



# Toward a Dynamical Equivalence between Brusselator and Oregonator: A Lie based approach

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**Abstract**— This paper explores a coordinate transformation defined by the composition of diffeomorphic maps as an equivalence criteria between two vector fields (i. e. ODEs) induced by different oscillatory chemical reaction networks (CRNs): (1) The Brusselator, a theoretical minimal Mass Action System (MAK) with limit cycle, and (2) the Oregonator, a minimal CRN designed to model the oscillations in the Belousov-Zhabotinsky (BZ) reaction. The diffeomorphic maps are constructed by means of Lie derivatives which creates a tangent space to the vector fields. These maps, through their inverses, makes possible to express the concentrations of chemical species of both CRNs as a function of the other, point by point in time.

**Keywords:** Brusselator, Oregonator, Chemical Reaction Networks, Lie derivatives, Dynamical equivalence.

## I. INTRODUCTION

Although chemical oscillations has been reported since 1828 (Epstein and Pojman, 1998), the theoretical framework which satisfactory explain them was developed until 1955, when Prigogine and coworkers pointed out that self-organization and chemical oscillations were well explained by their ideas of far-from equilibrium thermodynamics (Epstein and Pojman, 1998, and references there in). As an example of their theory, they designed a chemical oscillator of 4 reactions, later dubbed as the *Brusselator* (Prigogine and Lefever, 1968). Moreover, the *Brusselator* was also capable to display pattern formation (stripes and spirals) when diffusive terms were coupled to the Mass Action Kinetics (MAK) ODEs. This striking behavior was essentially the same observed by Belusov, when investigated a solution of bromate, citric acid, and ceric ions ( $Ce^{+4}$ ) in an unstirred cylinder, the solution exhibited traveling waves of yellow due the conversion from  $Ce^{+4}$  to  $Ce^{+3}$ . On the other hand, if the reaction takes place in a well stirred media, the solution oscillates from yellow to colorless.

In 1968, Zhabotinsky presented a better formulation than the Belusov's by replacing citric acid with malonic acid. In this way, the Belusov-Zhabotinsky (BZ) reaction caught the attention of several chemists. Among them, a group from the University of Oregon were the first to elucidate a

mechanism of 10 reactions showing qualitative agreement with the BZ reaction (Noyes *et al.*, 1972). Two years later, the same group reported a reduced version of 5 reactions, the so-called *Oregonator* (Field and Noyes, 1974). This minimal version was indeed able to account for the variety of oscillatory phenomena observed experimentally for the BZ reaction (Field and Noyes, 1974). It is noteworthy to mention that one of the most detailed mechanism reported for the BZ reaction has more than 40 reactions (Hegedus *et al.*, 2001).

The fact that two or more mechanisms might generate the same dynamics is known as the fundamental dogma of chemical kinetics. Thus, given the dynamics of chemical species concentrations (the experimentally "integrated" version of the set of MAK-ODEs), for some candidate mechanisms will be impossible to discriminate among them. Whether or not chemical mechanisms are indistinguishable can be thought as an *equivalent* problem. At this respect, recent results in (Craciun and Pantea, 2008), explores necessary and sufficient conditions for two or more mechanism to induce the *same* MAK-ODEs for some choice of kinetic constants, which are:

1. their *source complexes*, i. e the linear combination of chemical species at the left of the chemical arrow, must be the same, and
2. the intersection of the open convex cones generated by the set of reactions for each source complex, is not empty.

Mechanisms fulfilling these conditions are considered as *dynamically equivalent* (Craciun and Pantea, 2008). Moreover, under some conditions is possible to determine dynamical properties of some mechanism by analyzing other (possibly smaller and/or unrelated) mechanisms (Craciun and Pantea, 2008). In particular, for the *Brusselator* and *Oregonator*, the condition 1 is not fulfilled (see section II). Nevertheless, both mechanisms have common dynamical features.

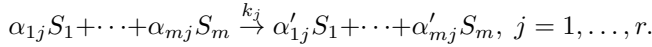
In this paper, we propose the composition of diffeomorphic maps such that chemical species concentrations for both, *Brusselator* and *Oregonator*, can be expressed as a

function of the other (equivalence). The equivalence it is also dynamic, because these maps are defined point by point in time for some accessible region in the space generated via Lie derivatives of the vectors fields.

This paper is organized as follows: section II is devoted to define concepts from the chemical engineering literature. In section III, we set the theoretical background necessary for construction of diffeomorphic maps via Lie derivatives of vector fields. Some numerical results are presented and discussed in section IV. Conclusions are drawn in section V.

## II. CHEMICAL REACTION NETWORKS AND MASS-ACTION KINETICS

Let us consider a chemical reaction system of  $r$  reactions and  $m$  reacting chemical species represented by:



where  $\alpha_{ij} \in \mathbb{R}$ , and chemical species are represented by  $S_i$ ,  $i = 1, \dots, s$ . The variable denoting chemical concentration for a chemical specie is  $x_i \in \mathbb{R}_+$  where  $\mathbb{R}_+ \triangleq \{x \in \mathbb{R} \mid x_i \geq 0, i = 1, \dots, n\}$  and  $\mathbb{R}_+ \triangleq \mathbb{R}_+ \setminus \{0\}$ . The rate constant,  $k_j \in \mathbb{R}_+$ ,  $j = 1, \dots, r$ , encode external factors influencing the velocity of  $j$ -th reaction and the concentrations of chemical species which are considered as constants throughout the reaction. The *stoichiometric coefficient*,  $n_{ij} = \alpha'_{ij} - \alpha_{ij}$ , is the net amount of  $i$ -th chemical specie which is consumed (or produced) in the  $j$ -th reaction. Stoichiometric coefficients are arranged in the *stoichiometric matrix*  $N \in \mathbb{R}^{s \times r}$ . The monomials of the *reaction rates*,  $v_j(k_j, x) = k_j \prod_{i=1}^m x_i^{\kappa_{ij}}$  are formed according to MAK law, where the *kinetic exponents*  $\kappa_{ij}$  encode the molecularity of the  $i$ -th specie in the  $j$ -th reaction. These kinetic exponents are arranged in the *kinetic matrix*,  $\kappa \in \mathbb{R}_+^{s \times r}$ . The MAK-ODEs induced by a chemical mechanism are defined as

$$\dot{x} = N \cdot v(k, x), \quad x(0) \geq 0 \quad (1)$$

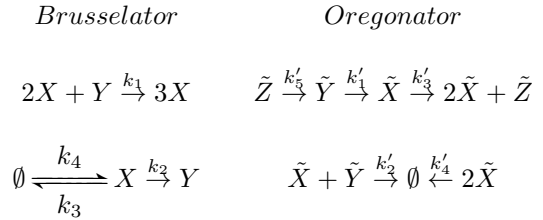
In general,  $N$  does not have maximal row rank. For  $d = \text{rank}(N)$ , there exist  $s - d$  conservation relations

$$W^T \cdot x = c \quad (2)$$

with  $W^T \cdot N = 0$  for a  $W \in \mathbb{R}^{s \times (s-d)}$ , where  $c \in \mathbb{R}_+$ .

A *reaction mechanism* is “a detailed description of the pathway leading from the reactants to the products, including as complete a characterization as possible of the composition, structure and other properties of reaction intermediates and transition states (Temkin *et al.*, 1996)”. Because some chemical species are present in excess, do not vary on time for practical purposes. These are named *external species* (Eiswirth *et al.*, 1991); those who do vary on time are called *internal species*. A *chemical reaction network* (CRN) is constructed using *pseudoreactions*, i.e. those remaining in the reaction mechanism by setting a  $\emptyset$  for every external specie, leaving the internal ones intact. The

linear combination of internal species before and after the chemical arrow in a CRN are named *complexes* (Feinberg, 1987). Of particular interest is the set of complexes that appears only at the left of the chemical arrow, the so-called *source complexes*. Monomials of MAK are derived from them, thus providing the velocity terms of the MAK-ODEs.



The associated CRNs for the *Brusselator* and *Oregonator* are depicted above, where the internal species for the former are denoted by  $X$  and  $Y$ , meanwhile for the latter are  $\tilde{X} = [HBrO_2]$ ,  $\tilde{Y} = [Br^-]$  and  $\tilde{Z} = [Ce^{+4}]$ . Source complexes for both CRNs are:  $\mathcal{C}_{0,BR} = \{2X + Y, X, \emptyset\}$  and  $\mathcal{C}_{0,OR} = \{\tilde{Z}, \tilde{Y}, \tilde{X}, \tilde{X} + \tilde{Y}, 2\tilde{X}\}$ , thus, condition 1 from section I does not hold, and Theorem 4.4 in (Craciun and Pantea, 2008) cannot be applied.

The stoichiometric matrices corresponding to the above CRNs are:

$$N = \begin{bmatrix} 1 & -1 & -1 & 1 \\ -1 & 1 & 0 & 0 \end{bmatrix}$$

$$\tilde{N} = \begin{bmatrix} 1 & -1 & 1 & -2 & 0 \\ -1 & -1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & -1 \end{bmatrix}$$

Note that neither of them has row rank deficiency, thus no conservation relations exists. The monomial vectors of reaction rates are

$$v(\mathbf{k}, \mathbf{x}) = \begin{bmatrix} k_1 x_1^2 x_2 \\ k_2 x_1 \\ k_3 x_1 \\ k_4 \end{bmatrix}, \quad \tilde{v}(\mathbf{k}', \tilde{\mathbf{x}}) = \begin{bmatrix} k'_1 \tilde{x}_2 \\ k'_2 \tilde{x}_1 \tilde{x}_2 \\ k'_3 \tilde{x}_1 \\ k'_4 \tilde{x}_1^2 \\ k'_5 \tilde{x}_3 \end{bmatrix}$$

Finally, the set of MAK-ODEs induced by the *Brusselator* are

$$\begin{aligned} \dot{x}_1 &= k_1 x_1^2 x_2 - k_2 x_1 - k_3 x_1 + k_4 \\ \dot{x}_2 &= -k_1 x_1^2 x_2 + k_2 x_1 \end{aligned} \quad (3)$$

and for the *Oregonator* we have

$$\begin{aligned} \dot{\tilde{x}}_1 &= k'_1 \tilde{x}_2 - k'_2 \tilde{x}_1 \tilde{x}_2 + k'_3 \tilde{x}_1 - 2k'_4 \tilde{x}_1^2 \\ \dot{\tilde{x}}_2 &= -k'_1 \tilde{x}_2 - k'_2 \tilde{x}_1 \tilde{x}_2 + k'_5 \tilde{x}_3 \\ \dot{\tilde{x}}_3 &= k'_3 \tilde{x}_1 - k'_5 \tilde{x}_3 \end{aligned} \quad (4)$$

The above sets of MAK-ODEs, beyond linear terms, are quite different, differing in one reaction. Even if we know in advance the set of parameters for the MAK-ODEs, it is difficult to elucidate a region in concentration space where both can be considered equivalent. In this sense, we seek for

conditions where chemical concentrations for both systems be equivalent. If such conditions exist and are fulfilled for any two CRNs, then, in some space, they are equivalent via a suitable mapping.

### III. COORDINATE TRANSFORMATION VIA LIE DERIVATIVES

In this section we construct diffeomorphic maps (i. e. differentiable bijective maps) via Lie derivatives of an observable function along the vector fields induced by the CRNs. These maps are a coordinate transformation from local coordinates to a local linear tangent space. By definition, the existence of a continuous inverse map is assured. These mathematical properties provide a suitable frame, via composition of functions, to write states from one system as a function of other states. In particular, because the ODEs (3-4) evolves in different dimensions ( $\mathbb{R}^2$  and  $\mathbb{R}^3$ , respectively), we can expect lost of some information after composition of functions. In other words, one system will be the projection of the other after composition.

We can write the set of MAK-ODEs as  $\dot{x} = f(x)$ , where  $f(x)$  is the vector field that maps points from some open set  $\mathcal{D} \subset \mathbb{R}^n$  to a tangent space,  $TM$ . Consider the existence of a smooth output function  $y = h(x)$ , where  $h : \mathbb{R}^n \rightarrow \mathbb{R}$ . In particular, for chemical reactions, any measurable chemical specie concentration will be valid as an output function. If the system  $\dot{x} = f(x)$ ,  $y = h(x)$  satisfies the observability rank condition about  $x_0$ , then, a coordinate transformation (diffeomorphism)  $z = \Phi(x)$  around  $x_0$  can be constructed via Lie derivatives as follows (Neijmeijer and van der Schaft, 1995)

$$\Phi(x) = (h(x), L_f h(x), \dots, L_f^{n-1} h(x)) \quad (5)$$

with the Lie derivative of the output along the vector field defined as

$$L_f h(x) = \sum_{k=1}^n f_k(x) \frac{\partial h(x)}{\partial x_k} \quad (6)$$

Using an output function  $y = h(x) = x_1$  for the *Brusselator*, the coordinate transformation is given by  $\Phi(\mathbf{x}_{BR}) = (h(x), L_f h(x))^T$   $z_{BR} = \Phi(\mathbf{x}_{BR})$ , thus

$$\begin{aligned} z_{BR} &= \Phi(\mathbf{x}_{BR}) \\ \Phi(\mathbf{x}_{BR}) &= (x_1, k_1 x_1^2 x_2 - k_2 x_1 - k_3 x_1 + k_4)^T \end{aligned} \quad (7)$$

which satisfies the (local) observability rank condition for the set  $\mathcal{U}_{BR} := \{(x_1, x_2) \in \mathbb{R}^2 \mid x_1 > 0, x_2 \geq 0\}$ , thus  $\Phi_{BR} : \mathcal{U}_{BR} \rightarrow \mathbb{R}_+ \times \mathbb{R}$ . The inverse of  $\Phi(\mathbf{x}_{BR})$  in terms of  $z$ 's is given by

$$\Phi^{-1}(z_{BR}) = (z_1, \frac{z_2 + (k_2 + k_3)z_1 - k_4}{k_1 z_1^2})^T \quad (8)$$

for  $z_1 \neq 0$ . Applying the same procedure for the *Oregonator* with  $\tilde{y} = h(\tilde{x}) = \tilde{x}_3$  as an output function we have

$$\tilde{z}_{OR} = \tilde{\Phi}(\tilde{\mathbf{x}}_{OR}) = (h(\tilde{x}), L_f h(\tilde{x}), L_f^2 h(\tilde{x}))^T$$

where

$$\begin{aligned} h(\tilde{x}) &= \tilde{x}_3 \\ L_f h(\tilde{x}) &= k'_3 \tilde{x}_1 - k'_5 \tilde{x}_3 \\ L_f^2 h(\tilde{x}) &= k'_3 ((k'_1 - k'_2 \tilde{x}_1) \tilde{x}_2 + (k'_3 - 2k'_4 \tilde{x}_1) \tilde{x}_1) \\ &\quad - k'_5 (k'_3 \tilde{x}_1 - k'_5 \tilde{x}_3) \end{aligned} \quad (9)$$

which is locally observable for the set  $\mathcal{U}_{OR} := \{(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3) \in \mathbb{R}^3 \mid \tilde{x}_1 \neq \frac{k'_1}{k'_2}, (\tilde{x}_2, \tilde{x}_3) \geq 0\}$ , thus  $\tilde{\Phi}_{OR} : \mathcal{U}_{OR} \rightarrow \mathbb{R}_+ \times \mathbb{R} \times \mathbb{R}$ . The associate inverse map  $\tilde{\Phi}^{-1}(\tilde{z}_{OR}) = (\tilde{\phi}_1^{-1}, \tilde{\phi}_2^{-1}, \tilde{\phi}_3^{-1})^T$  reads as follows

$$\tilde{\phi}_1^{-1} = \frac{\tilde{z}_2 + k'_5 \tilde{z}_1}{k'_3} \quad (10)$$

$$\tilde{\phi}_2^{-1} = \frac{\tilde{z}_3 - k'_3 (k'_3 - 2k'_4 \mu) \mu + k'_5 (k'_3 \mu - k'_5 \tilde{z}_1)}{k'_3 (k'_1 - k'_2 \mu)} \quad (11)$$

$$\tilde{\phi}_3^{-1} = \tilde{z}_1 \quad (12)$$

where  $\mu(\tilde{z}) = \frac{k'_5 \tilde{z}_1 + \tilde{z}_2}{k'_3}$ , such that  $\tilde{z}_2 + k'_5 \tilde{z}_1 \neq \frac{k'_1 k'_3}{k'_2}$ , to avoid singularity for  $\tilde{\phi}_2^{-1}$ . In order to get the chemical species concentrations of the *Brusselator* as function of the *Oregonator*'s concentrations, we define the following composition  $\mathbf{x}_{BR}^* = \Phi_{BR}^{-1}(\tilde{\Phi}_{OR}(\tilde{\mathbf{x}}_{OR}))$

$$\mathbf{x}_{BR}^* = \begin{pmatrix} \tilde{x}_3 \\ \frac{k'_3 \tilde{x}_1 + (k_2 + k_3 - k'_5) \tilde{x}_3}{k_1 \tilde{x}_3^2} \end{pmatrix} \quad (13)$$

where \* stands for the composed states. The *Oregonator*'s concentrations as function of *Brusselator*'s are defined according to  $\tilde{\mathbf{x}}_{OR}^* = \tilde{\Phi}_{OR}^{-1}(\Phi_{BR}(\mathbf{x}_{BR}))$

$$\tilde{\mathbf{x}}_{OR}^* = \begin{pmatrix} \frac{k_1 x_1^2 x_2 + (k'_5 - k_2 - k_3) x_1}{k'_3} \\ \frac{\tilde{z}_3 - k'_3 (k'_3 - 2k_4 \omega) \omega + k'_5 (k'_3 x_1 - k'_5 \omega)}{k'_3 (k'_1 - k'_2 x_1)} \\ x_1 \end{pmatrix} \quad (14)$$

where  $\omega(x_{BR}) = \frac{k_1 x_1^2 x_2 + (k'_5 - k_2 - k_3) x_1}{k'_3}$ . Note that  $\tilde{x}_{2,OR}^*$  depends also on  $\tilde{z}_3$ , which can be considered as zero because the *Brusselator* is a 2 dimensional system.

### IV. RESULTS AND DISCUSSION

An equivalence criterion for smooth vector fields is the concept of *dynamically (topologically) equivalent*. That is, two vector fields defined on the *same* state space are called dynamically equivalent if there is a homeomorphism (a bijection with a continuous inverse) of the state space that maps all orbits of the first vector field onto orbits of the second vector field, and preserves the direction of time along all the orbits (the time parameterization of the orbits is ignored). Of course, if two vector fields are topologically equivalent, then their phase portraits are *qualitatively* the same. In particular, via Lie derivatives, we compute diffeomorphic maps (a differentiable homeomorphism) for two systems defined in 2 and 3 dimensions, i. e we cannot map all the trajectories of one systems to the other. In this sense, one system will be a projection of the other for some region of interest. However, this do not exclude the fact that a qualitative behavior of trajectories cannot be preserved.

Of particular interest are the compositions defined in equations (13-14). Through these compositions it is possible to map trajectories from the *Brusselator's* concentration space to *Oregonator's* concentration space, and vice versa. That is,  $\Phi_{BR}^{-1} \circ \tilde{\Phi}_{OR} : \mathcal{U}_{OR} \rightarrow \mathcal{U}_{BR}$  and  $\tilde{\Phi}_{OR}^{-1} \circ \Phi_{BR} : \mathcal{U}_{BR} \rightarrow \mathcal{U}_{OR}$ . Looking at the equations (13-14), we have that  $x_{1,BR}^* = \tilde{x}_3$  and  $\tilde{x}_{3,OR}^* = x_{1,BR}$ . Although the remainder chemical concentrations are mapped by rational expressions to other scales of magnitudes,  $x_{1,BR}$ ,  $\tilde{x}_{3,OR}$  are mapped by the identity map (free of parameters), thus we can state that *Brusselator* and *Oregonator* are *partially dynamical equivalent* under this particular choice of  $(h(x), h(\tilde{x}))$ .

The regions of phenomenological interest for chemical species concentrations to be mapped are  $\mathcal{U}_{BR} \subset \mathbb{R}_+^2$ ,  $\mathcal{U}_{OR} \subset \mathbb{R}_+^3$ . To assure that trajectories from either subsets do not cross to the negative orthant, is not trivial because the composition maps depend on kinetic constants from both, *Brusselator* and *Oregonator* CRNs. Nevertheless, despite its apparent complexity, for the composition map  $\tilde{\Phi}_{OR}^{-1} \circ \Phi_{BR}$ , a set of kinetic constants and initial conditions, are readily find it as follows. From equation (14) we have  $\tilde{x}_{1,OR}^* = \frac{k_1 x_1^2 x_2 + (k_5' - k_2 - k_3)x_1}{k_3'}$ , and we want that  $\tilde{x}_{1,OR}^* > 0$ , thus

$$\begin{aligned} k_1 x_1^2 x_2 + (k_5' - k_2 - k_3)x_1 &> 0 \\ (k_1 x_1 x_2 + k_5' - k_2 - k_3)x_1 &> 0 \\ k_1 x_1 x_2 + (k_5' - k_2 - k_3) &> 0 \end{aligned}$$

and we arrive at the condition

$$x_{1,BR} > \left( \frac{k_3 + k_2 - k_5'}{k_1} \right) \left( \frac{1}{x_{2,BR}} \right) \quad (15)$$

Again, from equation (14),  $\tilde{x}_{2,OR}^* > 0$  is equivalent (after  $\omega$  factorization) to  $2k_3' k_4 \omega^2 - (k_3'^2 + k_5'^2)\omega + k_3' k_5' x_1 > 0$ . Doing the proper algebraic manipulations to solve for  $x_1$ , we arrive to the following inequality

$$x_{1,BR} > \left( \frac{\omega}{k_5'} \right) \left( k_3' + \frac{k_5'^2}{k_3'} - 2k_4 \omega \right) \quad (16)$$

which implies that

$$\omega < \left( \frac{1}{2k_4} \right) \left( k_3' + \frac{k_5'^2}{k_3'} \right) \quad (17)$$

Notice that  $\omega = \tilde{x}_{1,OR}^* > 0$ , if equation (15) holds.

The *Brusselator* undergoes a Hopf bifurcation for kinetics constants  $k_1 = k_3 = k_4 = 1$  and  $k_2 = 2$  (Nicolis and Prigogine, 1977). From (Field and Noyes, 1974), we set  $k_3' = 8 \times 10^3$ ,  $k_5' = 1$ . Then, equations (15-17) holds for initial conditions  $\mathbf{x}_{BR}(0, 0) = (1, 3)$ . This particular sets of parameters and initial conditions lead to  $\omega < 4000$ . Condition  $\tilde{x}_{3,OR}^* > 0$  is trivially satisfied. Fig. 1 shows that  $\tilde{\Phi}_{OR}^{-1} \circ \Phi_{BR}$  preserves the qualitative behavior of *Brusselator's* states in the *Oregonator's* state space.

On the other hand, conditions the map  $\Phi_{BR}^{-1} \circ \tilde{\Phi}_{OR}$  must satisfies in order to stay in the positive orthant can be

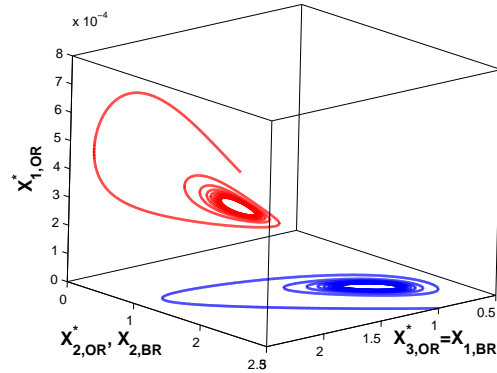


Fig. 1. Trajectories from Brusselator (blue) space mapped by (14) to  $\mathbb{R}_+^3$  (red).

derived from equation (16);  $x_{1,BR}^* > 0$  is trivially satisfied. The condition  $x_{2,BR}^* > 0$  is equivalent to  $k_3' \tilde{x}_1 + (k_2 + k_3 - k_5') \tilde{x}_3 - k_4 > 0$ , which can be written as

$$\tilde{x}_{1,OR} + \left( \frac{k_2 + k_3 - k_5'}{k_3'} \right) \tilde{x}_{3,OR} > \frac{k_4}{k_3'} \quad (18)$$

From this inequality is possible to proof the existence of kinetic constants such that (18) holds, if  $k_2 + k_3 > k_5'$ . Furthermore, upper and lower limits for  $\tilde{x}_{1,OR}$ ,  $\tilde{x}_{3,OR}$  can be derived from

$$\tilde{x}_{1,OR} > \frac{k_4}{k_3'} - \left( \frac{k_2 + k_3 - k_5'}{k_3'} \right) \tilde{x}_{3,OR} \quad (19)$$

which implies that  $\tilde{x}_{3,OR} < \frac{k_4}{k_2 + k_3 - k_5'}$ . On the other hand, assuming  $\tilde{x}_{3,OR} = 0$ , implies  $\tilde{x}_{1,OR} > \frac{k_4}{k_3'}$ . Using the above numerical values for kinetics constants, we have  $\tilde{x}_{1,OR} > 2.5 \times 10^{-3}$  and  $\tilde{x}_{3,OR} < 0.5$ . The problem is that, for this set of parameters,  $\tilde{x}_{1,OR} \rightarrow 1 \times 10^{-11}$  as  $t \rightarrow \infty$ , which is quite below condition  $\tilde{x}_{1,OR} > 2.5 \times 10^{-3}$ . In this sense, it is required to explore the parameters space in order to fulfill the above conditions. It might be possible that, for those parameters, the *Oregonator's* MAK-ODEs do not display oscillations or any nonlinear phenomena at all.

## V. CONCLUSIONS

The chemical species concentrations of two different oscillatory CRNs, not necessarily of the same dimension, can be expressed as function of the other, and vice versa, through composition of diffeomorphic maps. These maps were constructed via Lie derivatives of a suitable observable (a measure chemical specie) along the vector fields induced by the set of MAK-ODEs. For a set of kinetic constants and a suitable initial condition states, was possible to map trajectories from *Brusselator's* space onto *Oregonator's* space, preserving the qualitative dynamical nature displayed by the *Brusselator*. The opposite case, i. e mapping *Oregonator's* trajectories onto *Brusselator's* was partially achieved for  $x_{1,BR}^*$ , thus both chemical oscillators can be regarded as



*partially dynamic equivalent* for these chemical species. Conditions in parameters space that guarantee  $x_{2,BR}^* > 0$  cannot be fulfilled for typical values of both, *Brusselator* and *Oregonator* CRNs. In this sense, a broad parametric search need to be performed.

#### VI. ACKNOWLEDGMENTS

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