

Local controllability of reactions

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Received 28 May 1997; revised 21 April 1998

This paper is devoted to the study of local controllability of chemical reactions. After a brief introduction we give a sufficient condition of local controllability of chemical reactions. We show the use of our condition on a series of examples. In the last section we mention some unsolved problems.

1. Introduction

Classical control theory is mainly concerned with linear models. The equations of chemical kinetics are essentially nonlinear. Therefore, in order to treat the problem of controllability of reactions (so important from the point of view of chemical engineering science) one has to rely upon recent results on local controllability. As invariant manifolds (originated in conservation relations) also play an important role in kinetics, see Deák et al. [1], we use results on local controllability within an invariant manifold [10].

The present approach is theoretical. Similar approaches have been initiated by Samardzija [8], who introduced another kind of controllability and only investigated a special class of second-order reactions, and by Ramakrishna et al. [7], who investigated linear models arising in molecular dynamics by Lie algebraic methods. An interesting experimental approach has been initiated by Petrov et al. [6].

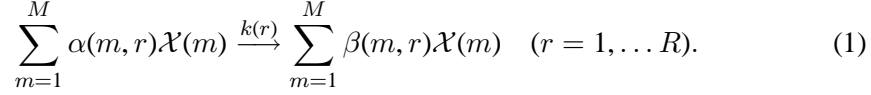
The structure of our paper is as follows. In section 1 we collect the basis of the mathematical model of chemical reactions. We recall the necessary part of the mathematical theory of controllability as well. Section 2 contains a general sufficient condition of local controllability of reactions. Section 3 presents a series of examples. Finally, section 4 discusses the results and formulates some open problems.

1.1. The model

Let us consider a well-mixed vessel of constant volume at constant temperature and pressure. Suppose the vessel contains a finite number of chemical components or species. Among these species chemical reactions take place and the quantities of

the components change. We are interested in the time evolution of the quantities of chemical components.

The usual way of displaying a complex chemical reaction is as follows:



Here M is the number of chemical components, R is the number of reaction steps, and $\mathcal{X}(m)$ is the m th chemical component. The nonnegative integers $\alpha(m, r)$ and $\beta(m, r)$ are the stoichiometric coefficients, and the positive real numbers $k(r)$ are the reaction rate constants. Let us denote the $M \times R$ matrices obtained from $\alpha(m, r)$ and $\beta(m, r)$ with α and β , respectively, and let $\gamma := \beta - \alpha$.

The usual, continuous time, continuous state deterministic model of the mass action type of reaction (1) is the differential equation

$$\dot{x}_m = \sum_{r=1}^R (\beta(m, r) - \alpha(m, r)) k(r) \prod_{m'=1}^M x_{m'}^{\alpha(m', r)} \quad (m = 1, \dots, M), \quad (2)$$

where $x_m(t)$ is to be interpreted as the concentration of the species $\mathcal{X}(m)$ at time t . Equation (2) is also said to be induced by reaction (1), it is the induced kinetic differential equation of (1). It is known that the set \mathbf{R}_+^M , i.e., the set of vectors having nonnegative coordinates, is invariant of every induced kinetic differential equation. As we mentioned, we are interested in invariant manifolds as well. Let us denote the subspace spanned by the columns of matrix γ with $S(\gamma)$. Let x^0 be an arbitrary vector in \mathbf{R}_+^M and consider $S(\gamma) + x^0$. The set obtained by $(S(\gamma) + x^0) \cap \mathbf{R}_+^M$ is said to be the reaction simplex belonging to x^0 . It is known that every reaction simplex is an invariant manifold of (2).

1.2. Controllability

From a technical point of view it is very important to control a chemical reaction. Furthermore, if we can control a reaction by changing a single rate constant we may realise the control by changing the temperature.

A well-known theorem on nonlinear systems says that, if the system, obtained by linearization around an equilibrium, satisfies the Kalman rank condition, then the nonlinear system is locally controllable into the equilibrium. Varga [10] extended this result to systems with an invariant manifold. We recapitulate his results.

Let $n, r \in \mathbf{N}$, $f \in C^1(\mathbf{R}^n \times \mathbf{R}^r, \mathbf{R}^n)$, $(x^*, u^*) \in \mathbf{R}^n \times \mathbf{R}^r$ such that $f(x^*, u^*) = \mathbf{0}$. Fix a $T > 0$ and, for every $\varepsilon > 0$, define

$$U_\varepsilon := \{u \in L_\infty^r[0, T]: |u(t)| \leq \varepsilon \text{ for a.e. } t \in [0, T]\}.$$

It is known that there exists an $\varepsilon_0 > 0$ such that, if

$$z \in \mathbf{R}^n, \quad |z - x^*| < \varepsilon_0, \quad u \in U_{\varepsilon_0},$$

then there is a unique absolutely continuous function $x \in W_{11}^n[0, T]$ with

- (i) $\dot{x}(t) = f(x(t), u^* + u(t))$ for a.e. $t \in [0, T]$,
- (ii) $x(0) = z$.

Definition 1. For $k \in \{1, \dots, n\}$, $S \subseteq \mathbf{R}^n$ is said to be a regular k -dimensional submanifold, if there exist an open set $G \subseteq \mathbf{R}^n$ and a function $\Phi \in C^1(G, \mathbf{R}^{n-k})$ such that $S = \Phi^{-1}(0)$ and, for all $x \in G$, $R_{\Phi'(x)} = \mathbf{R}^{n-k}$.

Now fix an arbitrary $\varepsilon \in (0, \varepsilon_0]$.

Definition 2. The above S is said to be a positively ε -invariant manifold of system (i) at x^* , if $z \in S$, $|z - x^*| < \varepsilon$ and $u \in U_\varepsilon$ imply that, for x in (i) and (ii), we have $x(t) \in S$ ($t \in [0, T]$).

Let S be a positively ε -invariant manifold of (i) at x^* .

Definition 3. System (i) is said to be locally controllable in S into $x^* \in S$ with respect to U_ε , if there exists an open neighbourhood $G(x^*)$ of x^* in \mathbf{R}^n with the property that, for every $z \in G(x^*) \cap S$, there is a $u \in U_\varepsilon$ such that, for the solution x of the initial value problem (i)–(ii), we have $x(T) = x^*$.

Now define $A := \partial_x f(x^*, u^*)$ and $B := \partial_u f(x^*, u^*)$. Varga [10] proved the following theorem.

Theorem 4. Let $S \subseteq \mathbf{R}^n$ be a regular k -dimensional submanifold which is a positively ε -invariant manifold of (i) at x^* with some $\varepsilon \in (0, \varepsilon_0]$. Then the condition

$$\text{rank}[B|AB|\dots|A^{n-1}B] = k$$

implies that (i) is locally controllable in S into x^* with respect to U_ε .

2. General results

It is easy to see that every reaction has at least one positively ε -invariant manifold, namely \mathbf{R}_+^M , which has dimension M . In some cases, there are other ε -invariant manifolds even with smaller dimension than M – as a consequence of conservation laws (cf. [1]). Thus we can apply in every case the condition of Varga.

2.1. Notations

We investigate the controllability of reactions in the following way. We choose the reaction rate constants as control parameters by taking $k(r) = 1 + u_r$. In every case we take $u_r^* = 0$ for $r = 1, \dots, R$, i.e., we are interested in controlling the system into an

equilibrium belonging to the system where every reaction rate constants are equal to 1. Such a reaction is said to be an uncontrolled reaction, and the corresponding induced kinetic differential equation is said to be an uncontrolled system. In the following we consider equilibrium points corresponding to uncontrolled systems or reactions. Matrices A and B will be calculated at (x^*, u^*) , where x^* is an equilibrium of the reaction where every reaction rate constant is equal to 1, i.e., x^* is an equilibrium of the uncontrolled system, and u^* is defined as above. We require that ε satisfy the condition $\varepsilon < \min\{\varepsilon_0, 1\}$, which yields that the controlled reaction rate constants are always larger than zero. In the following we simply say that a reaction is locally controllable if it satisfies definition 3 with x^* and u^* defined above.

2.2. Main theorem

Matrix B can be calculated easily because the right-hand side of an induced kinetic differential equation is linear in u . Now we formulate how $\text{rank}(B)$ can be obtained without explicitly calculating matrix B for each special case. The following theorem can be proved.

Theorem 5. Suppose that for $k(r) = 1$ ($r = 1, \dots, R$) the induced kinetic differential equation of (1) has a positive equilibrium point x^* . Then

$$\text{rank}(B) = \text{rank}(\gamma).$$

Proof. Let $k := \text{rank}(\gamma)$. Without loss of generality we can assume that the first k columns of γ are linearly independent. Then the corresponding reaction steps are the following:

$$\begin{aligned} \sum_{m=1}^M \alpha(m, 1) \mathcal{X}(m) &\xrightarrow{1+u_1} \sum_{m=1}^M \beta(m, 1) \mathcal{X}(m), \\ &\vdots \\ \sum_{m=1}^M \alpha(m, k) \mathcal{X}(m) &\xrightarrow{1+u_k} \sum_{m=1}^M \beta(m, k) \mathcal{X}(m). \end{aligned}$$

Thus the induced kinetic differential equation has the form

$$\begin{aligned} \dot{x}_1 &= (\beta(1, 1) - \alpha(1, 1))(1 + u_1) \prod_{m'=1}^M x_{m'}^{\alpha(m', 1)} + \dots \\ &\quad + (\beta(1, k) - \alpha(1, k))(1 + u_k) \prod_{m'=1}^M x_{m'}^{\alpha(m', k)} + g_1(x_1, \dots, x_M), \\ &\vdots \end{aligned}$$

$$\begin{aligned} \dot{x}_M = & (\beta(M, 1) - \alpha(M, 1))(1 + u_1) \prod_{m'=1}^M x_{m'}^{\alpha(m', 1)} + \dots \\ & + (\beta(M, k) - \alpha(M, k))(1 + u_k) \prod_{m'=1}^M x_{m'}^{\alpha(m', k)} + g_M(x_1, \dots, x_M), \end{aligned}$$

where the functions g_i , $i = 1, \dots, M$, are independent from u_1, \dots, u_k . Thus, as an easy calculation shows, the first k columns of matrix B are the following:

$$\begin{pmatrix} (\beta(1, 1) - \alpha(1, 1))a_1 \\ (\beta(2, 1) - \alpha(2, 1))a_1 \\ \vdots \\ (\beta(M, 1) - \alpha(M, 1))a_1 \end{pmatrix}, \quad \dots, \quad \begin{pmatrix} (\beta(1, k) - \alpha(1, k))a_k \\ (\beta(2, k) - \alpha(2, k))a_k \\ \vdots \\ (\beta(M, k) - \alpha(M, k))a_k \end{pmatrix},$$

where the positive constants a_1, \dots, a_k can be obtained by putting the coordinates x_1^*, \dots, x_M^* of the positive equilibrium x^* into the expressions

$$\prod_{m'=1}^M (x_{m'}^*)^{\alpha(m', 1)}, \quad \dots, \quad \prod_{m'=1}^M (x_{m'}^*)^{\alpha(m', k)}.$$

Let us denote by B_k the matrix with the above vectors as columns. Now it can be seen that

$$B_k = \gamma_k \cdot \text{diag}(a_1, \dots, a_k),$$

where $\text{diag}(a_1, \dots, a_k)$ is the diagonal matrix having a_1, \dots, a_k as its diagonal elements, and γ_k is the matrix obtained from matrix γ by taking only the first k columns. Since $\det(\text{diag}(a_1, \dots, a_k)) \neq 0$ and $\text{rank}(\gamma_k) = k$, it follows that $\text{rank}(B_k) = k$ and $\text{rank}(B) \geq k$. Suppose now that $\text{rank}(B) > k$. Then there exists a column, say the $(k + 1)$ th, of matrix B which is linearly independent from the columns of matrix B_k . If we add this $(k + 1)$ th column of matrix B to matrix B_k to obtain B_{k+1} having rank $k + 1$ we get the following:

$$B_{k+1} = \gamma_{k+1} \cdot \text{diag}(a_1, \dots, a_k, a_{k+1}),$$

where γ_{k+1} is an $M \times (k + 1)$ matrix which can be obtained from γ by taking only the first $k + 1$ columns. Using again the fact that $\det(\text{diag}(a_1, \dots, a_k, a_{k+1})) \neq 0$, it implies that $\text{rank}(\gamma_{k+1}) = k + 1$. Thus we get that the 1st, the 2nd, \dots , the k th and the $(k + 1)$ th columns of matrix γ are linearly independent, which is a contradiction. \square

We remark that the condition of positivity of the equilibrium x^* is indispensable to guarantee $\text{rank}(B) = \text{rank}(\gamma)$. We will see an example in section 3.4 where $\text{rank}(B) \neq \text{rank}(\gamma)$. Existence of a positive equilibrium is implied for reversible systems [5,9] and for weakly reversible systems of zero deficiency [3].

Corollary 6. Assume that a given reaction has a positive equilibrium and $\text{rank}(\gamma) = M$. Then the reaction is locally controllable in \mathbf{R}_+^M .

Proof. The conditions imply $\text{rank}(B) = M$; thus $\text{rank}[B|AB|\cdots|A^{M-1}B] = M$, and the condition of local controllability is satisfied. \square

Corollary 7. Suppose that a given reaction has a positive equilibrium and the column space of matrix B is an invariant subspace of matrix A . Then the reaction is locally controllable in the reaction simplex belonging to the positive equilibrium.

Proof. Since every reaction simplex is independent from the reaction rate constants, it is clear that every reaction simplex is an ε -invariant manifold of the reaction with arbitrary ε . The dimension of a reaction simplex is equal to the rank of matrix γ . Using our theorem we obtain $\text{rank}(B) = \text{rank}(\gamma)$, and using the condition that the subspace spanned by the columns of B is invariant under the multiplication of matrix A we obtain $\text{rank}[B|AB|\cdots|A^{M-1}B] = \text{rank}(B)$; thus the condition of local controllability in an invariant manifold is satisfied. \square

We remark that theorem 5 cannot only be applied for mass action type models. We used during the proof only the properties that the dependence on u is linear and the obtained constants a_1, \dots, a_R are positive. We will see a non mass action type example fulfilling these conditions in section 3.5.

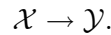
2.3. Reversibility

Next we study reversibility. Let us start with some notation. We will consider reactions with at least one positive equilibrium when all reaction rate constants are equal to 1. Assume that if we make a reaction step reversible (i.e., if we take the reversible closure of the reaction), the obtained reaction also has a positive equilibrium, say x^{**} , when all reaction rate constants are equal to 1. Let us denote the “new” matrix B of the obtained reaction by \tilde{B} , where \tilde{B} is calculated at (x^{**}, u^*) . The following theorem can be proved.

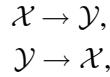
Theorem 8. Let us assume that a given reaction has a positive equilibrium. If we make a reaction step reversible and the obtained reaction also has a positive equilibrium then $\text{rank}(\tilde{B}) = \text{rank}(B)$.

Proof. It can be seen that if we make a reaction reversible then matrix $\text{rank}(\gamma) = \text{rank}(\tilde{\gamma})$, where $\tilde{\gamma}$ is the γ matrix of the obtained reaction. Since the obtained reaction also has a positive equilibrium, using theorem 5 we get that $\text{rank}(\tilde{B}) = \text{rank}(B)$. \square

We remark that it is possible that the rank of matrix B increases as we make a reaction step reversible. For example, let us consider the following reaction:



This reaction has no positive equilibrium. In every equilibrium concentration, $x_1^* = 0$. If we calculate matrix B in an equilibrium $x^* = (0, a)$, $u^* = 0$, where $a > 0$ constant, then we get the zero vector having zero rank. But if we make the only reaction step reversible to obtain the reaction



which has a positive equilibrium, and if we now calculate matrix \tilde{B} in an equilibrium $x^{**} = (a, a)$, $u^* = (0, 0)$, where $a > 0$ constant, then we get

$$\tilde{B} = \begin{pmatrix} -a & a \\ a & -a \end{pmatrix},$$

which has rank 1.

2.4. Reduction of the number of control parameters

From the technical point of view it is extremely important to reduce the number of control parameters. Up till now we have controlled every reaction rate constants. Next we investigate when we can control the system using a single parameter. We restrict ourselves to study only dimension 2 and controllability in \mathbf{R}_+^2 . If we control only one parameter then matrix B is reduced to a column vector. Without loss of generality we can assume that the first coordinate of B is not zero. Let us denote

$$B = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

and

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}.$$

We investigate the question: when will B and AB be linearly independent? We can answer this question easily. If we choose arbitrary a_{11} , a_{12} and a_{22} , the only constraint of choosing a_{21} is

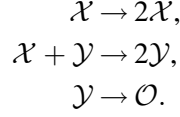
$$a_{21} \neq \frac{b_2}{b_1} \left(\frac{a_{11}b_1 + a_{12}b_2}{b_1} - a_{22} \right). \quad (3)$$

Thus, if we calculate vector B and matrix A and if the elements of A satisfy the above condition then we can control the reaction by controlling only the reaction corresponding to vector B .

3. Examples

In this section we investigate several formal chemical reactions. Our standard reference is [2] and the definition of the CIMA reaction (section 3.5) can be found in [4]. We are interested in the controllability of these reactions.

3.1. Lotka–Volterra model

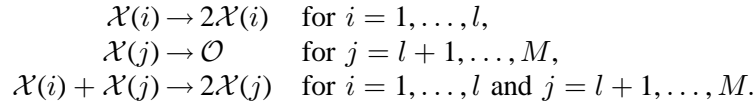


The induced kinetic differential equation of this reaction is

$$\begin{aligned}\dot{x}_1 &= (1 + u_1)x_1 - (1 + u_2)x_1x_2, \\ \dot{x}_2 &= (1 + u_2)x_1x_2 - (1 + u_3)x_2.\end{aligned}$$

The unique positive equilibrium of the uncontrolled system is $(1, 1)$ and matrix γ has rank 2; thus the reaction is locally controllable.

3.2. Generalized Lotka–Volterra model

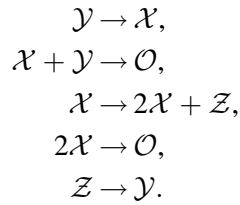


This model can be obtained by generalizing the previous predator–prey model to the case when there are l preys and $M - l$ predators present. To make the formulas simpler we only display the uncontrolled system

$$\begin{aligned}\dot{x}_1 &= x_1 - x_1x_{l+1} - \dots - x_1x_M, \\ &\vdots \\ \dot{x}_l &= x_l - x_lx_{l+1} - \dots - x_lx_M, \\ \dot{x}_{l+1} &= -x_{l+1} + x_1x_{l+1} + \dots + x_lx_{l+1}, \\ &\vdots \\ \dot{x}_M &= -x_M + x_1x_M + \dots + x_lx_M.\end{aligned}$$

Apart from the trivial zero equilibrium, the set of equilibria of the above system can be obtained by requiring the conditions $x_1^* + \dots + x_l^* = 1$ and $x_{l+1}^* + \dots + x_M^* = 1$. Thus the above system has positive equilibria, and one can notice that matrix γ has rank M . Applying our results we get that the generalized Lotka–Volterra model is locally controllable.

3.3. Oregonator (I)



The induced kinetic differential equation of the above reaction is the following:

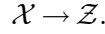
$$\begin{aligned}\dot{x}_1 &= (1 + u_1)x_2 - (1 + u_2)x_1x_2 + (1 + u_3)x_1 - 2(1 + u_4)x_1^2, \\ \dot{x}_2 &= -(1 + u_1)x_2 - (1 + u_2)x_1x_2 + (1 + u_5)x_3, \\ \dot{x}_3 &= (1 + u_3)x_1 - (1 + u_5)x_3.\end{aligned}$$

As an easy calculation shows, the unique positive equilibrium of the uncontrolled system is

$$x^* = \left(\frac{3 - \sqrt{5}}{\sqrt{5} - 1}, \frac{3 - \sqrt{5}}{2}, \frac{3 - \sqrt{5}}{\sqrt{5} - 1} \right) \quad \text{and} \quad \text{rank}(\gamma) = 3;$$

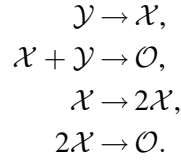
thus this reaction is locally controllable.

There exist a series of “stoichiometrically equivalent” models of the Belousov–Zhabotinsky reaction, all of which are called Oregonator. One of them is when instead of the original 3rd reaction step we write



It is very instructive to investigate the reaction with this 3rd reaction step because this modification destroys the applicability of our results. Namely, the obtained uncontrolled system does not have any positive equilibrium; furthermore, the only nonnegative equilibrium is the origin. If we calculate matrix B we get the zero matrix; thus the sufficient condition of local controllability is not satisfied in this case.

3.4. Oregonator (II)



The induced kinetic differential equation of Oregonator (II) is the following system:

$$\begin{aligned}\dot{x}_1 &= (1 + u_1)x_2 - (1 + u_2)x_1x_2 + (1 + u_3)x_1 - 2(1 + u_4)x_1^2, \\ \dot{x}_2 &= -(1 + u_1)x_2 - (1 + u_2)x_1x_2.\end{aligned}$$

The uncontrolled system has no positive equilibrium but has a unique non-zero non-negative equilibrium, namely $x^* = (1/2, 0)$. Now we cannot apply our results; we have to calculate matrix A and B to get

$$B = \begin{pmatrix} 0 & 0 & 1/2 & -1/2 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

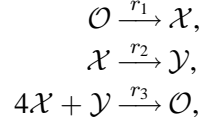
and

$$A = \begin{pmatrix} -1 & 1/2 \\ 0 & -3/2 \end{pmatrix}.$$

One can notice that $\text{rank}(B) \neq \text{rank}(\gamma)$ in this case. Since $\text{rank}[B|AB] = 1$, the sufficient condition of local controllability is not satisfied.

3.5. CIMA reaction

This reaction is not a mass action type reaction, but it can be seen that our results can be applied according to the remark at the end of section 2.2. Now we write the reaction rates above the reaction steps:



where

$$r_1 = 1 + u_1, \quad r_2 = (1 + u_2)x_2, \quad r_3 = (1 + u_3)\frac{x_1x_2}{u + x_1^2},$$

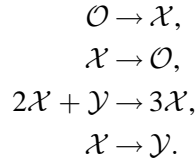
and u is a positive constant. The induced kinetic differential equation of the system is

$$\begin{aligned}\dot{x}_1 &= (1 + u_1) - (1 + u_2)x_1 - 4(1 + u_3)\frac{x_1x_2}{u + x_1^2}, \\ \dot{x}_2 &= (1 + u_2)x_2 - (1 + u_3)\frac{x_1x_2}{u + x_1^2}.\end{aligned}$$

As an easy calculation shows, if $u < 1/4$ then the uncontrolled system has positive equilibrium and $\text{rank}(\gamma) = 2$; thus the CIMA reaction is locally controllable if $u < 1/4$.

We remark that the CIMA reaction is locally controllable even if we control only the first reaction rate constant since condition (3) is satisfied.

3.6. Brusselator



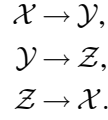
The induced kinetic differential equation is the following system:

$$\begin{aligned}\dot{x}_1 &= (1 + u_1) - (1 + u_2)x_1 + (1 + u_3)x_1^2x_2 - (1 + u_4)x_1, \\ \dot{x}_2 &= -(1 + u_3)x_1^2x_2 + (1 + u_4)x_1.\end{aligned}$$

The unique positive equilibrium of the uncontrolled system is $(1, 1)$ and $\text{rank}(\gamma) = 2$; thus the reaction is locally controllable.

Using condition (3) we get that the above reaction is locally controllable by controlling only the first reaction rate constant.

3.7. Triangle reaction



The induced kinetic differential equation is the following:

$$\begin{aligned}\dot{x}_1 &= -(1 + u_1)x_1 + (1 + u_3)x_3, \\ \dot{x}_2 &= (1 + u_1)x_1 - (1 + u_2)x_2, \\ \dot{x}_3 &= (1 + u_2)x_2 - (1 + u_3)x_3.\end{aligned}$$

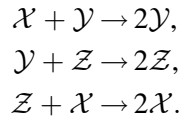
The uncontrolled system has many positive equilibrium points, but all of them have the same form (a, a, a) , where a is an arbitrary positive constant. In order to apply our results we should get $\text{rank}(\gamma) = 3$, but in this case matrix γ has rank 2. Thus we have to calculate matrices A and B . After this calculation we could see that

$$\text{rank}[B|AB|A^2B] = 2,$$

or, in other words, the condition of local controllability in \mathbf{R}_+^3 is violated.

On the other hand, we can apply our results which claim local controllability in manifolds with dimension smaller than M , since the subspace spanned by the columns of matrix B is invariant for the matrix A . As a result we get that the reaction is locally controllable into (a, a, a) in the reaction simplex belonging to vector (a, a, a) .

3.8. Ivanova reaction



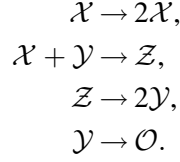
The induced kinetic differential equation is

$$\begin{aligned}\dot{x}_1 &= -(1 + u_1)x_1x_2 + (1 + u_3)x_1x_3, \\ \dot{x}_2 &= (1 + u_1)x_1x_2 - (1 + u_2)x_2x_3, \\ \dot{x}_3 &= (1 + u_2)x_2x_3 - (1 + u_3)x_1x_3.\end{aligned}$$

The positive equilibrium points of the uncontrolled system are $x^* = (a, a, a)$ again, where a is an arbitrary positive constant, but $\text{rank}(\gamma) = 2$; thus we cannot apply our results. After calculating matrices A and B we get $\text{rank}[B|AB|A^2B] = 2$, and the condition of local controllability is not satisfied.

Since matrix A is invariant for the subspace spanned by the columns of matrix B , the reaction is locally controllable in the reaction simplex belonging to the positive equilibrium.

3.9. Explodator

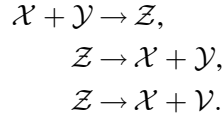


The induced kinetic differential equation is the following system:

$$\begin{aligned}\dot{x}_1 &= (1 + u_1)x_1 - (1 + u_2)x_1x_2, \\ \dot{x}_2 &= -(1 + u_2)x_1x_2 + 2(1 + u_3)x_3 - (1 + u_4)x_2, \\ \dot{x}_3 &= (1 + u_2)x_1x_2 - (1 + u_3)x_3.\end{aligned}$$

The only nonnegative equilibrium is $x^* = (0, 0, 0)$ and matrix B is the zero matrix; thus the local controllability condition is violated.

3.10. Michaelis–Menten reaction



The induced kinetic differential equation is

$$\begin{aligned}\dot{x}_1 &= -(1 + u_1)x_1x_2 + (1 + u_2)x_3 + (1 + u_3)x_3, \\ \dot{x}_2 &= -(1 + u_1)x_1x_2 + (1 + u_2)x_3, \\ \dot{x}_3 &= (1 + u_1)x_1x_2 - (1 + u_2)x_3 - (1 + u_3)x_3, \\ \dot{x}_4 &= (1 + u_3)x_3.\end{aligned}$$

There are two types of the nonnegative equilibria, namely $x^* = (a, 0, 0, b)$ or $x^* = (0, a, 0, b)$. The calculation shows in every case that matrix B is the zero matrix again.

4. Discussion, open problems

We start with some general remarks. Throughout the paper, the condition of existence of at least one positive equilibrium played a central role in our results. On the other hand, it is enough to know that the positive equilibrium exists since we did not use the coordinates of the positive equilibrium explicitly. According to our results, one can notice that one could get the rank of matrix B without calculating explicitly the equilibrium.

As a trivial consequence of theorem 8 we mention that if we make a reaction step reversible such that the obtained reaction also has positive equilibrium we cannot get $\text{rank}(\tilde{B}) = M$ when the original reaction has matrix B with smaller rank than M . In other words, if we are interested in controllability in dimension M we cannot influence

the satisfaction of our condition by making reaction steps reversible in the previous case.

One can think that obtaining $\text{rank}(B) = M$ is a positive result. It is not the case when we investigate local controllability in manifolds with dimension smaller than M . In this case we cannot even apply theorem 4.

Now we formulate some open problems. It would be interesting to investigate some other possible choices of the control parameters. To consider matrix A is not as simply as to consider matrix B . One could ask what kind of further conditions could be derived by considering matrix A .

The other part of the open problems is when we build up another model for chemical reactions. If we deal with diffusion or with a stochastic model it would be useful to investigate controllability questions. Furthermore, if we could claim something about controllability of reactions with diffusion or something about stochastic models, it would be very interesting to compare this new results to the results obtained by investigating the usual deterministic model.

The question of local observability of chemical reactions will be (partially) answered in a forthcoming paper.

Acknowledgements

The author would like to thank János Tóth, Zoltán Varga and Vilmos Gáspár for their useful advice and their conscientious work of reading the manuscript. The referee was kind to call the author's attention to the paper [7]. This work was partially supported by the National Scientific Research Fund No. T014480.

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