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# Dynamical Analysis of a Class of Distributed Parameter Fixed Bed Reactors

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**Abstract**

This paper deals with the dynamical properties (observability, reachability, stabilizability, detectability) of fixed bed reactors. The class of processes considered here are plug flow reactors in which sequential reactions take place (at the exclusion of reversible reactions, and "loop" reactions). The analysis is based on a linear distributed parameter model of the process. It is shown that the system is stable, whence detectable and stabilizable when the control inputs are the influent reactant concentrations. But it is not approximately reachable. Besides observability is studied when either the concentrations of the process components or the products of the sequential reactions' endpoints are measured at the reactor output.

## 1 Introduction

The dynamics of fixed bed reactors are described by partial differential equations (PDE's) derived from mass and energy balances (e.g. [1]). Either for (dynamic) simulation or for control design, the PDE's model is commonly reduced to a set of ordinary differential equations (ODE's) by using approximation methods (e.g. finite differences, orthogonal collocation,...)[2], [3]. The approximation procedure may result in extensive computation studies before obtaining a satisfactory model approximation. For finite differences, the number of ODE's may easily become excessively high. And for orthogonal collocation (which presents the advantage of substantially reducing the number of required ODE's), in spite of interesting attempts, e.g. [4], there exists no systematic procedures for choosing the reduction parameters (like the number of collocation points, or the value of the parameters $\alpha$ and $\beta$ of the Jacobi polynomial, which influence the location of the discretization points); the properties of the space derivatives' approximation may be even be surprising (see [5]). Beside this computation burden, it may be difficult generally speaking to know the connection between the original distributed parameter model and its discretized version, and as it is mentioned in [6], the dynamical properties of both models may be different.

This paper is dedicated to the analysis of a class of fixed bed reactors, viz. plug flow reactors involving sequential reactions for which the kinetics only depends on the concentrations of the reactants involved in the reaction. The analysis is carried out by using the tools of the distributed parameter (i.e. infinite dimensional state space) linear system theory (see e.g. [7], [8] and the references therein), and is based on the linearized tangent model of the (generally) nonlinear PDE's model. In that sense this work is intended to try to reconcile the abstract distributed parameter system theory and the practical process control problems. The concepts of observability and reachability that will be considered here are those used in [9]. It is shown that the linearized tangent PDE's model is stable, whence that it is detectable and stabilizable. On the other hand, it is shown that it is not approximately reachable. The system is observable if the component concentrations are measured at the reactor output. Moreover no physical value (positive concentration) of the state is unobservable if the products at the sequential reactions' endpoints are measured at the reactor output.

The paper is organized as follows. Section 2 is dedicated to the dynamical models : we first introduce the *basic* dynamical model of a plug flow reactor for one isothermal reaction with one reactant and one product. The dynamical analysis of the *basic* dynamical model is carried out in Section 3. In order to have a paper as easy to read as possible, particularly for non-experts in infinite dimensional systems, we have deliberately written the paper with a pedagogical intention by starting Section 3 with a short introduction of the basic concepts of infinite-dimensional systems. Extensions of the results to other cases of

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sequential reactions are discussed in Section 4.

## 2 Basic Dynamical Model

Let us consider a fixed bed reactor without dispersion in which the following reaction takes place :

$$A \longrightarrow bB \tag{1}$$

The dynamics of this process are given by the following mass balance equations :

$$\begin{aligned} \frac{\partial x_1'}{\partial t} &= -u\frac{\partial x_1'}{\partial z} - r(x_1') & (2)\\ \frac{\partial x_2}{\partial t} &= -u\frac{\partial x_2}{\partial z} + br(x_1') & (3)\\ x_1'(z &= 0,t) = x_{in}(t),\ x_2(z=0,t)=0 & (4)\end{aligned}$$

for all $t \geq 0$ and for all $z \in [0, L]$, where $x_1'$ and $x_2$ are the concentrations (mole/l) of $A$ and $B$ respectively, $u > 0$ is the fluid superficial velocity (m/s), $r$ is the reaction rate (mole/l.s), and $x_{in}$ is the influent reactant concentration. Here we also assume that the kinetics only depend on the reactant concentration $x_1'$. In order to get a linear distributed parameter system with homogeneous boundary conditions, we consider the following change of variable :

$$x_1 = x_1' - x_{in}. \tag{5}$$

Then the dynamical model (2)-(4) reads as follows:

$$\begin{aligned} \frac{\partial x_1}{\partial t} &= -u\frac{\partial x_1}{\partial z} - r(x_1, x_{in}) - \frac{dx_{in}}{dt} & (6)\\ \frac{\partial x_2}{\partial t} &= -u\frac{\partial x_2}{\partial z} + br(x_1, x_{in}) & (7)\\ x_1(z &= 0,t) = 0,\ x_2(z=0,t)=0. & (8)\end{aligned}$$

If the reaction is characterized by first order kinetics or if we consider the linearized tangent model of (2)-(4) in case of nonlinear kinetics,then the dynamical model (6)-(8) takes the following form

$$\begin{aligned} \frac{\partial x_1}{\partial t} &= -u\frac{\partial x_1}{\partial z} - k_0x_1 - k_0x_{in} - \frac{dx_{in}}{dt} & (9)\\ \frac{\partial x_2}{\partial t} &= -u\frac{\partial x_2}{\partial z} + bk_0x_1 + bk_0x_{in} & (10)\\ x_1(z &= 0,t) = 0,\ x_2(z=0,t)=0, & (11)\end{aligned}$$

where $k_0$ is the kinetics constant ($s^{-1}$). Equations (9)-(11) together with suitable initial conditions define the *basic* dynamical model on which the dynamical analysis will first be performed. In the analysis below, this model is seen as a system with a single control input, viz. $x_{in}$. Now observe that the basic dynamical model can be written in the following operator matrix form:

$$\begin{aligned} \frac{dx}{dt} &= Ax + Bv,\ x(0) = x_0 \ \in\ D(A), & (12)\\ A &= \begin{pmatrix} -u\frac{\partial}{\partial z} - k_0 & 0 \\ bk_0 & -u\frac{\partial}{\partial z}\end{pmatrix}, & (13)\\ B &= \begin{pmatrix} -k_0 & -1 \\ bk_0 & 0\end{pmatrix}\Delta_w(\cdot), & (14)\end{aligned}$$

where $\Delta_w(\cdot)$ denotes a finite unit impulse of window width w, i.e. an approximate Dirac delta distribution at $z = 0$, and where the state x and the input v are defined respectively by $x = (x_1, x_2)$ and $v = (x_{in}, \frac{dx_{in}}{dt})$. This description is analyzed in detail in the following section.

## 3 Dynamical Aanalysis of the Basic Dynamical Model

### 3.1 Uncontrolled model

Since our objective is the dynamical analysis of the fixed bed reactor model by using the linear distributed parameter system theory tools (see e.g. [7], [8], [10]), an important prior step is to obtain a description of the model as an infinite-dimensional Hilbert state space system (12), where $x(t)$ belongs to a real separable Hilbert space $X$, and $A$ is the (infinitesimal) generator of a strongly continuous ($C_0$-) semigroup of bounded linear operators $(e^{At})_{t\geq 0}$ on $X$. Here we use the (Hilbert) state space $X = L^2(0, L) \oplus L^2(0, L)$ , where $L^2(0, L)$ is the set of measurable square–integrable real–valued functions $f : [0, L] \rightarrow I\!R$, i.e. such that $\int_0^L \mid f(z) \mid^2 dz < \infty$, and where $X \oplus Y$ denotes the Hilbert space obtained as the cartesian product of the Hilbert spaces $X$ and $Y$ endowed with the inner product defined by $< z_1, z_2 >=< x_1, x_2 > + < y_1, y_2 >$ for all $z_1 = (x_1, y_1)$, $z_2 = (x_2, y_2) \in X \oplus Y$. $L^2(0, L)$ is a Hilbert space with inner product and norm defined $\forall\, f, g \ \in\ L^2$ respectively by

$$< f, g >_2 = \int_0^L f(z)g(z)dz, \tag{15}$$

$$\| f \|_2 = \sqrt{< f, f >_2} = (\textstyle\int_0^L \mid f(z) \mid^2 dz)^{\frac{1}{2}}.$$

We first concentrate on the free (i.e. uncontrolled) system (for $x_{in} = 0$):

$$\frac{dx}{dt} = Ax,\ x(0) = x_0 \ \in\ D(A), \tag{16}$$

where the operator A is given by (13), which can be rewritten more concisely as follows :

$$A = \begin{pmatrix} A_1 & 0 \\ D & A_2 \end{pmatrix}. \tag{17}$$

#### 3.1.1 Operator $A_1$

This operator is given by

$$\begin{aligned} A_1 : D(A_1) &\longrightarrow L^2(0, L)\\ x_1 &\mapsto A_1x_1 = -u\frac{\partial x_1}{\partial z} - k_0x_1 \quad (18)\end{aligned}$$

on its domain $D(A_1) = \{\, x_1 \in L^2(0, L)$: $x_1$ is absolutely continuous, $\frac{dx_1}{dz} \in L^2(0, L)$, $\ x_1(0) = 0\}$. By e.g. [8], if $A_1$ is the generator of a $C_0$-semigroup of bounded linear operators $(e^{A_1 t})_{t\geq 0}$ on $L^2(0,L)$, then the (homogeneous) Cauchy problem

$$\frac{dx_1}{dt} = A_1 x_1,\ t \geq 0,\ x_1(0) = x_{10} \in D(A_1) \qquad (19)$$

has a unique solution $x_1(\cdot)$, which is given by

$$x_1(t) = e^{A_1 t} x_{10},\ t \geq 0. \qquad (20)$$

**Assertion 1 :** The operator $A_1$ is the generator of a $C_0$-semigroup $(e^{A_1 t})_{t\geq 0}$ of bounded linear operators on $L^2(0,L)$ which is given for any initial state $x_{10} \in L^2(0,L)$ by

$$(e^{A_1 t} x_{10})(z) = \begin{cases} e^{-k_0 t} x_{10}(z-ut) & \text{if } z \geq ut \\ 0 & \text{if } z < ut \end{cases}$$

for all $t \geq 0$ and for all $z \in [0,L]$ . Moreover the $C_0$-semigroup $(e^{A_1 t})_{t\geq 0}$ is exponentially stable; more precisely

$$\| e^{A_1 t} \| \leq e^{-k_0 t},\ \forall t \geq 0, \qquad (21)$$

where $\| \cdot \|$ denotes the uniform operator norm. □

Indeed, observe that

$$< A_1 x, x > \leq -k_0 \| x \|_2^2 \ \ \forall x \in D(A_1), \qquad (22)$$

$$< A_1^* x, x > \leq -k_0 \| x \|_2^2 \ \ \forall x \in D(A_1^*), \qquad (23)$$

where the adjoint operator $A_1^*$ is given by $A_1^* x_1 = u\frac{\partial x_1}{\partial z} - k_0 x_1$ for every $x_1$ in its domain $D(A_1^*) = \{ x_1 \in L^2(0,L)$: $x_1$ is absolutely continuous, $\frac{dx_1}{dz} \in L^2(0,L)$ , $x_1(L) = 0$ $\}$. Observe that $k_0 > 0$; hence, by e.g. Corollary 2.2.3. of [8], it follows from (22)-(23) that $A_1$ is the generator of an exponentially stable $C_0$-semigroup $(e^{A_1 t})_{t\geq 0}$ such that (21) holds. Now, by considering the Laplace transform with respect to $t$ and the expression (18), eq. (19) becomes :

$$u\frac{\partial \hat{x}_1}{\partial z} = -(s+k_0)\hat{x}_1 + x_{10},\ \hat{x}_1(0,s) = 0,$$

where $\hat{x}_1(z,s)$ is the Laplace transform of $x_1(z,t)$. The integration of the above differential equation with respect to the spatial coordinate gives

$$\hat{x}_1(z,s) = \frac{e^{-\frac{s+k_0}{u}z}}{u} \int_0^z e^{\frac{s+k_0}{u}\eta} x_{10}(\eta) d\eta. \qquad (24)$$

Finally observe that the above expression is the Laplace transform (with respect to t) of

$$e^{-k_0 t} x_{10}(z-ut),\ t \geq 0,\ 0 \leq z \leq L. \qquad (25)$$

Remark 1 : The $C_0$-semigroup property of $(e^{A_1 t})_{t\geq 0}$ is characterized by the following conditions, [7], [8]: (i) for all $t \geq 0$, $e^{A_1 t}$ is a bounded linear operator, such that

$$\| e^{A_1 t} \| = \sup_{x \in L^2, x\neq 0} \frac{\| e^{A_1 t} x \|_2}{\| x \|_2} < \infty;$$

(ii) [Semigroup property] for every $x \in L^2(0,L)$, $e^{A_1 t} x_{|t=0} = x$ and $e^{A_1 (t+s)} = e^{A_1 (t)} e^{A_1 (s)}$ for all $t,\ s \geq 0$ ; (iii) [Strong continuity] for every $x \in L^2(0,L)$ , $\| e^{A_1 t} x - x \|_2 \rightarrow 0$ as $t \rightarrow 0^+$ .

#### 3.1.2 Operator $A_2$

Observe that $A_2 = A_1 + k_0 I$ and $D(A_2) = D(A_1)$. In view of Assertion 1, it follows e.g. by Theorem 3.2.1 of [8] that the following result holds.

**Assertion 2 :** The operator $A_2$ is the generator of a $C_0$-semigroup $(e^{A_2 t})_{t\geq 0}$ of contractions on $L^2(0,L)$, (i.e. $\| e^{A_2 t} \| \leq 1$ for all $t \geq 0$), which is given for any initial state $x_{20} \in L^2(0,L)$ by

$$(e^{A_2 t} x_{20})(z) = \begin{cases} x_{20}(z-ut) & \text{if } z \geq ut \\ 0 & \text{if } z < ut \end{cases}$$

for all $t \geq 0$ and for all $z \in [0,L]$ . Moreover the $C_0$-semigroup $(e^{A_2 t})_{t\geq 0}$ is exponentially stable, i.e. there exist constants $M_2 > 0$ and $k_1 > 0$ such that

$$\| e^{A_2 t} \| \leq M_2\, e^{-k_1 t},\ \forall t \geq 0. \square \qquad (26)$$

Remark 2 : Observe that, for any $x_{20} \in L^2(0,L)$,

$$\int_0^\infty \| e^{A_2 t} x_{20} \|_2^2\, dt \leq \frac{L}{u} \| x_{20} \|_2^2 < \infty .$$

Hence, by e.g. Lemma 5.1.2 of [8], the $C_0$-semigroup $(e^{A_2 t})_{t\geq 0}$ is exponentially stable.

#### 3.1.3 Operator $A$

We are taking advantage of the lower triangular form of the operator $A$, which is the generator of the $C_0$-semigroup $e^{At}$ (see e.g. Lemma 3.2.2 of [8]) :

$$e^{At} = \begin{pmatrix} e^{A_1 t} & 0 \\ S(t) & e^{A_2 t} \end{pmatrix}, \qquad (27)$$

$$S(t)x = \int_0^t e^{A_2 (t-s)} D e^{A_1 s} x ds, \qquad (28)$$

where $e^{A_1 t}$ and $e^{A_2 t}$ are the $C_0$-semigroups generated respectively by $A_1$ and $A_2$. Besides since

$$\| e^{A_i t} \| \leq M_i e^{\omega_i t},\ i = 1,2,\ \omega_1 = -k_0,\ \omega_2 = -k_1$$

then $e^{At}$ is also bounded as follows :

$$\| e^{At} \| \leq M e^{\omega t},\ \omega = max(\omega_1, \omega_2) < 0, \qquad (29)$$

whence the $C_0$-semigroup $(e^{At})_{t\geq 0}$ is exponentially stable. Observe also that the value of $S(t)x_{10}$, where $x_{10}$ is in $L^2(0,L)$, is equal to :

$$\begin{aligned} (S(t)x_{10})(z) &= \int_0^t (e^{A_2 (t-s)} D e^{A_1 s} x_{10})(z) ds \\ &= b \cdot (1 - e^{-k_0 t}) \cdot x_{10}(z-ut), \end{aligned}$$

if $z \geq ut$, and $(S(t)x_{10})(z) = 0$ otherwise.

### 3.2 Solution $x(z,t)$

In view of the previous developments, we can write the solution $x(t) = e^{At} x_0$ of the basic dynamical model (9)–(11) as follows, for all $t \geq 0$ and for all $z \in [0, L]$,

$$\begin{aligned} x_1(z,t) &= x_2(z,t) = 0, \; if\; z < ut, & (30) \\ x_1(z,t) &= e^{-k_0 t} x_{10}(z - ut), & (31) \\ x_2(z,t) &= x_{20}(z - ut) + \\ b \cdot (1 - e^{-k_0 t}) &\cdot x_{10}(z - ut), if\; z \geq ut. & (32) \end{aligned}$$

The above expression will be used in the subsequent dynamical analysis. Note that the spectrum of the operator $A$ is empty, i.e. that $(sI - A)^{-1}$ is a bounded linear operator on X for all complex numbers s (see [8])(hence the transfer function has no singularity, and in particular no poles). Because of the stability of $(e^{At})_{t \geq 0}$, the system (9)–(11) is stabilizable (i.e. there exists a stabilizing feedback K such that A + BK generates an exponentially stable $C_0$-semigroup) and detectable (i.e. there exists a stabilizing injection F such that A + BF generates an exponentially stable $C_0$-semigroup).

### 3.3 Observability Analysis

Let us first define an output function $y(.)$ by

$$y(t) = (Cx)(t), \; t \geq 0, \qquad (33)$$

where $C : X \rightarrow I\!R^p$ , with $p = 1$ or 2, is a bounded linear operator. For a linear system (12),(33), i.e. $(C, A)$, the *unobservable subspace* $NO(C, A)$ is the subspace of all initial states $\xi \in X$ producing a zero output, i.e. $Ce^{At}\xi = 0 \; for\; all\; t \geq 0$. The sytem (12), (33), i.e. $(C, A)$, is said to be *observable* if and only if $NO(C, A) = \{0\}$.

Remark 3 : The above observability concept is also known as *approximate* observability in [8] and *weak* observability in [10].

Let us consider measurements at the reactor output $(z = L)$. In this case, the output function $y(\cdot)$ is defined as follows: we consider a (very small) finite length interval at the reactor output $[L - w, L]$, i.e. :

$$y(t) = (Cx)(t) \;\; = \;\; \int_0^L \Delta_w(L - z)\tilde{C}x(z,t)dz$$

where $\Delta_w(\cdot)$ is given as in (14) (i.e. $\Delta_w(z) = w^{-1}$ for $z \in [0, w)$ and $\Delta_w(z) = 0$ elsewhere), and $\tilde{C}$ is either the 2-by-2 identity matrix when both components $x_1$ and $x_2$ are measured, or a unit row vector if only one of them is available for measurement. Observe that $x_1(z,t)$ is only a function of $x_{10}$ while $x_2(z,t)$ is a (positive) weighted sum of both initial reactant and product profiles. If we consider that both variables $x_1$ and $x_2$ are measured, the observability map is written as follows:

$$Ce^{At}\xi = \begin{pmatrix} e^{-k_0 t} S_1(t) \\ b(1 - e^{-k_0 t}) S_1(t) + S_2(t) \end{pmatrix}, \qquad (34)$$

with $S_i(t) = \frac{1}{w} \int_{L-w}^{L} \xi_i(z - ut)dz$, i = 1, 2.
By the Lebesgue differentiation theorem (see e.g. Theorem 8.17 of [11]), and by (Lemma p. 177 of [11]), the following result holds:

**Lemma:** If f $\in L^2(0, L)$ $(\subset L^1(0, L))$ and if $\int_0^x f(z)dz = 0$ for all $x \in [0, L]$, then $f = 0 \in L^2(0, L)$, i.e. $f(z) = 0$ for almost every $z \in [0, L]$. □

From this lemma, we can deduce that the observability map is equal to zero for all $t \geq 0$, i.e. for all $t \in [0, \frac{L}{u}]$ , if and only if $\xi_1(z - ut) = \xi_2(z - ut) = 0$, for all $t \in [0, \frac{L}{u}]$ and for almost all $z \in [L - w, L]$, or equivalently $\xi_1 = \xi_2 = 0 \in L^2(0, L)$.

**Assertion 3 :** The system (12), (33) is observable if the process components $x_1$ and $x_2$ are measured at the reactor output. □

Remark 4 : a) By Assertion 3 and by e.g. pp. 32-34 of [10], the system state can be determined uniquely from the knowledge of the output.
b) Obviously the system is not observable if only $x_1$ is available for measurement at the reactor output (in this case, the observability map reduces to the first component of (34)).

It is also interesting to analyze the observability when only the product $x_2$ is measured at the reactor output. Indeed it has been shown in [5] that the values of reactant and product concentrations in a plug flow reactor remain *positive* (and bounded) for all t. Therefore, by considering this positivity property, the observability map (which is now given by the second component of (34)) is equal to zero for all $t \in [0, \frac{L}{u}]$ if and only if $\xi_1(z - ut) = \xi_2(z - ut) = 0$, for all $t \in [0, \frac{L}{u}]$ and for almost all $z \in [L - w, L]$. This leads to the following result.

**Assertion 4 :** No (positive) physical value of the state of the system (12),(33), i.e. $(C, A)$, is unobservable from the measurement of the product concentration $x_2$ at the reactor output: more precisely, for any $\xi \in X$ such that $\xi \geq 0$ almost everywhere on $t \geq 0$, if $Ce^{At}\xi = 0$ for all $t \geq 0$, then $\xi = 0 \; \in X$ . □

Remark 5 : Presently we do not know whether Assertion 4 is sufficient for determining uniquely the (positive) state from the knowledge of the output, when only the product $x_2$ is measured at the reactor output.

### 3.4 Reachability Analysis

Here we consider the dual property of observability, i.e. (approximate) reachability. The latter concept is more convenient from a control engineering point of view, because it is less restrictive than exact controllability. Moreover there exist computational tests for checking observability (resp. reachability) for large classes of linear distributed parameter systems, see e.g. [8].
For a linear system (12), i.e. $(A, B)$, the *reachable subspace* $R(A, B)$ is the subspace of all states which can be (approximately) reached from the origin, i.e. $R(A, B)$ is the closure of the set of all $\xi \in X$ such that there exist a time $\tau \geq 0$ and a square-integrable input $u : [0, \tau] \rightarrow I\!R$ such that $\xi = \int_0^\tau e^{A(\tau - s)}Bu(s)ds$. The system (12), i.e. $(A, B)$ is said to be *reachable* if and only if $R(A, B) = X$, or equivalently $NO(B^*, A^*) = \{0\}$, since $R(A, B)$ is the

orthogonal complement of $NO(B^*, A^*)$, see e.g. [9]. Consider a (very small) finite length interval at the reactor input $[o, w]$ for the control input $x_{in}$ , i.e.

$$(b_1 v_1)(z,t) = \begin{pmatrix} -k_0 \\ bk_0 \end{pmatrix} \Delta_w(z) x_{in}(t), \qquad (35)$$

where $b_1 \in X$ is the first column of the operator $B$ , (14). The derivation of the adjoints $b_1^* =< b_1, \cdot >$ and $e^{A^* t}$ gives after some straightforward computations: for $z \in [0, L]$ and $t \geq 0$ ,

$$\begin{aligned} b_1^* \xi &= \frac{k_0}{w} \int_0^w (b\xi_2 - \xi_1)(z) dz, \\ e^{A^* t} \xi &= \begin{pmatrix} e^{-k_0 t} \xi_1(\zeta) + b(1 - e^{-k_0 t}) \xi_2(\zeta) \\ \xi_2(\zeta) \end{pmatrix} \end{aligned}$$

if $\zeta = z + ut \leq L$, and $e^{A^* t} \xi = 0$ otherwise. Then the adjoint of the reachability map is equal to

$$b_1^* e^{A^* t} \xi = \frac{k_0}{w} e^{-k_0 t} \int_0^w (b\xi_2 - \xi_1)(\zeta) 1(L - \zeta) dz,$$

where $1(\cdot)$ denotes the unit step function, i.e. $1(t) = 1$ for $t \geq 0$ and $1(t) = 0$ elsewhere. We can set the right hand side to zero by considering values of $\xi_1$ and $\xi_2$ such that $b\xi_2 = \xi_1$. Therefore the following result holds.

**Assertion 5 :** The system (12) with a single control input, namely $x_{in}$, i.e. $(A, b_1)$, where $b_1 \in X$ is the first column of the control operator $B$ given by (14), is not (approximately) reachable. □

# 4 Generalization to Sequential Reactions

Let us now consider a plug flow reactor with sequential reactions (at the exclusion of reversible reactions and reaction loops) for which the kinetics only depends on the reactant concentrations. For the observability, the generalization is based on the extension of the result of the preceding section to two typical cases : a sequence of 3 reactions, and a reaction with more than one reactant.

## 4.1 Observability

### 4.1.1 Sequence of 3 reactions

Let us consider the following sequential reaction scheme :

$$A \longrightarrow bB \qquad (36)$$
$$B \longrightarrow cC \qquad (37)$$

The state operator is then equal to :

$$A = \begin{pmatrix} -u\frac{\partial}{\partial z} - k_1 & 0 & 0 \\ bk_1 & -u\frac{\partial}{\partial z} - k_2 & 0 \\ 0 & ck_2 & -u\frac{\partial}{\partial z} \end{pmatrix}$$

where $k_1$ and $k_2$ are the kinetics constants of reactions 1 and 2, respectively. Here again, $A$ is a lower triangular matrix : therefore we can use the step-by-step approach which has been considered in the basic model case to determine the solution of $x_1$, $x_2$ and $x_3$ (i.e. the concentration of the product $C$). This gives if $z - ut \geq 0$ :

$$\begin{aligned} x_1(z,t) &= e^{-k_1 t} x_{10}(z - ut), \\ x_2(z,t) &= e^{-k_2 t} x_{20}(z - ut) + \frac{bk_1}{k_1 - k_2} \\ & \quad (e^{-k_2 t} - e^{-k_1 t}) x_{10}(z - ut), \\ x_3(z,t) &= x_{30}(z - ut) \\ & + c(1- e^{-k_2 t}) x_{20}(z - ut) \\ & + bc(1- \frac{k_1 e^{-k_2 t} - k_2 e^{-k_1 t}}{k_1 - k_2}) x_{10}(z - ut). \end{aligned}$$

Note that here again, the values of $x_1$, $x_2$ and $x_3$ are a weighted sum of the initial profiles, with positive coefficients. Therefore Assertions 3 and 4 are readily extended for the process components $x_1$, $x_2$ and $x_3$ (Assertion 3), and for $x_3$ (Assertion 4).

### 4.1.2 Reaction with more than one reactant

Let us consider the folowing reaction scheme :

$$A + bB + cC \longrightarrow dD \qquad (38)$$

Let us denote by $x_1$, $x_2$, $x_3$ the concentrations of $A$, $B$ and $C$ normalized with respect to their influent concentrations (as we did in section 2 for the reactant $A$), and $x_4$ the concentration of the product $D$. If we consider the linearized tangent model of the process, the state operator $A$ related to the 3 reactants is equal to :

$$\begin{pmatrix} -u\frac{\partial}{\partial z} - k_1 & -k_2 & -k_3 \\ -bk_1 & -u\frac{\partial}{\partial z} - bk_2 & -bk_3 \\ -ck_1 & -ck_2 & -u\frac{\partial}{\partial z} - ck_3 \end{pmatrix}$$

where the coefficients $k_i$ (i = 1 to 3) are defined from the reaction rate $r(x_1, x_2, x_3$ (= $k_0 f(x_1, x_2, x_3)$ with $k_0$ the kinetic constant) as follows :

$$k_i = k_0 \frac{\partial r}{\partial x_i}, \; i = 1 \; to \; 3. \qquad (39)$$

Triangularisation of the operator $A$ is obtained by considering the following state transformation for the reactants :

$$\zeta_i = x_i + \sum_{j=i+1}^{N} \frac{k_j}{k_i} x_j, \; i = 1 \; to \; N, \qquad (40)$$

where $N$ is the number of reactants involved in the reaction. Since the new variables $\zeta_i$ are positive sums of the original variables, the above line of reasoning applies for measurements of $x_4$ at the reactor output.

### 4.1.3 General observability property

The above two examples cover the typical situations encountered in sequential reactions. Therefore we may conjecture that the following general result holds: the system is observable from measurements of the component concentrations at the reactor output, and no (positive) physical value of the state of the linearized tangent model of a plug flow reactor with sequential reactions are unobservable if the products at the endpoints of the reaction sequences are measured at the reactor output. Note that, since the result is - generally speaking - based on a linearized model, the result is local. It is also worth noting that this result is in line with the results obtained for sequential reactions in multi-tank CSTR's, for which it has been emphasized that the system is (locally) observable when the concentrations of the products at the endpoints of the reaction scheme are measured at the reactor output (see [12]).

### 4.2 Approximate reachability

The reachability result (Assertion 5) can also be generalized to the cases considered above: nothing will be gained in terms of reachability properties by adding reactions and process components in a reaction sequence. However, since the system is stable (as it can be readily noticed from the above arguments), the system is stabilizable, i.e. it is possible to maintain the system state variables in stable conditions in closed loop by an appropriate control design, yet without being able to act arbitrarily on the closed loop dynamics of the whole state.

## 5 Conclusions

In this paper we have analyzed the dynamical properties of a class of fixed bed reactors, viz. plug flow reactors involving sequential reactions for which the kinetics only depends on the concentrations of the reactants involved in the reaction. The analysis has been carried out by using the tools of the distributed parameter, and wass based on the linearized tangent model of the (generally) nonlinear PDE's model. It has been shown that the linearized tangent PDE's model is stable, whence that it is detectable and stabilizable. On the other hand, it is shown that it is not approximately reachable. The system is observable if the component concentrations are measured at the reactor output. Moreover no physical value (positive concentration) of the state is unobservable if the products at the sequential reactions' endpoints are measured at the reactor output.

Our present investigations are oriented towards the analysis of (parabolic) distributed parameter reactor models with diffusion (dispersion).

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## References

[1] S. Feyo de Azevedo, M.A. Romero-Ogawa, and A.P. Wardle. Modelling of tubular fixed-bed catalytic reactors : a brief review. *Trans. I.Chem.E.*, 68(Part A):2–8, 1990.

[2] C. Georgakis, R. Aris, and R. Amundson. Studies in the control of tubular reactors - I. General considerations. *Chem. Eng. Sci.*, 32:1359–1369, 1977.

[3] S.B. Jorgensen. Fixed bed reactor dynamics and control - A review. *Proc. IFAC Control of Distillation Columns and Chemical Reactors, Pergamon*, pages 11–24, 1986.

[4] Y.S. Cho and B. Joseph. Reduced-order steady state and dynamic models. part I and II. *AIChE J.*, 29(2):261–276, 1983.

[5] D. Dochain. "Contribution to the Analysis and Control of Distributed Parameter Systems with Application to (Bio)chemical Processes and Robotics". Thèse d'aggrégation de l'enseignement supérieur, Université Catholique de Louvain, Belgium, 1994.

[6] W.H. Ray. *"Advanced Process Control"*. Butterworths Series in Chemical Engineering, Boston, 1981.

[7] A. Pazy. *Semigroups of Linear Operators and Applications to Partial Differential Equations.* Springer-Verlag, New York, 1983.

[8] R. Curtain and H. Zwart. *Lecture Notes on Distributed Parameter Systems.* Springer Verlag, Berlin, 1994.

[9] F.M. Callier and J. Winkin. LQ-optimal control of infinite-dimensional systems by spectral factorization. *Automatica*, 28 (4):757–770, 1992.

[10] A. ElJai and A.J. Pritchard. *Sensors and Controls in the Analysis of Distributed Systems.* Ellis-Horwood, Chichester, 1988.

[11] W. Rudin. *Real and Complex Analysis.* McGraw Hill, New York, 1974.

[12] M. Perrier and D. Dochain. Dynamical analysis of multi-tank reactors with application to hydrometallurgy. *submitted for publication*, pages 41–88, 1994.