18)$$

$$D^* + \bar{Y} \to D + R \quad (fast) \qquad (19)$$

with a net effect of $\bar{Y} \to R$.

With respect to Eq. (10) and its associated term "$-4\bar{x}$", we can explain it via:

$$E + \bar{X} \xrightarrow{k_8} E^* + \bar{X} \quad (slow), \quad JR_3 = k_8\bar{x} \qquad (20)$$

$$E^* + \bar{Z} \to E + R \quad (fast) \qquad (21)$$

The resulting net effect is $\bar{Z} \to R$.

3.4 Sinks

We have only one term for degradation of a chemical species in Eq. (9), that is "$-\bar{y}$", and expressed as a chemical reaction of the form:

$$\bar{Y} \xrightarrow{k_9} R, \quad JE_1 = k_9\bar{y} \qquad (22)$$
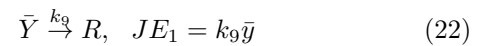
Thus, in accordance with Eq. (6), the current vectors for the Wang and Chen system derived from the above reactions are:

$$\mathbf{J}_S = \begin{bmatrix} JS_1 \\ JS_2 \\ JS_3 \end{bmatrix}, \quad \mathbf{J}_C = \begin{bmatrix} JC_1 \\ JC_2 \\ 0 \end{bmatrix}, \qquad (23)$$

$$\mathbf{J}_R = \begin{bmatrix} JR_1 \\ JR_2 \\ JR_3 \end{bmatrix}, \quad \mathbf{J}_E = [JE_1] \qquad (24)$$

whereas the corresponding stoichiometric matrices are:

$$\mathbf{N}_S = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{N}_C = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}, \qquad (25)$$

$$\mathbf{N}_R = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad \mathbf{N}_E = \begin{bmatrix} 0 \\ -1 \\ 0 \end{bmatrix} \qquad (26)$$

Resumed below is the chemical reaction network representation of the Wang-Chen system:

$$S \xrightarrow{k_1} \bar{X}$$
$$S \xrightarrow{k_2} \bar{Y}$$
$$S \xrightarrow{k_3} \bar{Z}$$
$$A + \bar{Y} + \bar{Z} \xrightarrow{k_4} \bar{X} + \bar{Y} + \bar{Z}$$
$$B + 2\bar{X} \xrightarrow{k_5} \bar{Y} + 2\bar{X}$$
$$C + \bar{Y} \xrightarrow{k_6} C^* + \bar{Y} \quad (slow) \qquad (27)$$
$$C^* + \bar{X} \rightarrow R + C \quad (fast)$$
$$D + \bar{X} \xrightarrow{k_7} D^* + \bar{X} \quad (slow)$$
$$D^* + \bar{Y} \rightarrow D + R \quad (fast)$$
$$E + \bar{X} \xrightarrow{k_8} E^* + \bar{X} \quad (slow)$$
$$E^* + \bar{Z} \rightarrow E + R \quad (fast)$$
$$\bar{Y} \xrightarrow{k_9} R$$
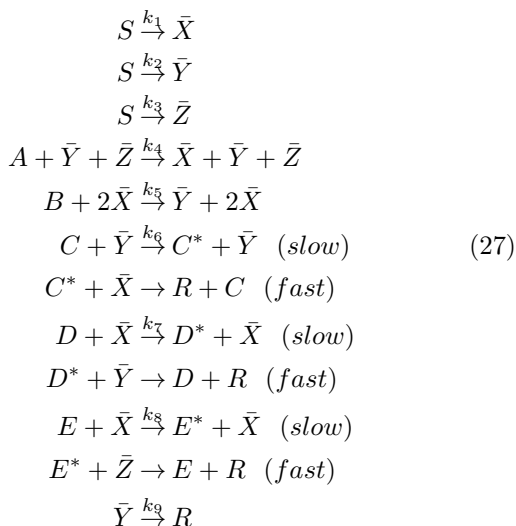
Now, we turn our attention to the polynomial ODEs that such reaction network induces. For chemical species X the associated ODEs takes the form:

$$\frac{d\bar{x}}{dt} = JS_1 + JC_1 - JR_1$$
$$\frac{d\bar{x}}{dt} = k_1 + k_4\bar{y}\bar{z} - k_6\bar{y} \qquad (28)$$

Comparing Eq.(28) with Eq.(8),

$$\frac{d\bar{x}}{dt} = a + \bar{y}\bar{z} - \Delta\bar{y} \qquad (29)$$

we have that:

$$k_1 = a, \ k_4 = 1, \ k_6 = \Delta \qquad (30)$$

For the chemical species Y we have that:

$$\frac{d\bar{y}}{dt} = JS_2 + JC_2 - JR_2 - JE_1 \qquad (31)$$
$$\frac{d\bar{y}}{dt} = k_2 + k_5\bar{x}^2 - k_7\bar{x} - k_9\bar{y} \qquad (32)$$

Comparison of Eq. (9) with Eq.(32),

$$\frac{d\bar{y}}{dt} = \Delta^2 + \bar{x}^2 - 2\Delta\bar{x} - \bar{y} \qquad (33)$$

lead to the following kinetic constants values:

$$k_2 = \Delta^2, \ k_5 = 1, \ k_7 = 2\Delta, \ k_9 = 1 \qquad (34)$$

Finally, chemical species Z ODE is:

$$\frac{d\bar{z}}{dt} = JS_3 - JR_3 \qquad (35)$$
$$\frac{d\bar{z}}{dt} = k_3 - k_8\bar{x} \qquad (36)$$

A direct comparison of Eq.(36) with Eq.(10),

$$\frac{d\bar{z}}{dt} = (1 + 4\Delta) - 4\bar{x} \qquad (37)$$

gives the kinetic constant values:

$$k_3 = 1 + 4\Delta, \ k_8 = 4 \qquad (38)$$

Let us consider the ODEs derived from the chemical representation of Wang and Chen system Wang and Chen (2012):

$$\frac{d\bar{x}}{dt} = k_1 + k_4\bar{y}\bar{z} - k_6\bar{y}$$
$$\frac{d\bar{y}}{dt} = k_2 + k_5\bar{x}^2 - k_7\bar{x} - k_9\bar{y} \qquad (39)$$
$$\frac{d\bar{z}}{dt} = k_3 - k_8\bar{x}$$

with $\Delta = 3$ and $a = 0.006$, the kinetic constant values are:

$$k_1 = 0.006, \ k_2 = 9, \ k_3 = 13, \ k_4 = 1, \ k_5 = 1$$
$$k_6 = 3, \ k_7 = 6, \ k_8 = 4, \ k_9 = 1$$

System (39) has a unique stable equilibrium point, $\mathbf{E}^*$:

$$\bar{x}^* = \frac{k_3}{k_8} = 3.25 \qquad (40)$$
$$\bar{y}^* = \frac{(k_2k_8^2 + k_3^2k_5 - k_3k_7k_8)}{(k_8^2k_9)} = 0.0625 \qquad (41)$$
$$\bar{z}^* = \frac{((k_2k_8^2 + k_3^2k_5 - k_3k_7k_8)k_6 - k_1k_8^2k_9)}{k_4(k_2k_8^2 + k_3^2k_5 - k_3k_7k_8)} = 2.9 \ (42)$$

Numerical integration of system (39) is depicted in Figs. 3 and 4. The eigenvalues associated to the equilibrium point $\mathbf{E}^*$ are the same as those for $\mathbf{E}$. Numerical computation (Wolf et al., 1985) of the Lyapunov exponents [1] of system (1) gives $\bar{L}_1 = 0.0633$, $\bar{L}_2 = 0$, and $\bar{L}_3 = -1.0612$, indicating the existence of chaotic behaviour (see Fig. 5).
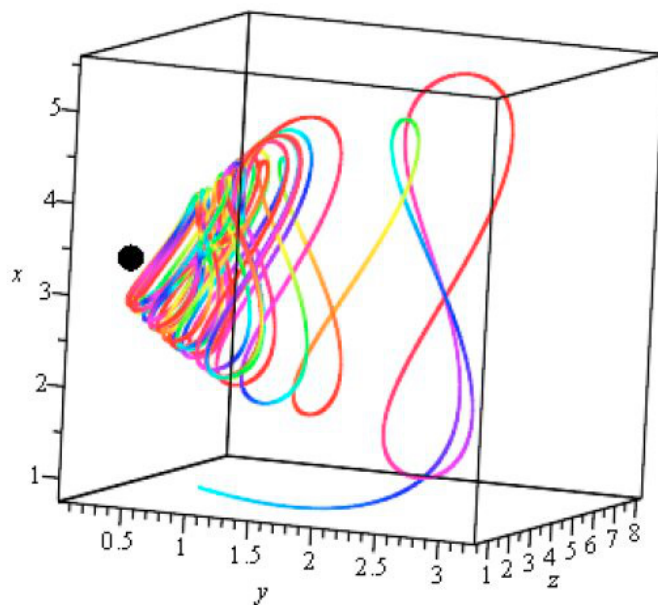

Fig. 3. Three dimensional behaviour of the chemical representation of Wang and Chen system with $a = 0.006$ and $\Delta = 3$. Black solid dot is the unique and stable equilibrium point, $\mathbf{E}^*$. Initial conditions: $[1, 1, 1]$. Bars over lower case letters were omitted seeking simplicity.

4. DISCUSSION

Loosely speaking we can say that two or more entities are equivalent if they have a common feature that enables us

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[1] Lyapunov Exponents Toolbox (LET), a Matlab code written by Steve Siu. Available at: http ://www.mathworks.com/matlabcentral/fileexchange
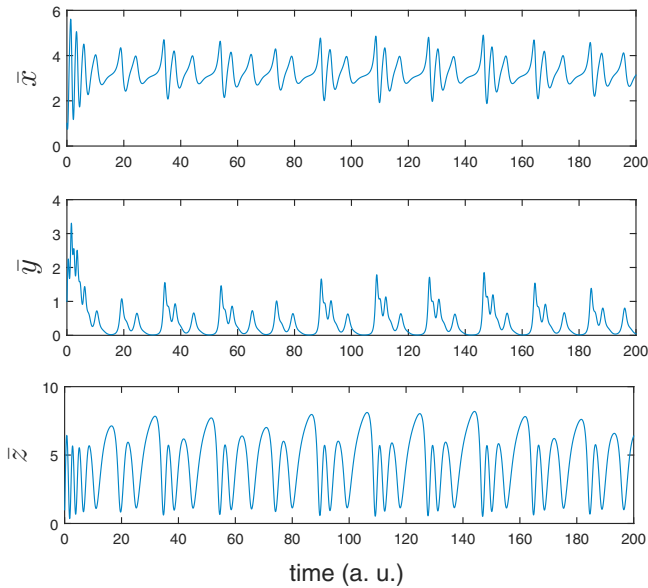
Fig. 4. Time series of the chemical representation of Wang and Chen system with $a = 0.006$ and $\Delta = 3$. Initial conditions: $\mathbf{x}_0 = [1,\ 1, 1]$.
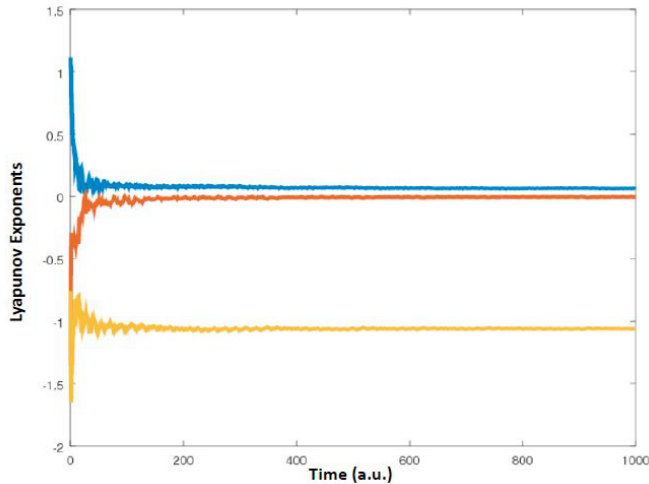

Fig. 5. Lyapunov exponents of the Wang-Chen chemical based dynamical system (1).

to declare them as the same. Within dynamical systems theory there are several equivalence definitions (Arnold, 1992). A particularly easy one to verify is the Topological Equivalence (TE) concept (Arnold, 1992).

Let us consider two linear systems:

$$\dot{\mathbf{x}}(t) = \mathbf{A}\mathbf{x}(t) \text{ and } \dot{\mathbf{x}}(t) = \mathbf{B}\mathbf{x}(t),\ \mathbf{x} \in \mathbb{R}^s \qquad (43)$$

where $(\mathbf{A}, \mathbf{B}) : \mathbb{R}^{s \times s} \rightarrow \mathbb{R}^s,\ \mathbf{x} \in \mathbb{R}^s$, with all their eigenvalues having a *nonzero* real part and denote the number of negative real eigenvalues by m_- whereas the number of positive real eigenvalues with m_+, so that $m_- + m_+ = n$. Then, it can be said that two linear systems are TE if the following theorem's conditions hold:

Theorem 1. A necessary and sufficient condition for *topological equivalence* of two linear systems having no eigenvalues with zero real part is that the number of eigenvalues

with negative (or positive) real part be the same for both systems: $m_-(A) = m_-(B),\ m_+(A) = m_+(B)$.

Theorem 1 implies that all *stable* equilibrium points (*unstable*, respectively), classified as nodes and foci, are TE to each other but not equivalent to a saddle type equilibrium point. Additionally, theorem 1 holds locally for *nonlinear* polynomial ODEs, that is, in the vicinity of an equilibrium point the set of polynomial ODEs is topologically equivalent to its linear approximation (Arnold, 1992).

As shown in the previous section, the theorem's condition holds for the eigenvalues of system (39); moreover, these eigenvalues are the same as in system (1). Hence the new chemical based dynamical system, (39), is topological equivalent to the Wang and Chen (2012) system, (1), in the vicinity of the unique and stable equilibrium point.

Other invariance properties, such as Lyapunov exponents and Lyapunov dimension (D_L), have been used as an equivalence criteria between dynamical systems (Eichhorn et al., 2001). For a three dimensional dynamical system with $L_2 = 0$, the Lyapunov dimension can be computed using the following equation (Chlouverakis and Sprott, 2005):

$$D_L = \frac{3}{2} + \frac{1}{2}\sqrt{1 - \frac{8L_1}{L_3}} \qquad (44)$$

where L_1 is the largest positive Lyapunov exponent and L_3 stands for the negative one. Using equation (44), the chemical based dynamical system (39) has a Lyapunov dimension $D_{\bar{L}} = 2.1077$, whereas Wang and Chen (2012) originally reported a Lyapunov dimension of $D_L = 2.048$ given $L_1 = 0.0510,\ L_2 = 0,\ L_3 = -1.0510$ for parameter value $a = 0.006$. Comparing these invariance properties we can say that both dynamical systems are indeed equivalent and that the chemical representation obtained is coherent with the original dynamical system developed by Wang and Chen (2012). In this sense, if a real chemical reaction can be explained by reaction network (27), then we might find a far dull behaviour to that expected by the existence of a unique and stable equilibrium point.

However, let us point out that the set of polynomial ODEs induced by the chemical representation of the Wang-Chen system does not belong to the *mass action kinetics* polynomial ODEs and hence equations in (39) are not positively invariant (Chellaboina et al., 2009). In other words, solutions starting inside the positive orthant does not remain within the positive orthant, a clear violation of a fundamental property of polynomial mass action kinetics ODEs (Chellaboina et al., 2009). This violation is shown in Fig. 6.

Therefore, further investigation is needed in order to characterise the basin of attraction of the chaotic regime that is lurking in the vicinity of the unique and stable equilibrium point as well as the implementation of other approaches to derive a mass action kinetic polynomial ODEs with the same dynamical properties of the Wang-Chen system. A second approach to be pursued is the so-called "X-factorable" transformation, which allows to rewrite a polynomial set of ODEs into a chemical kinetic set of ODEs (Guo Xu and Shu Li, 2003). The finding or design of a real chemical reaction that can be explained by the same reactions (or some of them) derived here remains
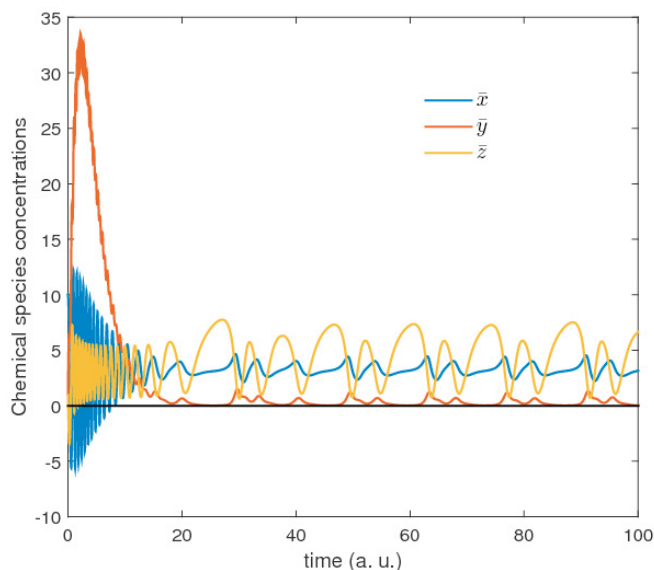
Fig. 6. Time series of the chemical representation of Wang-Chen system with $a = 0.006$ and $\Delta = 3$. Note the crossing to the negative orthant during the transient behaviour of $\bar{x}$ and $\bar{z}$. Initial conditions: $[10, 1, 1]$.

an interesting challenge. Recently, the rise of Artifical Intelligence (AI) and deep learning algorithms within the pharmaceutical industry has led to major improvements in the discovery of drug molecules and their reaction pathways (Segler et al., 2018). A similar procedure might be exploited to explore and synthesize chemical reaction networks with the dynamical characteristics explained in this paper.

5. CONCLUSION

A chemical representation of the chaotic dynamical system reported by Wang and Chen (2012) was obtained using cooperative catalysis and slow-fast reactions. The chemical based dynamical system preserved the same eigenvalues as well as the Lyapunov exponents and the associated Lyapunov dimension of the original chaotic Wang-Chen dynamical system. However, the derived chemical representation does not induce polynomial mass action kinetic ODEs, which are guarantee to be positively invariant.

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