

**FUNDAMENTAL CONCEPTS AND METHODS
FOR SYSTEMS MODELING:
A Mathematical Foundation for the Description of
Physical, Chemical, and Biological Processes**

Outline of Lecture Unit 4

**INTRODUCTORY CONCEPTS AND APPLICATIONS FROM THE
STATE SPACE DESCRIPTION OF FINITE DIMENSIONAL PROCESS SYSTEMS**

prepared by

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1 INTRODUCTION

1.1 Motivation for Study

State space representation of process systems offers a unified methodology for analyzing and simplifying complex systems by taking into account topological, metric and spectral (modal) properties of linear vector spaces and linear (and other) operators defined on these spaces. As just a simple introduction we discuss briefly composition or stoichiometric state spaces.

2 ELEMENTARY STATE SPACE CONCEPTS: COMPOSITION AND REACTION SPACES

Note: This brief discussion is essentially nothing more but a “hint” for solving problems like 4.1 (in Homework problem Set # 3).

The state of a system of n_S chemical species A_1, A_2, \dots, A_{n_S} , that participate in n chemical reactions, n_R of which are independent reactions

$$\alpha_{1,j}A_1 + \alpha_{2,j}A_2 + \dots + \alpha_{n_S,j}A_{n_S}, \quad j = 1, 2, 3, \dots, n_R, \dots, n$$

can be represented by a vector \mathbf{a} in an n_S -dimensional linear vector space \mathcal{E}_S , the *composition space* or *species space*.

$$\mathbf{a} = [a_1, a_2, \dots, a_{n_S}]$$

where a_j is the number of moles of species A_j (an extensive state variable) or, under appropriate conditions an intensive state variable such as concentration or mole fraction.

In general one can write

$$\mathbf{a} = \mathbf{a}_0 + \mathbf{b}$$

where \mathbf{a}_0 is the initial composition vector and \mathbf{b} represents deviations in composition from \mathbf{a}_0 (or one can define \mathbf{a}_0 as the origin of a translated space).

The time evolution of the state of the system will correspond to a continuous path or trajectory confined in an n_R -dimensional subspace \mathcal{E}_R of \mathcal{E}_S , the *stoichiometric or reaction subspace*. The following relation holds:

$$n_S = n_R + n_L$$

where n_L is the dimension of \mathcal{E}_L , the orthogonal supplement of \mathcal{E}_R with respect to \mathcal{E}_S .

\mathcal{E}_R is spanned by the *reaction vectors* or *vectors of stoichiometric coefficients* (positive for products, negative for reactants), which include n_R linearly independent vectors.

$$\mathbf{f}_j = [\alpha_{1,j}, \alpha_{2,j}, \dots, \alpha_{n_S,j}], \quad j = 1, 2, \dots, n_R$$

\mathcal{E}_L is spanned by n_L linearly independent vectors

$$\mathbf{g}_j = [g_1, g_2, \dots, g_{n_S}], \quad j = 1, 2, \dots, n_L$$

In practice, as various experiments are performed information becomes available on values of the vector \mathbf{b} (for various \mathbf{a}_0). Then, the following important relations connects \mathbf{g}_j with \mathbf{f} and $\mathbf{b} = \mathbf{a} - \mathbf{a}_0$:

$$(\mathbf{g}_j \cdot \mathbf{b}) = 0, \quad (\mathbf{g}_j \cdot \mathbf{f}_j) = 0$$

expressing the fact that \mathbf{b} 's have to be stoichiometrically consistent.

These relations allow the determination of n_R as well as of acceptable reaction vectors (i.e. linear combinations of species) via standard matrix algebra methods (e.g. finding the rank of the matrix formed by either the \mathbf{f} or \mathbf{g} vectors).

3 BASIC TOOLS: THE SOLUTION OF LINEAR ODE SYSTEMS

A linear differential operator of arbitrary order can be set in matrix form, as a finite system of first order ordinary differential equations:

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x} = \mathbf{A}\mathbf{x}$$

This equation is governs a wide variety of linear “lumped parameter” or “finite-dimensional” models of process systems.

A most important theorem of mathematics states that:

(a) The differential equation

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x}$$

always has a nontrivial solution when

$$\det(\mathbf{A}) \neq 0$$

and

(b) The initial value problem

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x}, \mathbf{x}(t_0) = \mathbf{x}_0$$

has one and only one solution.

Furthermore, the set of solutions of

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x}$$

is a linear vector space.

Consider the case where \mathbf{A} is an $n \times n$ matrix. The vector function

$$\mathbf{x}(t) = \exp(\lambda t)\mathbf{v}$$

is a solution of

$$\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x}$$

if and only if λ is an eigenvalue of \mathbf{A} and \mathbf{v} is an eigenvector associated with λ . Indeed, $\mathbf{x}(t) = \exp(\lambda t)\mathbf{v}$ would be a solution of $\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x}$ if and only if $\lambda \exp(\lambda t)\mathbf{v} = \exp(\lambda t)\mathbf{A}\mathbf{v}$. Since $\exp(\lambda t)$ is never zero the result $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$ is obtained directly.

Each eigenvalue λ determines an infinite number of solutions of the form $\mathbf{x}(t) = \exp(\lambda t)\mathbf{v}$; the number of independent solutions depends on the number of independent eigenvectors associated with λ . If there are n independent eigenvectors $\{\mathbf{v}_i\}$ of \mathbf{A} , then

$$\mathbf{x}_1(t) = e^{\lambda_1 t}\mathbf{v}_1, \mathbf{x}_2(t) = e^{\lambda_2 t}\mathbf{v}_2, \dots, \mathbf{x}_n(t) = e^{\lambda_n t}\mathbf{v}_n$$

form a basis for the solution space of $\frac{d\mathbf{x}}{dt} = \mathbf{A}\mathbf{x}$ and therefore the general form of the solution is

$$\mathbf{x}(t) = c_1 e^{\lambda_1 t}\mathbf{v}_1 + c_2 e^{\lambda_2 t}\mathbf{v}_2 + \dots + c_n e^{\lambda_n t}\mathbf{v}_n$$

4 PROBLEMS FOR THE MATERIAL OF LECTURE UNIT 4

A problem set covering material of this lecture unit and lectures units 3 and 5 is given with this outline.