Properties of the Equations Describing a Tank Reactor

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Contents

Abstract

1. INTRODUCTION
   Isothermic Reactors
   Adiabatic Reactors
   Reactors with cooling

2. BATCH REACTORS

3. THE STIRRED TANK REACTOR

4. LINEARIZED ANALYSIS

5. ACKNOWLEDGEMENT

6. REFERENCES

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Abstract

Mathematical models describing the dynamics of tank reactors are well-known in literature. The equations are strongly nonlinear which makes the analysis hard. It has been shown for batch reactors that there exist invariants which make it possible to reduce the order of the equations. Based on linearized analysis it has also been shown that the equations for tank reactors have asymptotic invariants. The purpose of this note is to show that the nonlinear equations for tank reactors have asymptotic invariants. A simplified derivation of the results for the linearized equations is also given.

1. INTRODUCTION

Consider a tank reactor where n constituents react in m reactions. Let c be a vector whose i:th component is the concentration of the i:th constituent in the reactor, let r be a vector whose i:th component is the rate of the i:th reaction, let α be the ratio of volumetric flow and reactor volume, A the transpose of the stoichiometric matrix. It is assumed that the columns of A are linearly independent. The mass balance for the reactor can then be written as

$$\frac{dc}{dt} = \alpha(c_f - c) + A\, r(c,T) \tag{1.1}$$

where the vector c_f denotes the concentration of the feed. Notice that the reaction rate r depends on the concentration and on temperature. The temperature can be determined from an enthalpy balance. This may take different forms depending on the practical arrangement of the reactor. Three cases will be considered i.e. isothermic, adiabatic and reactors with cooling.

Isothermic Reactors

In the isothermic case the temperature T is constant and the reactor is described by (1.1).

$$\frac{dc}{dt} = \alpha(c_f - c) + A\, r(c) \tag{1.2}$$

Adiabatic Reactors

In the adiabatic case the enthalpy balance becomes

$$\frac{dh}{dt} = \alpha(h_f - h) + a\, r(c,T) \tag{1.3}$$

where h_f is the enthalpy of the feed, a is a row vector whose i:th component denotes the enthalpy per mole generated in the i:th reaction and r(c,T) is the reaction rate as before. Since T is a function of h we thus find that the reaction rate is given by

$$r = r_1(c,h) = r(c,T(h)) \tag{1.4}$$

Introducing the vector

$$x = \begin{bmatrix} c \\ \\ h \end{bmatrix} \tag{1.5}$$

and the matrix

$$\tilde{A} = \begin{bmatrix} A \\ \\ a \end{bmatrix} \tag{1.6}$$

the equation for an adiabatic reactor can thus be written as

$$\frac{dx}{dt} = \alpha(x_f - x) + \tilde{A}\, r(x) \tag{1.7}$$

which is identical in form to (1.4).

We thus find that (1.7) describes both the adiabatic and the isothermic cases.

The matrix A has m columns in both cases. Notice that the dimension k of the state vector of (1.7) equals n in the isothermic case and n+1 in the adiabatic case.

Reactors with cooling

A complete description of a reactor with cooling requires an enthalpy balance. The nice structure of the equations is then lost and it is difficult to make general statements as can be done for isothermic and adiabatic reactors.

2. BATCH REACTORS

First consider batch reactors i.e. $\alpha=0$. The equation (5) then reduces to

$$\frac{dx}{dt} = Ar(x) \tag{2.1}$$

Let V be the subspace of R^k that is spanned by the columns of A and U its orthogonal complement which is of dimension k-m. Any vector $x \in X$ can then be rewritten as

$$x = u + Av \tag{2.2}$$

where $v \in R^m$ and

$$u^T A = 0 \tag{2.3}$$

Introducing (2.2) into (1.5) gives

$$\frac{dx}{dt} = \frac{du}{dt} + A\frac{dv}{dt} = Ar(u+Av)$$

Projecting this equation on U and V gives

$$\frac{du}{dt} = 0 \tag{2.4}$$

$$\frac{dv}{dt} = r(u+Av) \tag{2.5}$$

We thus find that

$$u(t) = u_o = \text{constant} \tag{2.6}$$

which means that there are k-m invariants, (n-m in the isothermic case and n-m+1 in the adiabatic case) and that the analysis of the batch reactor can be reduced to the analysis of the equation

$$\frac{dv}{dt} = r(u_o + Av) \tag{2.7}$$

where $v \in R^m$.

Using the explicit form of the projection operator the reaction invariants can also be written as

$$\left[I - A(A^TA)^{-1} A^T \right] \left[x(t) - x(o) \right] = 0 \tag{2.8}$$

3. THE STIRRED TANK REACTOR

Now consider the general case i.e. $\alpha \neq 0$. Proceeding as before to partition the state space into U and V and introduce (2.2) into (1.5) we get

$$\frac{dx}{dt} = \frac{du}{dt} + A\frac{dv}{dt} = \alpha(u_f + Av_f - u - Av) + Ar(u + Av) \tag{3.1}$$

Projecting this equation on U and V respectively and we find

$$\frac{du}{dt} = \alpha(u_f - u) \tag{3.2}$$

$$\frac{dv}{dt} = \alpha(v_f - v) + r(u + Av) \tag{3.3}$$

The reactor is thus described by the equations (3.2) and (3.3). In this case there are no true invariants. Notice however that the equation (3.2) can be solved explicitely

$$u(t) = u_f + u_o \cdot e^{-\alpha t} \tag{3.4}$$

In this case there are no true invariants since

It follows from (3.4) that

$$\lim_{t \to \infty} u(t) = u_f \tag{3.5}$$

Since dim U = k-m we thus find that there are k-m asymptotic invariants. In analogy with (2.8) these asymptotic invariants can be expressed as

$$\lim_{t\to\infty} \left[I - A(A^TA)^{-1} A^T\right]\left[x(t) - x(o)\right] = 0 \qquad (3.6)$$

Introducing (3.5) into (3.3) we find

$$\frac{dv}{dt} = \alpha(v_f - v) + r(u_f + u_o \cdot \exp(-\alpha t) + Av) \qquad (3.7)$$

and we find that the reactor can be described by an equation of dimension m. Notice that (3.7) is not autonomous. However when t goes to infinity the equation (3.7) will converge to

$$\frac{dv}{dt} = \alpha(v_f - v) + r(u_f + Av) \qquad (3.8)$$

If $u(t) = u_f$ the space U is an uncontrollable subspace of (3.1) if the feed is considered as the control variable. This means that if $u(t) = u_f$, the reactor will be described by (3.8) even if the feed is changed.

Also notice that if the input composition x_f is changed in such a way that it remains in the subspace spanned by the columns of A, u(t) remains constant.

4. LINEARIZED ANALYSIS

Assuming small perturbations around a reference solution we find that the perturbations δx satisfies the equation

$$\frac{d}{dt}\delta x = -\alpha\delta x + (A\ B)\delta x = (-\alpha I + A\ B)\delta x \qquad (4.1)$$

where

$$B = r_x$$

and r_x denotes the matrix of partial derivatives of r evaluated of the reference solution. Similarly linearization of (3.6) around a reference solution with $u = u_f$ gives

$$\frac{d}{dt}\delta v = -\alpha\delta v + BA\delta v = (-\alpha I + BA)\delta v \qquad (4.2)$$

The character of the solutions of (4.1) and (4.2) in the neighbourhood of the reference solutions are thus given by the matrices AB and BA. Notice that A is an k x m matrix ($k \geq m$) and B is an m x k matrix.

The relation between the eigenvectors of the matrices AB and BA will now be explored.

Let e be an eigenvector of AB corresponding to the eigenvalue λ then

$$AB\ e = \lambda e \tag{4.3}$$

Multiplication of this equation by B from the left gives

$$BA(Be) = B\lambda e = \lambda(Be)$$

Hence if e belongs to the subspace spanned by the rows of B, Be is nonzero and we thus find that Be is an eigenvector of BA corresponding to the eigenvalue λ. If B is of rank m there are then m eigenvectors such that Be is not zero and we thus find that at least in the case of distinct eigenvalues all eigenvalues of BA are among those of AB and furthermore that the eigenvectors are simply related.

5. ACKNOWLEDGEMENT

I became aware of this problem when beeing opponent on Dr. Fjelds dissertation.

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