Modelling & Simulation of Chemical Engineering Systems

٥٠١ هعم : تمثيل الأنظمة الهندسية على الحاسب الآلى

Department of Chemical Engineering
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Course Information

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- Lectures: Monday, 6-9 pm, Unit operation lab PC room

Course Objectives

To enable you to:

1. model steady and dynamic behaviour of chemical engineering systems
2. understand the underlying mathematical problems, and some awareness of the available analytical and numerical solution techniques.

Course Structure

- I. Mathematical Models in Chemical Engineering (3 weeks)
  - Fundamentals, Classification,Building a model, Fundamental laws, Model solution and validation, Examples of Chemical processes
- II. Initial Value Ordinary differential Equations (3 weeks)
  - Linear Initial value ODE’s
  - Nonlinear Initial value ODE’s

Course structure

- III. Boundary value ordinary differential equations (5 weeks)

  Fundamentals, Shooting method, Finite difference method, Collocation method, Applications

- IV. Partial differential equations (4 weeks)
  - Fundamentals, Classification,
  - Finite difference method for elliptic and parabolic problems

Course Marks

The course marks will be allocated as follows:

- Weekly Assignments (30%)
- Midterm Exams (30%)
- Final Exam (40%)

Course References

1. Alkis Constantinides & Navid Mostoufi "Numerical Methods for Chemical Engineers with MATLAB Applications", Prentice Hall, 1999.
2. Stanley Walas, "Modeling Differential Equations in Chemical Engineering", Butterworth-Heinemann, 1991.
3. Steven Chapra & Raymond Canale, " Numerical Methods for Engineers", 4^{th} edition, McGraw Hill, 2002.
4. S. Pushpavanam, "Mathematical Methods in Chemical Engineering", Prentice Hall, 1998.

LECTURE #1

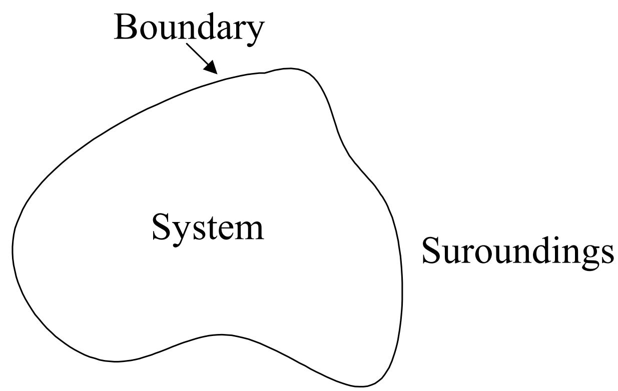
What does "Model" mean?

- Representation of a physical system by mathematical equations
  - (**<u>Models at their best are no more than approximation of the real process)</u>**
  - Equations are based on fundamental laws of physics (conservation principle, transport phenomena, thermodynamics and chemical reaction kinetics).

What does “Simulation” mean?

- Solving the model equations analytically or numerically.
  - **Modeling & Simulation are valuable tools: safer and cheaper to perform tests on the model using computer simulations rather than carrying repetitive experimentations and observations on the real system**.

System



Classification based on thermodynamic principles

- Isolated system.
- Closed system.
- Open system.

Classification based on number of phases

- Homogeneous system.
- Heterogeneous system.

Models

Theoretical

based on fundamental principles

Empirical

based on experimental plant data.

Semi-empirical

Steady state VS. dynamic
Lumped VS. distributed parameters
Linear Vs Non-linear
Continuous VS discrete
Deterministic VS probabilistic models

What does “Steady state and Dynamic” means?

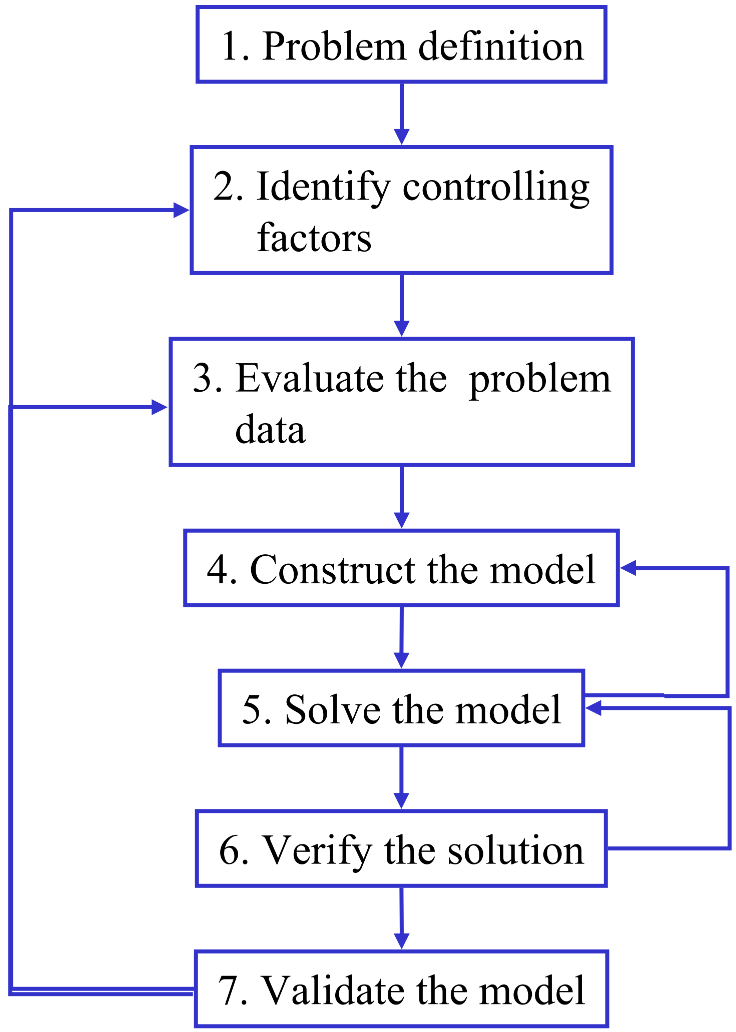
- In all processes of interest, the operating conditions (*e.g.*, temperature, pressure, composition) inside a process unit will be varying over time.
- Steady-state: process variables will not be varying with time

Why Dynamic Behaviour?

A subject of great importance for the:

1. Study of operability and controllability of continuous processes subject to small disturbances
2. Development of start-up and shut-down procedures
3. Study of switching continuous processes from one steady-state to another
4. Analysis of the safety of processes subject to large disturbances
5. Study of the design and operation procedures for intrinsically dynamic processes (batch/periodic/separation)

Systematic Model Building



(inputs, outputs, etc.)

(chemical reaction, diffusion, fluid flows, etc.)

(compare with experiments)

Ingredients of Process Models

1. Assumptions
   - Time, spatial characteristics
   - Flow conditions

2. Model equations and characterising variables
   - Mass, energy, momentum

3. Initial conditions
4. Boundary conditions
5. Parameters

Process Classification: Batch *vs*. Continuous

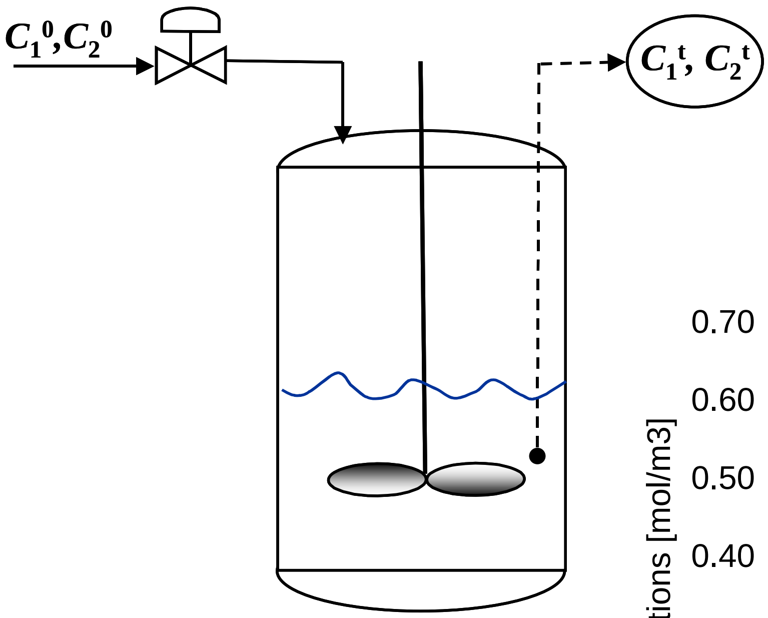
Batch:

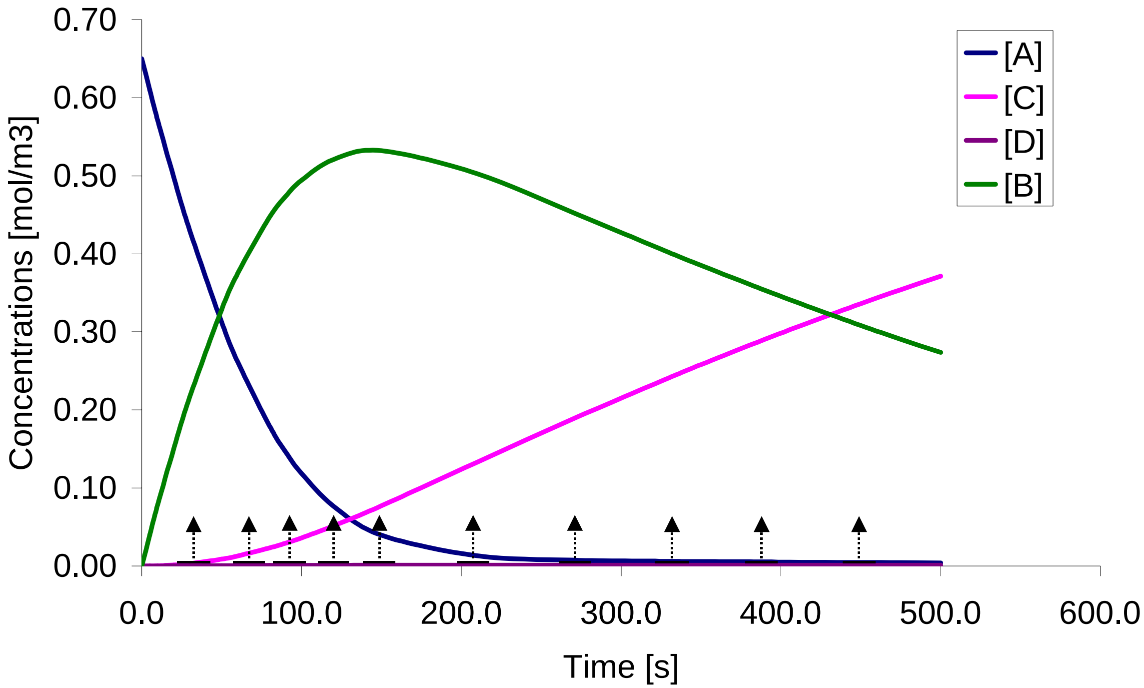
- feedstocks for each processing step (*i.e.*, reaction, distillation) are charged into the equipment at the start of processing; products are removed at the end of processing

- transfer of material from one item of equipment to the next occurs discontinuously – often via intermediate storage tanks

- batch processes are intrinsically dynamic – conditions within the equipment vary over the duration of the batch

Batch Example: Kinetics





Variations on Batch Operation

Semi-batch (fed-batch):

- One or more feedstocks to a batch unit operation to be added during the batch

Semi-continuous:

- Some products are removed during the batch

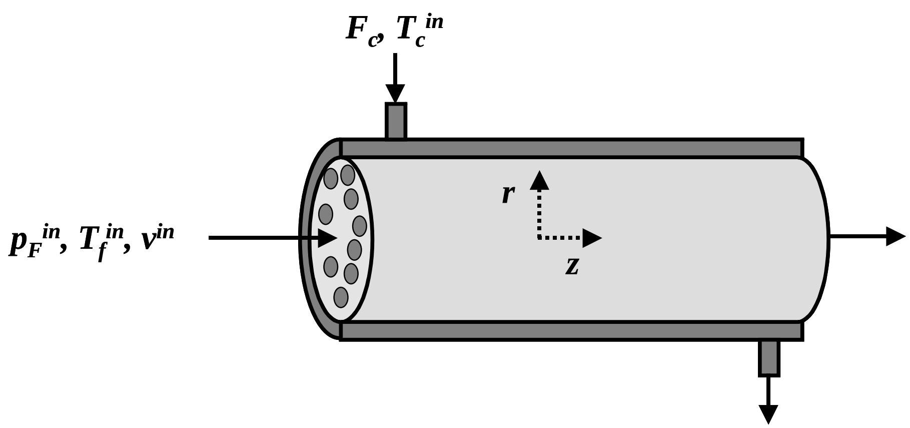
Process Classification: Batch *vs.* Continuous

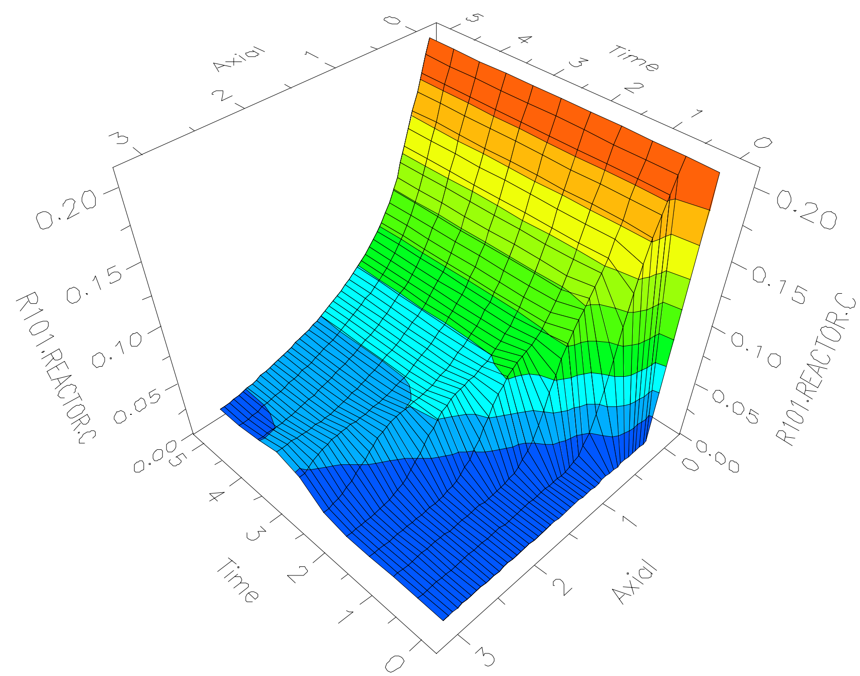
Continuous:

- Involve continuous flows of material from one processing unit to the next

- Usually designed to operate at steady-state; due to external disturbances, even continuous processes operate dynamically

Continuous Example: PFR





Variations on Continuous Operation

Periodic:

- Continuous processes subjected to a periodic (e.g., sinusoidal or square wave) variation of one or more of the material/energy input streams

Industrially Important Examples

- Periodic adsorption – periodic conditions (pressure/temperature) regulates preferential adsorption and desorption of different species over different parts of the cycle
- Periodic catalytic reaction – involves variation of feed composition; under certain conditions the average performance of the reactor is improved

Lumped *vs*. Distributed

Lumped Operations:

(Almost) perfect mixing – at any particular time instant, the values of operating conditions are (approximately) the same at all points within the unit

Distributed Operations:

Imperfect mixing will result in different operating conditions at different points even at the same time $\rightarrow$ existence of distributions of conditions over spatial domains

Lumped *vs.* Distributed:
Mathematical Considerations

Lumped Operations:

- Characterised by a single independent variable (time)
- Their modelling can be effected in terms of ordinary differential equations (ODEs)

Distributed Operations:

- Introduce additional independent variables (e.g., one or more spatial co-ordinates, particle size, molecular weight, etc.)
- Involves partial differential equations (PDEs) in time

Lumped *vs*. Distributed:
How do I decide?

Deciding on whether to model a system as lumped or distributed operations is a matter of judgement for the modeller.

Must Consider:

- Objectives of the model being constructed (control, optimisation, operating procedures)
- Required predictive accuracy
- Information available for model validation

Conservation Laws

Mathematical Modelling:

– Encoding physical behaviour as a set of mathematical relations

– Involves application of fundamental physical laws

– Consider a subset of the universe as a system of interest – the position of the boundary separating the system and its surroundings may vary with time

Conservation Laws:
General Form

Conservation laws describe the variation of the amount of a "conserved quantity" within the system over time:

$$\begin{pmatrix} \text{rate of} \\ \text{accumulation} \\ \text{of conserved} \\ \text{quantity} \\ \text{within system} \end{pmatrix} = \begin{pmatrix} \text{rate of} \\ \text{flow of} \\ \text{conserved} \\ \text{quantity} \\ \text{into system} \end{pmatrix} - \begin{pmatrix} \text{rate of} \\ \text{flow of} \\ \text{conserved} \\ \text{quantity} \\ \text{from system} \end{pmatrix} + \begin{pmatrix} \text{rate of} \\ \text{generation of} \\ \text{conserved} \\ \text{quantity} \\ \text{within system} \end{pmatrix} \quad (1.1)$$

Conserved Quantities

Typical conserved quantities:

- Total mass (kg)
- Mass of an individual species (kg)
- Number of molecules/atoms (mol)
- Energy (J)
- Momentum (kg.m/s)

Conservation Laws: Comments

- Conservation laws provide a simple and systematic "balance"
- With a generation term, conservation laws may be written for any physical quantity
- The usefulness of a particular law depends on whether or not we possess the necessary physical knowledge to quantify each term
- Often, the rate of generation of one quantity is related to the rate of generation (or consumption) of another – this may affect the quantities to which we can apply a conservation law
  - *e.g.*, $A \longrightarrow B$

$$\begin{pmatrix} \text{rate of} \\ \text{generation} \\ \text{of B} \end{pmatrix} = \begin{pmatrix} \text{rate of} \\ \text{consumption} \\ \text{of A} \end{pmatrix}$$

  - If we cannot characterise the either rate, a conservation law will not prove to be useful
  - A conservation law on (A+B) will since it does not involve a generation term

Distributed Systems:Microscopic balance

- **The balance equation is written over a differential element within the system to account for the variation of the state variables from point to point in the system, besides its variation with time**.

- **Each state variable *V* of the system is assumed to depend on the three coordinates *x*,*y* and *z* plus the time**. i.e. $V = V(x,y,z,t)$.

- **The selection of the appropriate coordinates depends on the geometry of the system under study. It is possible to convert from one coordinate system to an other.**

Perfect Mixing Assumption

All intensive properties of the stream(s) leaving a perfectly mixed system are identical to those inside the system.

Macroscopic balance

For lumped parameter systems the process state variables are uniform over the entire system, that is each state variable V do not depend on the spatial variables, i.e. x,y and z in cartesian coordinates but only on time t.

In this case the balance equation is written over the whole system using macroscopic modeling.

Accumulation Terms in Conservation Laws

Extensive variables: mass, volume

Intensive variables: mass fraction, temperature, pressure, specific volume

Accumulation terms should be formulated in terms of a single extensive variable, with use of additional algebraic relations used to express relationships between the extensive variables used and the intensive properties

Model Completeness

A dynamic model of a process will be deemed complete if, given the time variation of all extensive/intensive properties associated with the process inlets, it can determine unique time trajectories for all other variables in the model.

Conservation Laws:
Energy

Accumulation: takes account of all forms of energy

Internal energy	random movement of molecules/atoms of fluid; intermolecular/interatomic forces
Kinetic energy	bulk motion of the liquid (e.g., agitation)
Potential energy	by virtue of its position in a gravitational force field

Inlet/Outlet: make contributions proportional to their flowrate

Specific enthalpy (rather than internal energy) is used – the difference between them accounts for the energy (work) required to force an element of fluid in the inlet stream into the fluid in the system.

Conservation Laws:
Energy

Interaction with Surroundings: account for mechanical work

(i) Mechanical agitation device

rate of energy addition ≈ power output of device

(ii) Work done on the system by the atmosphere (open systems)

$$-P_{atm}\frac{dV}{dt} = \text{work imparted to system}$$

+ve if level moves downwards (atmosphere carries out work on the system)

-ve if level moves upwards (system is pushing back the atmosphere)

Assumptions in Modelling

Assumptions should be introduced only when <u>not introducing</u> them results in:

1. Substantial increase in computational complexity (*i.e.*, perfect mixing $\rightarrow$ CFD)
2. Need to characterise phenomena which are not well understood and/or cannot easily be quantified

Next Lecture

- Elements of conservations laws:
  - Transport rates:bulk and diffusion flow;
  - Thermodynamic relations;
  - Phase equilibria
  - Chemical kinetics
  - Control laws

- Degree of freedom
- Modeling of lumped parameter chemical systems