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

**Outline of Lecture Unit 0**

**- BASIC CONCEPTS -**

prepared by
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# 1 PHYSICO-CHEMICAL/BIOCHEMICAL SYSTEMS

## 1.1 Disciplines Defining Physico-chemical and Biochemical Systems Modeling

- Transport phenomena
- Reversible and irreversible thermodynamics
- Chemical kinetics and reactor theory

In the following the terms Physico-chemical/Biochemical Systems (or Subsystems) and Process Systems (Subsystems) will be used interchangeably. These include: Single-Medium and Multimedia Environmental and Microenvironmental Systems, Biological and Physiological Systems, Industrial Process Systems, etc.

# 2 THE MATHEMATICAL STUDY OF PROCESS SYSTEMS (MODELING)

## 2.1 Basic Classification of Mathematical Models for Process Systems

### 2.1.1 Phenomenological

These use "observations" to derive *input-output* relations; they are used for both deterministic and stochastic process systems
also called: data-driven models, black box models, statistical models

### 2.1.2 Mechanistic

These are based on fundamental physical and chemical principles - describe what happens *inside* the system as well as the *input-output* relations; they are used for both deterministic and stochastic process systems
also called: physicochemical models (and, depending on the application, transport phenomena models, etc.)
(misleading name for this class of models: "deterministic" models)

### 2.1.3 Hybrid Data-Mechanism models

These are the most common type in practice: observations are combined with fundamental principles to parameterize usable mathematical descriptions of process systems
*(in the following the use of the term mechanistic model will typically refer to a hybrid model)*

## 2.2 The Equations of Mechanistic Process Modeling

All equations relevant to process systems are either *balance laws* or *constitutive relations.* Any usable (i.e. "closed") equation (e.g. Navier Stokes for fluid flow, heat conduction equation, etc.) contains both.
These equations apply to variables that are:

- extensive or intensive
- through or across

## 2.3 The Steps of Mechanistic Mathematical Modeling

1. Specify purpose and objectives of the mathematical description.
2. Identify geometrical attributes of the system under consideration (extent, boundaries).
3. Identify temporal attributes of the system under consideration (stationarity of phenomena, transients, time lags, frequencies, etc.).
4. Develop a conceptual structure (model) that is as simple as possible but still "mimics" observed or desired effects.
5. Identify subsystems ("elements") of the conceptual model.
6. Specify variables of interest for each subsystem.
7. Identify boundary and initial conditions for these variables (for each subsystem and the entire system).
8. Identify/develop physicochemical constitutive (material) relations for the variables in each subsystem.
9. Apply physical laws of conservation, continuity and compatibility (typically derived through Reynolds' Transport Theorem) to subsystems to develop (in conjunction with the constitutive relations and the initial and boundary conditions) a closed system of equations (algebraic, differential, integral, ...).
10. Use scaling to further simplify the equations if possible.
11. Implement transformations to bring the equations into "manageable" form.
12. Examine the possibilities of existence of exact analytical solutions (possibly under constraining conditions - i.e. exact solutions of an approximate problem), and of approximate analytical solutions. Then establish the need for a numerical solution. (Symbolic computation methods - such as those offered by Mathematica, Macsyma, Maple - could also be considered in this step.)
13. Select the appropriate numerical methods for computational solution; select or develop the appropriate computational algorithms.
14. Implement the computational algorithms into code (traditional code, i.e. Fortran, C, etc.; object oriented code, i.e. Objective Fortran or C, C++; higher level language, e.g. ACSL, CSMP, etc.; integrated mathematical package, e.g. Mathematica, MatLab, etc.) and perform simulations.
15. Codify (visually, statistically, etc.) the simulation results into usable forms.
16. Analyze results and compare them with the real world using a formal statistical performance evaluation of the model.
17. Analyze sensitivity and robustness of the model.
18. Evaluate uncertainties in the model, the input data and the performance evaluation data.
19. Modify/refine model as necessary and repeat the above steps.

# 3 CLASSIFICATIONS OF MECHANISTIC MATHEMATICAL MODELS FOR PROCESS SYSTEMS

## 3.1 Classification According to the Dynamics of the Process System that are Incorporated in the Model

### 3.1.1 Deterministic or Stochastic (or Chaotic)

### 3.1.2 Linear or Nonlinear (or Quasilinear)

### 3.1.3 Steady State or Nonsteady State (or Mixed/Multiscale)

### 3.1.4 Lumped Parameter or Distributed Parameter (or Mixed)

### 3.1.5 Continuous Time or Discrete Time

### 3.1.6 Homogeneous or Nonhomogeneous

### 3.1.7 Local or Nonlocal

### 3.1.8 Constant Coefficient or Nonconstant Coefficient

The mathematical description of a process system will be characterized as a combination of the above attributes.

## 3.2 Classification According to the Level of Internal Physical Detail Incoprporated in the Mathematical Description

*Note:This classification follows and modifies/extends the classical Himmelblau-Bischoff approach.*

### 3.2.1 Macroscopic

*Extent of Use by Chemical/Biochemical and Environmental Engineers and Scientists:* Very widely used.
*Topical Designations:* Process engineering, unit operations, classical kinetics and thermodynamics.
*Typical Parameters for Analysis:* Interphase transport coefficients; macroscopic kinetic constants; friction factors.
*Typical Form of Governing Equations:* Algebraic equations; ordinary differential and difference equations.

### 3.2.2 Maximum Gradient

*Extent of Use by Chemical/Biochemical and Environmental Engineers and Scientists:* Used for various continuous "plug" flow systems.
*Topical Designations:* Laminar and turbulent transport phenomena; reactor design.
*Typical Parameters for Analysis:* Interphase transport coefficients; macroscopic kinetic constants.
*Typical Form of Governing Equations:* Deterministic ordinary differential and difference equations.

### 3.2.3 Multiple Gradient

*Extent of Use by Chemical/Biochemical and Environmental Engineers and Scientists:* Applicable to special cases; gaining more widespread acceptance with availability of computational resources.
*Topical Designations:* Laminar and turbulent transport and reaction phenomena; transport in porous media.

*Typical Parameters for Analysis:* "Effective" or "apparent" transport coefficients.
*Typical Form of Governing Equations:* Deterministic partial differential and integrodifferential equations.

#### 3.2.4 Population Distribution

*Extent of Use by Chemical/Biochemical and Environmental Engineers and Scientists:* Applicable to special cases.
*Topical Designations:* Discrete entities treated via simplified statistical mechanics; reaction phenomena in nonideal mixing conditions; disperse multiphase phenomena; reactor design.
*Typical Parameters for Analysis:* Population distribution functions.
*Typical Form of Governing Equations:* Deterministic ordinary and partial differential or integrodifferential equations.

#### 3.2.5 Microscopic or Macroparticle (Stochastic)

*Extent of Use by Chemical/Biochemical and Environmental Engineers and Scientists:* Applicable to special cases; gaining more widespread acceptance with availability of computational resources.
*Topical Designations:* Discrete entities treated by kinetic theory and statistical mechanics; laminar and turbulent transport and reaction phenomena; transport in porous media.
*Typical Parameters for Analysis:* Distribution functions; correlations.
*Typical Form of Governing Equations:* Stochastic ordinary differential and integrodifferential equations; deterministic partial differential and integrodifferential equations.

#### 3.2.6 Molecular and Atomic (Stochastic)

*Extent of Use by Chemical/Biochemical and Environmental Engineers and Scientists:* Fundamental background research.
*Topical Designations:* Discrete entities treated by kinetic theory, statistical mechanics and thermodynamics, and quantum mechanics.
*Typical Parameters for Analysis:* Distribution functions; collision integrals.
*Typical Form of Governing Equations:* Integrodifferential and partial integrodifferential equations (stochastic and deterministic).

## 4 MATHEMATICAL TOOLS FOR THE MECHANISTIC STUDY OF PROCESS SYSTEMS

### 4.1 Exact Analytical Methods

- Linear Algebra and Finite-Dimensional Linear Space Methods
  *(Equilibrium and diffusive phenomena; monomolecular reaction systems.)*
  - Implementation of numerical methods
  - Analysis of stoichiometric systems
  - Solution of discretized transport problems at equilibrium
  - Data analysis methods
  - Reaction network simplifications
  - Reaction network dynamics/path analysis

- Infinite-Dimensional Linear Space Methods
  *(Equilibrium and diffusive phenomena; monomolecular reaction systems.)*
  - Ordinary differential equations
  - Partial differential equations
  - Integral equations
  - Integrodifferential equations
  - Other functional equations (e.g. delay-difference equations)
- Nonlinear Methods
  *(Advective phenomena; multimolecular reaction kinetics.)*
  - Special types of ordinary and partial differential equations
  - Stability properties, limit cycles, qualitative theory of NL-ODES
  - Chaotic dynamics
- Stochastic Methods (linear and nonlinear)
  *(Turbulent transport, mixing and reaction; transport in porous media.)*
  - Ordinary stochastic differential equations (Langevin)
  - deterministic partial differential equations (Fokker-Planck)
  - Integrodifferential equations
  - Other functional equations

## 4.2 Approximate Analytical Methods

- Series expansions
- Boundary layer methods
- Perturbation methods
- Variational methods

## 4.3 Numerical Methods

- Ordinary differential equations
  - Simple systems methods
  - Stiff systems methods
- Partial differential equations
  - Finite difference methods
  - Finite element methods
- Integral equations