Journal of Mathematical Chemistry 24 (1998) 15–22 

# On local observability of chemical systems

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Received 28 October 1997; revised 21 April 1998

In this paper we consider the question of local observability of chemical systems. We deal with the problem of reducing the number of observed coordinates. The main goal of our paper is to prove sufficient conditions which will guarantee local observability.

## 1. Introduction

In a previous paper we investigated the problem of local controllability of chemical reactions [3]. This paper is devoted to the study of the "dual" problem, namely local observability. The problem of observability is to find some coordinates with the property that if these coordinates of two solutions are equal then all coordinates are equal. Uniqueness of solutions implies that every system will be observable by observing all coordinates. Thus the further problem is to reduce the number of observed coordinates, which is very important from the point of view of applications.

Our theoretical investigations will be applied to a special class of polynomial differential equations, namely the kinetic differential equations. These equations are interpreted as a deterministic model of chemical reactions. Kinetic differential equations are essentially nonlinear. Conservation relations imply that kinetic differential equations have invariant manifolds; thus we use results on local observability within an invariant manifold [4]. The above naive definition of observability can be translated into the language of chemistry to get that in experiments it is enough to follow the time evolution of concentration of some chemical components.

Our paper is organized as follows. In the next section we introduce the definitions of the mathematical theory of local observability and the mass action kinetic model. In section 3 there follow the sufficient conditions for local observability, and in section 4 we give three examples. We will discuss our results in section 5.

## 2. Preliminaries

In this section we introduce the investigated model of chemical reactions and collect the basis of the mathematical theory of local observability as well.

### 2.1. The mass action type model

Let us assume that the physical circumstances are ideal, i.e., in the given reaction the temperature the pressure and the volume of the vessel are constant and there are only finitely many chemical components denoted by $\mathcal{X}(m),\ m = 1, \dots, M$. In the chemical reaction the following $R$ reaction steps take place:

$$\sum_{m=1}^{M} \alpha(m,r)\mathcal{X}(m) \xrightarrow{k(r)} \sum_{m=1}^{M} \beta(m,r)\mathcal{X}(m) \quad (r = 1, \dots, R). \tag{1}$$

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. We use three $M \times R$ matrices $\alpha,\ \beta$, obtained from $\alpha(m,r),\ \beta(m,r)$, respectively, and define $\gamma := \beta - \alpha$.

The mass action type model of reaction (1) is the differential equation

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

where $x_m(t)$ is to be interpreted as the concentration of the chemical component $\mathcal{X}(m)$ at time $t$. Equation (2) is said to be the induced kinetic differential equation of reaction (1).

### 2.2. Local observability

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 $f(x^*, u^*) = 0$. Fix a $T > 0$ and, for every $\varepsilon > 0$, define

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

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

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

then there is a unique absolutely continous function $x \in W_{11}^n[0,T]$, where $W_{11}^n[0,T]$ denotes the set of absolutely continous $x : [0,T] \to \mathbf{R}^n$ functions, with

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

(ii) $x(0) = z$.

Now fix an arbitrary $\varepsilon \in (0, \varepsilon_0]$ and $k \in \{1, \dots, n\}$. Let $S \subset \mathbf{R}^n$ be a $k$-dimensional positively $\varepsilon$-invariant submanifold of system (i). The latter means that, roughly speaking, any solution starting from a point of $S$ near enough the equilibrium $x^*$, will remain in $S$, at least for small controls. To be more precise, $S$ is said to be an $\varepsilon$-invariant manifold of system (i) at $x^*$ if the conditions $z \in S,\ |z - x^*| < \varepsilon,\ u \in U_\varepsilon$ imply that

for $x$ in (i) and (ii) we have $x(t) \in S$ ($t \in [0, T]$). Consider the following observation system:

$$\dot{x} = f \circ (x, u^* + u), \tag{3}$$

$$y = h \circ x, \tag{4}$$

where $h \in C^1(\mathbf{R}^n, \mathbf{R}^m)$ with $m \in \mathbf{N}$, $h(x^*) = 0$, and $x$ in equation (4) is the solution of the initial value problem (i)–(ii). The function $y$ is called the observation corresponding to $x$.

**Definition 1.** System (3)–(4) is said to be locally observable at $x^*$ in $S$ with respect to $U_\varepsilon$ if

(a) $u \in U_\varepsilon$,

(b) $z^i \in S$, $|z^i - x^*| < \varepsilon$, $x^i \in W_{11}^n[0, T]$,
$\dot{x}^i = f \circ (x^i, u^* + u)$, $x^i(0) = z^i$ for $i = 1, 2$,

(c) $h \circ x^1 = h \circ x^2$

imply that $z^1 = z^2$ (thus $x^1 = x^2$).

Let $A := \partial_x f(x^*, u^*)$, $C := h'(x^*)$,

$$Q := \begin{bmatrix} C \\ CA \\ \vdots \\ CA^{n-1} \end{bmatrix},$$

and let us denote the tangent space of manifold $S$ at $x^*$ with $T_{x^*}(S)$ which is to be considered as a linear subspace of $\mathbf{R}^n$. We will use the following theorem due to Varga [4]:

**Theorem 2.** If

$$T_{x^*}(S) \cap \operatorname{Ker} Q = \{0\},$$

then system (3)–(4) is locally observable at $x^*$ in $S$ with respect to $U_\varepsilon$ with some $\varepsilon \in (0, \varepsilon_0)$.

## 3. Sufficient conditions

First we investigate local observability questions in dimension $M$, i.e., in $\mathbf{R}_+^M$. It is known that the $M$-dimensional manifold $\mathbf{R}_+^M$ is a positively invariant manifold of every induced kinetic differential equation (see [1]). In some cases there are other invariant manifolds, even of smaller dimension than $M$. These cases will be considered in section 3.2.

### *3.1. The case of dimension $M$*

We start with a linear algebraic lemma which will help us to prove a general result.

**Lemma 3.** Let $u_1, \ldots, u_n$ and $v_1, \ldots, v_n$ two basis in $\mathbf{R}^n$. For all $I \subset \{1, \ldots, n\}$, exists $J_I \subset \{1, \ldots, n\}$ with $|I \cup J_I| = n$ such that $\{u_i, v_j \mid i \in I,\ j \in J_I\}$ forms a basis in $\mathbf{R}^n$.

*Proof.* Without loss of generality we can assume that if $|I| = l$ then $I = \{1, \ldots, l\}$. We will prove with induction. If $l = 1$ then using $u_1 = \sum_{i=1}^{n} \lambda_i v_i$ and the fact that there exists $j$ such that $\lambda_j \neq 0$ we get that

$$\frac{1}{\lambda_j} u_1 - \sum_{i \neq j} \frac{\lambda_i}{\lambda_j} v_i = v_j,$$

which shows that $J_I := \{1, \ldots, n\} \backslash \{j\}$ is a good choice.

If we know the result for $l = k$ we can prove it for $l = k + 1$ in the following way. Let us denote the $J_I$ set for $I = \{1, \ldots, k\}$ by $J_k$. Then $u_{k+1} = \sum_{i \in J_k} \lambda_i v_i + \sum_{i=1}^{k} \mu_i u_i$, and there exists a $j \in J_k$ such that $\lambda_j \neq 0$, since vectors $u_1, \ldots, u_{k+1}$ are linearly independent. Thus the set defined $J_I := J_k \backslash \{j\}$ is a good choice, and the lemma is proved. □

**Theorem 4.** If $\det A \neq 0$ then there exists a $C \in \mathbf{R}^{\lceil M/2 \rceil \times M}$ which satisfies the condition of local observability with $h'(x^*) \equiv C$.

*Proof.* Let us use the above lemma with $u_1 := e_1,\ \ldots,\ u_n := e_n$, where $e_i$ is the $i$th unit vector, $v_1 := a_1,\ \ldots,\ v_n := a_n$, where $a_i$ is the $i$th row of matrix $A$, and $I := \{1, \ldots, \lceil M/2 \rceil\}$. Then lemma 3.1 claims that, after renumbering, the rows of matrix $A$, $e_1, \ldots, e_{\lceil M/2 \rceil}, a_1, \ldots, a_{\lfloor M/2 \rfloor}$ forms a basis of $\mathbf{R}^n$. This means that if we define

$$C := \begin{bmatrix} e_1 \\ \vdots \\ e_{\lceil M/2 \rceil} \end{bmatrix},$$

then the matrix

$$\begin{bmatrix} C \\ CA \end{bmatrix}$$

has full rank; thus, matrix $Q$ has full rank as well. As a result, we get that the condition of local observability is satisfied with $C$ defined above. □

*Remark 1.* The above theorem gives us the possibility to construct the observation function. For example, $h(z) := C(z - x^*)$ is a linear observation function which satisfies the condition of local observability.

*Remark 2.* The proof of the above general theorem is constructive. Recalling the naive definition of observability we can say theorem 4 means that if the first $\lfloor M/2 \rfloor$ coordinates of two solutions are equal then all coordinates are equal.

*Remark 3.* If $R = M$ and every coordinate of equilibrium $x^*$ is equal to 1 then the condition $\det A \neq 0$ and conditions $\det \gamma \neq 0$ and $\det \alpha \neq 0$ are equivalent because the following equality holds:

$$A = \gamma \begin{bmatrix} k(1) & & \\ & \ddots & \\ & & k(R) \end{bmatrix} \alpha.$$

Now let us reduce the number of the rows of matrix $C$. The following theorem deals with the optimal case, i.e., when the number of the rows is equal to 1. Let $g_A$ denote the minimal polynomial of matrix $A$.

**Theorem 5.** If $\operatorname{gr} g_A = M$ then there exists a $C \in \mathbf{R}^{1\times M}$ which satisfies the local observability condition with $h'(x^*) \equiv C$.

*Proof.* From linear algebra we know that if the degree of the minimal polynomial is maximal then there is a vector which generates a maximal dimensional $A$-invariant subspace. This vector can be choosen as $C$. □

*Remark 4.* The above theorem means that a suitable linear combination can be observed but, in contrast to theorem 4, the proof is not constructive.

### *3.2. The case of dimension $k < M$*

As we mentioned earlier, in this section observability questions will be investigated with smaller dimension manifolds than $M$. Reaction simplices will be chosen as these manifolds, i.e., the translations of the subspace spanned by the columns of matrix $\gamma$. This subspace will be denoted by $S(\gamma)$. In this section we consider reactions which satisfy the inequality $R < M$. The following theorem deals with the optimal case again.

**Theorem 6.** If the columns of matrix $\gamma$ are eigenvectors of matrix $A$ and the corresponding eigenvalues are different then there exists a $C \in \mathbf{R}^{1\times M}$ which satisfies the sufficient condition for local observability with $h'(x^*) \equiv C$. Furthermore, we can choose any $C$ satisfying $C \notin \operatorname{Span}\{\gamma_1, \ldots, \gamma_R\}^{\perp}$, where $\gamma_1, \ldots, \gamma_R$ are the columns of matrix $\gamma$.

*Proof.* Let $C$ be an arbitrary vector satisfying $C \notin \mathrm{Span}\{\gamma_1, \ldots, \gamma_R\}^{\perp}$. We have to show that $\mathrm{Ker}\, Q \cap S(\gamma) = \{0\}$ holds or, equivalently, $s \in S(\gamma),\ Qs = 0$ imply $s = 0$. Since any $s$ from $S(\gamma)$ is the linear combination of vectors $\gamma_1, \ldots, \gamma_R$, it is enough to show that the vectors $s_i := Q\gamma_i,\ i = 1, \ldots, R$, are linearly independent. Since

$$Q\gamma_i = \begin{bmatrix} C \\ CA \\ \vdots \\ CA^{M-1} \end{bmatrix} \gamma_i = \begin{bmatrix} C\gamma_i \\ CA\gamma_i \\ \vdots \\ CA^{M-1}\gamma_i \end{bmatrix} = \begin{bmatrix} C\gamma_i \\ \lambda_i C\gamma_i \\ \vdots \\ \lambda_i^{M-1} C\gamma_i \end{bmatrix},$$

where $\lambda_i$ denotes the eigenvalue corresponding to $\gamma_i$, and using the condition $C\gamma_i \neq 0$ it is enough to prove that the vectors

$$\begin{bmatrix} 1 \\ \lambda_i \\ \vdots \\ \lambda_i^{M-1} \end{bmatrix}, \quad i = 1, \ldots, R,$$

are linearly independent, which is obvious since the eigenvalues are different. □

We remark that although the conditions of the previous theorem seem to be restrictive, only matrix $\gamma$ is fixed and there is a possibility to choose matrix $A$, namely matrix $A$ depends not only on the coordinates of the equilibrium but on the coordinates of $u^*$ as well.

## 4. Examples

In this section we will give three examples to demonstrate our results.

### *4.1. An example for dimension $M$*

Consider the Lotka–Volterra model, i.e., the following reaction:

$$\begin{aligned} \mathcal{X} &\to 2\mathcal{X}, \\ \mathcal{X} + \mathcal{Y} &\to 2\mathcal{Y}, \\ \mathcal{Y} &\to \mathcal{O}. \end{aligned}$$

After building up the kinetic differential equation and calculating matrix $A$ one can see that the minimal polynomial of matrix $A$ is equal to $\lambda^2 + 1$; thus, the reaction satisfies the condition of theorem 5. This means that we can observe a suitable linear combination of the two variables. On the other hand, one can check that $\det A \neq 0$; thus we can apply theorem 4 giving the possibility to construct one suitable vector $C$. Following the proof of theorem 4 one can notice that $e_1, a_1$ forms a basis, where $a_1$ is the first row of matrix $A$. This means that $C = e_1$ is a good choice and (by remark 1) $h(z) = z_1 - 1$ is an observation function.

### 4.2. An example for dimension $k < M$

Let us consider the following reaction:

$$\begin{aligned} \mathcal{X}_1 &\to \mathcal{X}_2, \\ &\vdots \\ \mathcal{X}_{2M-1} &\to \mathcal{X}_{2M}. \end{aligned}$$

The induced kinetic differential equation is

$$\begin{aligned} \dot{x}_1 &= -u_1 x_1, \\ \dot{x}_2 &= u_1 x_1, \\ &\vdots \\ \dot{x}_{2M-1} &= -u_M x_{2M-1}, \\ \dot{x}_{2M} &= u_M x_{2M-1}. \end{aligned}$$

If we calculate matrix $A$ in an equilibrium $x^* = (0, a_1, \ldots, 0, a_M)$, $u^* = (1, 1, \ldots, M, M)$ we get

$$A = \text{blockdiag}\left( \begin{bmatrix} -1 & 0 \\ 1 & 0 \end{bmatrix}, \ldots, \begin{bmatrix} -M & 0 \\ M & 0 \end{bmatrix} \right).$$

Let us denote the columns of matrix $\gamma$ by $\gamma_i$ ($i = 1, \ldots, M$). It is easy to see that $A\gamma_i = -i\gamma_i$ ($i = 1, \ldots, M$). This equality implies local observability after applying theorem 6.

### 4.3. Michaelis–Menten reaction

Consider the following reaction (see [2]):

$$\begin{aligned} \mathcal{X} + \mathcal{Y} &\to \mathcal{Z}, \\ \mathcal{Z} &\to \mathcal{X} + \mathcal{Y}, \\ \mathcal{Z} &\to \mathcal{X} + \mathcal{V}. \end{aligned}$$

The induced kinetic differential equation is

$$\begin{aligned} \dot{x}_1 &= -u_1 x_1 x_2 + u_2 x_3 + u_3 x_3, \\ \dot{x}_2 &= -u_1 x_1 x_2 + u_2 x_3, \\ \dot{x}_3 &= u_1 x_1 x_2 - u_2 x_3 - u_3 x_3, \\ \dot{x}_4 &= u_3 x_3. \end{aligned}$$

If we calculate matrix $A$ in an equilibrium $x^* = (a, 0, 0, 0)$, $u^* = (1, 1, 1)$ one can notice that none of our results can be applied, namely $\det(A) = 0$, $\operatorname{gr} g_A < 4$, and the columns of matrix $\gamma$ are not eigenvectors of matrix $A$.

## 5. Discussion

First, we return to the problem of reducing the number of control parameters as it was investigated in [3]. As we mentioned in [3], it is very important to reduce the number of control parameters from the point of view of chemical engineering science, since if there is a single control parameter then we may happen realise the control by changing the temperature. In [3] we gave a condition of reducing the number of control parameters to a single control parameter in dimension 2. To be more general, we can use the condition of theorem 5, namely if $\operatorname{gr} g_A < M$ then it is impossible to reduce the number of control parameters to a single one.

It would be interesting to investigate reaction–diffusion models as well or to improve our results by considering not only mass action type models.

## Acknowledgements

The author acknowledges János Tóth and Zoltán Varga for their advice and Róbert Freud for his help in proving theorem 5. This work was partially supported by the National Scientific Research Fund under number T014480.

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