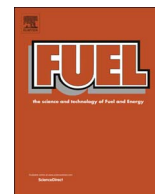




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Full Length Article

# Controllability and reachability of reactions with temperature and inflow control

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## ARTICLE INFO

## Keywords:

Lie-algebra  
Temperature control  
Inflow control  
Fuel cell

## ABSTRACT

Knowing the controllability properties of reactions may be critical in the design phase of controlled systems. Analysis of the controllability properties of reactions is done here with control inputs being the temperature of the reaction, and the inflow rates of some species. The analysis is based on the Lie-algebra generated by the vector fields related to the differential equation of the reaction. We prove that the chemical reactions are strongly reachable on a subspace that has the same dimension as the number of independent reaction steps in every point except where the concentration of reactant species is zero, and show that this result holds for reactions in continuously stirred tank reactors as well. Finally, we analyze the controllability of the anode and cathode reactions of a polymer electrolyte membrane fuel cell with the inflow rates of hydrogen and oxygen being the control inputs and show that by using the inflow rates as control inputs the dimension of the subspace on which the system is controllable can be greater than the number of independent reaction steps.

## 1. Introduction

Controlling chemical reactions is a key issue in modern chemical engineering science [1–3], see e.g. [4,5], where control of nonlinear chemical reactors is considered. The controllability properties of a system can tell us how we can affect the system by using some control law, e.g. whether we can affect the resulting equilibrium state of a system, that may be the case for a controllable system, or we can only affect the speed and certain qualities of the transient, as it may be the case for a system that is only reachable, but not controllable. Thus, analysis of the controllability properties is desirable before the design of control systems.

The controllability of chemical reactions is usually checked only locally using linear tests, i.e. approximation of the nonlinear differential equations with linear ones, and using results from the control theory of linear systems, see one of the first papers by [6] on the observability and controllability of continuously stirred tank reactors (CSTRs). Controllability of chemical reactions that have a positive equilibrium is established in [7] based on the linearized dynamics. In [8], controllability analysis of a liquid-phase catalytic oxidation of toluene to benzoic acid was done based on linearization at five different operating points, and controllability analysis of polymerization in different operating points was done in [9]. Controllability analysis of protein

glycosylation was done based on a linear model identified from measurements in [10]. The connection of controllability and structure of chemical reaction was analyzed in [11], while controllability of chemical processes was analyzed in [12–16].

A key issue in the formulation of the control problem is the control input. In [7] the reaction is considered as a multiple input system, where the rates of the reaction steps can be controlled independently, thus the control inputs were the reaction rates of the reaction steps. The controllability of such a system was proved in a positive equilibrium, provided that such an equilibrium exists. This result was further generalized in [17], and it was shown that the controllability is a global property if we can control all the reaction rates independently, and the possibility of reducing the required number of control inputs was also investigated. However, implementation of control by altering the reaction rates has some problems from the practical point of view. Here we will consider the temperature of the reaction and inflow rate of some species as control inputs.

Controllability analysis in operating points, however, only gives local results. The application of Lie-algebra rank condition was suggested for the controllability analysis of chemical reactions in [18], however no general results were given. The Lie-algebra generated by the vector fields of the reaction was used for controllability analysis of reactions whose control inputs are the reaction rates in [17]. A review

Abbreviations: PEMFC, polymer electrolyte membrane fuel cell; CSTR, continuously stirred tank reactor

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<http://dx.doi.org/10.1016/j.fuel.2017.09.095>

Received 10 February 2017; Received in revised form 23 August 2017; Accepted 26 September 2017  
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of controllability analysis of chemical reactions was done in [19]. An alternative method for controllability analysis is shown in [20].

We give the definitions of the controllability properties and the conditions used for controllability analysis in Section 2. The mass action kinetic model used to model reactions is discussed in Section 3. We give the model of temperature dependence of the reaction rate coefficients, and the dynamics of the temperature of the reaction.

We analyze the controllability properties of chemical reactions in the case if the controlled variable is the temperature of the reaction in Section 4. We extend the acquired results for reactions in CSTRs. Finally, we analyze the controllability properties of a modified polymer electrolyte membrane fuel cell (PEMFC) model with the control input being the inflow rate of the oxygen, and the inflow rate of oxygen and hydrogen.

## 2. Controllability and reachability

Consider a nonlinear system whose dynamics is governed by the differential equation

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t)) + \mathbf{g}(\mathbf{x}(t))u(t) \quad (1)$$

at time instant  $t \in \mathbb{R}^+$ , with  $\mathbf{x}(t) \in \mathbb{R}^M$  being the state of the system at time instant  $t$ ,  $\mathbf{f}$  is a smooth vector field (i.e.  $\mathbf{f} \in \mathcal{C}^\infty(\mathbb{R}^M, \mathbb{R}^M)$ ) called the drift vector field,  $\mathbf{g}$  is a smooth vector field (i.e.  $\mathbf{g} \in \mathcal{C}^\infty(\mathbb{R}^M, \mathbb{R}^M)$ ) called the control vector field, and  $u(t)$  is the control input at time instant  $t$ .

**Definition 1.** [17] Define the following sets, called the reachability (or accessibility) sets:

- $\mathcal{R}(\mathbf{x}_0, T) = \{\text{the set of the states of the system (1) at time } T \text{ if the initial condition is } \mathbf{x}(0) = \mathbf{x}_0 \text{ with all possible inputs such that } \mathbf{u} \in \mathcal{L}^\infty([0, T], \mathbb{R}) \text{ provided that the solution is defined on } [0, T]\}.$
- $\mathcal{R}(\mathbf{x}_0) = \bigcup_{t \geq 0} \mathcal{R}(\mathbf{x}_0, t)$ , i.e. all the states of the system that can be reached in arbitrary time with the initial condition  $\mathbf{x}(0) = \mathbf{x}_0$  and an arbitrary bounded input.

**Definition 2.** The system described with the differential Eq. (1) is called strongly reachable (or strongly accessible) from the point  $\mathbf{x}^*$  if the set  $\mathcal{R}(\mathbf{x}^*, T)$  has an interior point for all  $T > 0$ .

**Definition 3.** The system described with the differential Eq. (1) is called locally controllable in the point  $\mathbf{x}^*$  if  $\mathbf{x}^*$  is the interior point of  $\mathcal{R}(\mathbf{x}^*)$ .

**Definition 4.** The system described with the differential Eq. (1) is called small-time locally controllable in the point  $\mathbf{x}^*$  if  $\mathbf{x}^*$  is the interior point of  $\mathcal{R}(\mathbf{x}^*, T)$  for arbitrary  $T > 0$ .

The Lie-bracket of two smooth vector fields  $\mathbf{f}_1, \mathbf{f}_2 \in \mathcal{C}^\infty(\mathbb{R}^M, \mathbb{R}^M)$  is defined as

$$[\mathbf{f}_1, \mathbf{f}_2] = \mathbf{f}_1 \mathbf{f}_2 - \mathbf{f}_2 \mathbf{f}_1 \quad (2)$$

We use the ad operator to denote the application of the Lie-bracket as

$$\text{ad}_{\mathbf{f}_1}^0 \mathbf{f}_2 = \mathbf{f}_2 \quad (3)$$

$$\text{ad}_{\mathbf{f}_1}^1 \mathbf{f}_2 = [\mathbf{f}_1, \mathbf{f}_2] \quad (4)$$

$$\text{ad}_{\mathbf{f}_1}^2 \mathbf{f}_2 = [\mathbf{f}_1, \text{ad}_{\mathbf{f}_1}^1 \mathbf{f}_2]. \quad (5)$$

**Definition 5.** The Lie-algebra generated by the vector fields  $\mathbf{f}_1$  and  $\mathbf{f}_2$  denoted by  $\text{Lie}\{\mathbf{f}_1, \mathbf{f}_2\}$  is the smallest Lie-algebra (subspace) that satisfies the following conditions:

1.  $\mathbf{f}_1, \mathbf{f}_2 \in \text{Lie}\{\mathbf{f}_1, \mathbf{f}_2\}$ .
2. For any two vector fields  $\tau_1, \tau_2 \in \text{Lie}\{\mathbf{f}_1, \mathbf{f}_2\}$  it is true that  $[\tau_1, \tau_2] \in \text{Lie}\{\mathbf{f}_1, \mathbf{f}_2\}$ .

**Theorem 1.** [21] The system defined by the differential Eq. (1) is strongly reachable from a point  $\mathbf{x}^* \in \mathbb{R}^M$  if and only if the Lie-algebra generated by the vector fields  $\mathbf{g}$  and  $[\mathbf{f}, \mathbf{g}]$  is  $M$ -dimensional at  $\mathbf{x}^* \in \mathbb{R}^M$ .

Note that it may happen that the dimension of  $\text{Lie}\{\mathbf{g}, [\mathbf{f}, \mathbf{g}]\}$  is  $N < M$ , in this case we say that the system is strongly reachable on an  $N$ -dimensional subspace of  $\mathbb{R}^M$ . Otherwise, we say the system is (completely) strongly reachable.

Strong reachability is not the same as local controllability; the condition for strong reachability is only a necessary condition for local controllability [21]. The following example shows a system that is strongly reachable, but not locally controllable.

**Example 1.** Consider the system described by the differential equations

$$\dot{x}_1(t) = x_2^2(t) \quad (6)$$

$$\dot{x}_2(t) = u(t). \quad (7)$$

Using the input  $u$  we can drive state  $x_2$  anywhere, however, we can not decrease the state  $x_1$ , so the set of reachable states from an initial point  $\mathbf{x}(0)$  is  $\mathcal{R}(\mathbf{x}(0)) = \{x_1(t) \geq x_1(0), x_2(t) \in \mathbb{R}, t \geq 0\}$ .

This system is not locally controllable, since if we leave the point  $x_1(t)$ , we can not drive the system back to that point. However, the following system is locally controllable everywhere (and globally controllable as well):

**Example 2.**

$$\dot{x}_1(t) = x_2(t) \quad (8)$$

$$\dot{x}_2(t) = u(t). \quad (9)$$

Using the input  $u$  we can drive the state  $x_2$  anywhere, and by utilizing the effect of  $x_2$  on  $x_1$ , we can drive that state anywhere too, thus the set of reachable states from an initial point  $\mathbf{x}(0)$  is  $\mathcal{R}(\mathbf{x}(0)) = \{x_1(t) \in \mathbb{R}, x_2(t) \in \mathbb{R}, t \geq 0\}$ .

There are some sufficient conditions for small-time local controllability that can be found in the literature, see e.g. [22,23]. These conditions involve checking the Lie-brackets of the vector fields, one has to check whether the effect of bad Lie-brackets (iterated Lie-brackets not vanishing at equilibrium points containing the control vector field even times, referring to polynomials in the differential equation with even power) can be compensated with good Lie-brackets (iterated Lie-brackets not vanishing at equilibrium points containing the control vector field odd times, referring to polynomials in the differential equation with odd power). In order to formulate this condition more precisely, we need the following definition.

**Definition 6.** Let  $S^1(\mathbf{g}, \mathbf{f})$  denote the subspace spanned by all iterated Lie-brackets of  $\mathbf{g}$  and  $\mathbf{f}$  that contains the vector field  $\mathbf{g}$  exactly one time, i.e.  $S^1(\mathbf{g}, \mathbf{f}) = \text{span}\{\mathbf{g}, [\mathbf{f}, \mathbf{g}], [\mathbf{f}, [\mathbf{f}, \mathbf{g}]], \dots\}$ . Similarly, let  $S^k(\mathbf{g}, \mathbf{f})$  denote the subspace spanned by iterated Lie-brackets of  $\mathbf{f}$  and  $\mathbf{g}$  that contains  $\mathbf{g}$  exactly  $k$  times.

**Theorem 2.** [22] If the vector fields of the system defined by the differential Eq. (1) satisfy the condition  $S^{2k}(\mathbf{g}, \mathbf{f})(\mathbf{x}^*) \subseteq S^{2k-1}(\mathbf{g}, \mathbf{f})(\mathbf{x}^*)$  at an equilibrium  $\mathbf{x}^*$  of (1) for each  $k = 1, 2, \dots$ , then the system is small-time locally controllable in  $\mathbf{x}^*$ .

Note that if the conditions of Theorem 2 hold not just in equilibrium points, but in the points of a trajectory of the system, we say that the system is small-time locally controllable on that trajectory [23].

## 3. Kinetic differential equations with temperature dependence

Consider a chemical reaction with  $M$  species, and let the species be denoted by  $X_1, X_2, \dots, X_M$ . Moreover, let  $R$  be the number of reaction steps. Call the linear combination of the species on the left-hand side of a reaction step the reactant complex, and the linear combination of the

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