Chapter 1

INTRODUCTION

1.1 Terminology

Process An actual series of operations or treatments of materials or physical, chemical, biological phenomena involved in these operations or treatments

- large scale: chemical plant $\mathcal{O}(10-100)$ m
- medium scale: unit operation, distillation column, chemical reactor, CVD reactor $\mathcal{O}(1)$ m
- small scale: drop formation, combustion of coal particles, reaction on the catalyst surface $\mathcal{O}(1)$ mm
- micro scale: deposition of metal on the wafer, diffusion through porous catalyst $\mathcal{O}(1)$ m
- nano scale: nano crystal formation, molecular reaction $\mathcal{O}(1)$ Å- nm

Model Mathematical description of the real process

Simulation Substitution of real process

- Numerical simulation
- Experimental simulation

1.2 Model

- Deterministic model: eg. Transport phenomena model
- Stochastic model: eg. Population balance model
- Empirical model: eg. Use of polynomial to fit empirical data

1.3 Process analysis step

See Fig.1-1

1.4 Goal of modelling and simulation

- Understanding $\longrightarrow$ insight
- Solution $\longrightarrow$ numbers

1.5 Mathematical model

1. Mathematically well-posed
    (a) Existence
    (b) Continuity
2. Discretization
    (a) time: $t \rightarrow \Delta t$
    (b) space: $x, y, z \rightarrow \Delta x, \Delta y, \Delta z$
        - finite difference method
            - finite volume method
        - finite element method
            - spectral method

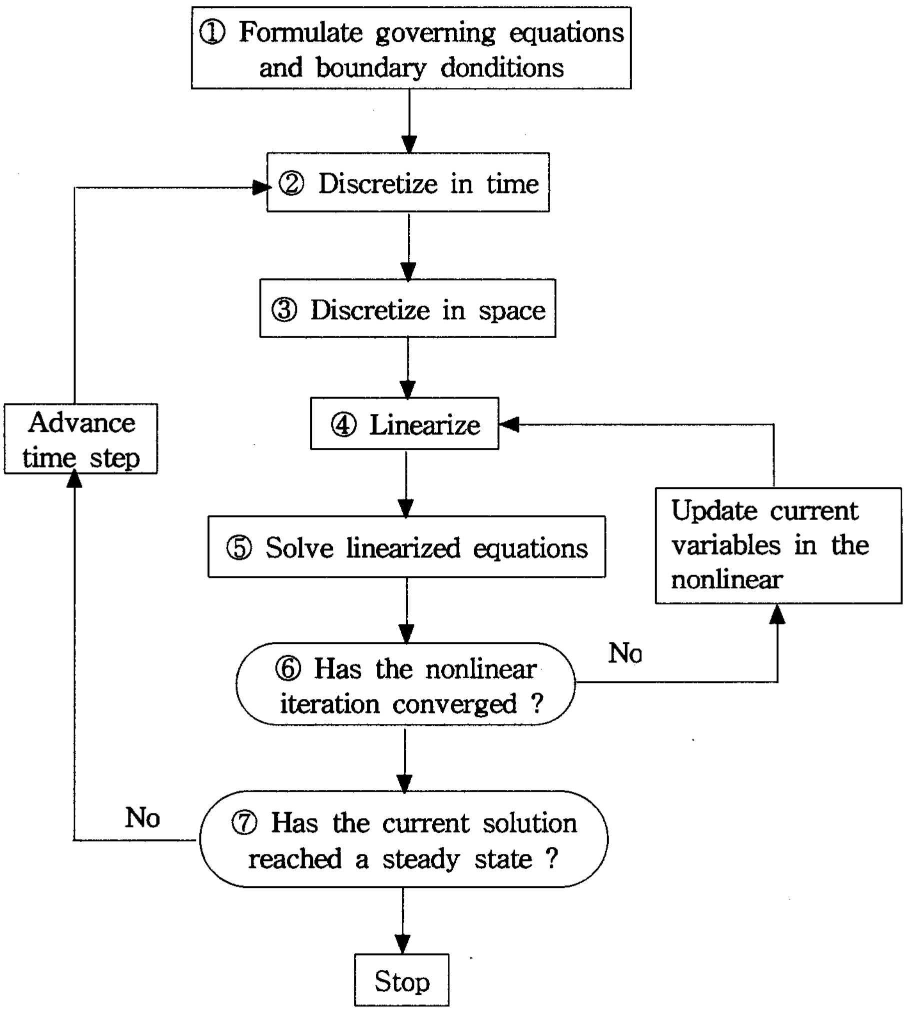

Figure 1.1: Process analysis step.

$$
\begin{array}{ccl}
\text{PDE} & \xrightarrow{\text{discretize}} & \frac{d\boldsymbol{u}}{dt} = \boldsymbol{R}(\boldsymbol{u}) \\
(t, x, y, z) & & \quad\text{(ODE)} \\
 & \xrightarrow{\text{time integration}} & \text{Nonlinear algebraic equation} \\
 & \xrightarrow{\text{linearize}} & \text{Linear algebraic equation} \\
 & \longrightarrow & \text{solution}
\end{array}
$$

3. Is the numerical solution right?

   - function approximation
   - convergence of discrete set (As $\Delta x \to 0, \varepsilon \to 0$))
   - stability theorem

1.6 Lax equivalence theorem

Lax equivalence theorem: Given a properly posed initial boundary balue problem and a finite difference approximation to it that satisfies consistency condition, then stability is the necessary and sufficient condition for convergence.

- Consistency
  Finite difference equation is said to be consistent (compatible) with the differential equation if the local truncation errors tend to zero as $\Delta t, \Delta x \to 0$.

- Stability

$$|\varepsilon^n| < K(n\Delta t) \quad (n\Delta t \ \text{ fixed}, n \to \infty, \Delta t \to 0)$$

- Convergence

$$\|\theta^n - \Theta^n\| \to 0 \quad (n\Delta t \ \text{ fixed}, n \to \infty, \Delta t \to 0)$$

Chapter 2

BASICS OF LINEAR ALGEBRA

2.1 Matrices and Determinants

2.1.1 Matrix

Matrix: Array of elements arranged in rows and columns

$$\underline{\underline{A}} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}$$

$m \times n$ matrix, $\underline{\underline{A}} \in \Re^{m\times n}$

where

$\{a_{ij}\}, i = 1, \ldots, m$ and $j = 1, \ldots, n$: set of elements of $\underline{\underline{A}}$

Column vector: $m \times 1$ matrix

$$\underline{a}_1 = \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{m1} \end{bmatrix}$$

2.1.2 Diagonal matrix

Diagonal matrix: $a_{ij} = 0$ for $i \neq j$.

$$a_{ij} = a_j \delta_{ij}, \quad \text{where } \delta_{ij} = \left(\begin{array}{ll} 0 & i \neq j \\ 1 & i = j \end{array} \right.$$

2.1.3 Triangular matrices

Upper triangular matrix $\underline{\underline{U}} = \begin{bmatrix} 1 & 2 & 3 \\ 0 & 3 & 4 \\ 0 & 0 & 2 \end{bmatrix}$

Lower triangular matrix $\underline{\underline{L}} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 3 & 0 \\ 1 & 4 & 2 \end{bmatrix}$

2.1.4 Transpose

Transpose: $\underline{\underline{A}}^T$ (elements: a_{ij}^T)

$$a_{ij}^T = a_{ji}$$

$\underline{a}^T$: row vector (transpose of column vector)

2.1.5 Symmetric matrix

For symmetric matrix,

$$\begin{aligned} \underline{\underline{A}} &= \underline{\underline{A}}^T \\ a_{ij} &= a_{ji} \end{aligned}$$

2.1.6 Partitioned matrix

$$\underline{\underline{A}} = \begin{bmatrix} \underline{\underline{A}}_{11} & \underline{\underline{A}}_{12} & \cdots & \underline{\underline{A}}_{1l} \\ \underline{\underline{A}}_{21} & \underline{\underline{A}}_{22} & \cdots & \underline{\underline{A}}_{2l} \\ \vdots & \vdots & \ddots & \vdots \\ \underline{\underline{A}}_{k1} & \underline{\underline{A}}_{k2} & \cdots & \underline{\underline{A}}_{kl} \end{bmatrix}$$

where each $\underline{\underline{A}}_{ij}$ is a $m_i \times n_j$ matrix.

Partitioning with column vector

$$\underline{\underline{A}} = [\underline{a}_1, \underline{a}_2, \ldots, \underline{a}_n]$$

For $\underline{\underline{A}}\,\underline{x} = \underline{b}$,

$$\begin{aligned} \underline{\underline{A}}\,\underline{x} &= [\underline{a}_1, \underline{a}_2, \ldots, \underline{a}_n] \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \\ &= x_1\underline{a}_1 + x_2\underline{a}_2 + \cdots + x_n\underline{a}_n \\ &= \underline{b} \end{aligned}$$

This says that $\underline{\underline{A}}\,\underline{x}$ is a linear combination of the columns of $\underline{\underline{A}}$.

2.1.7 Rank

Rank of $\underline{\underline{A}} \in \Re^{m \times n}$

If all matrices formed from $\underline{\underline{A}}$ of greater than order r have determinants equal to zero, but at least one matrix of order r has non-zero determinant,
then $\text{rank}(\underline{\underline{A}}) = r$.

Ex) For the matrix

$$\underline{\underline{A}} = \begin{bmatrix} 2 & 1 & 3 & 4 \\ -1 & 1 & -2 & -1 \\ 0 & 3 & -1 & 2 \end{bmatrix}$$

det of all 3×3 matrices $= 0 \longrightarrow \text{rank}(\underline{\underline{A}}) = 2$.

- For a square matrix $\underline{\underline{A}}$ of order n,
  If $\text{rank}(\underline{\underline{A}}) < n$, then $\det(\underline{\underline{A}}) = 0$. That is, $\underline{\underline{A}}$ is singular.

2.1.8 Conforming matrices

If $\underline{\underline{A}} \in \Re^{n\times m}, \underline{\underline{B}} \in \Re^{p\times q}$, then the two matrices are conformable if $m = p$. Multiplication of two conforming matrices is defined as $\underline{\underline{A}}\,\underline{\underline{B}} = \underline{\underline{C}}$, where

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$$

- If $\underline{\underline{B}}$ is non-singular and $\underline{\underline{A}}$ and $\underline{\underline{B}}$ are conformable, then

$$\text{rank}(\underline{\underline{B}} \cdot \underline{\underline{A}}) = \text{rank}(\underline{\underline{A}})$$

2.1.9 Identity matrix operation

1. $\underline{\underline{I}}_{ij}$ is the identity matrix (or idemfactor) with rows i and j interchanged.

   - Example

$$\underline{\underline{I}}_{23} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \longrightarrow \det(\underline{\underline{I}}_{23}) = -1$$

- $\det(\underline{\underline{I}}_{ij}) = -1$
- $\underline{\underline{I}}_{ij}\underline{\underline{A}}$: change ith row and jth row of $\underline{\underline{A}}$.

2. $\underline{\underline{J}}_{ij}(k)$: $\underline{\underline{I}}$ with k in (i, j) position

   - Example

   $$\underline{\underline{J}}_{23}(k) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & k \\ 0 & 0 & 1 \end{bmatrix}$$

   - $\det(\underline{\underline{J}}_{ij}(k)) = 1$ except when $k = 0$ and $i = j$.
   -

   $$\begin{aligned} \underline{\underline{J}}_{23}(k) \cdot \underline{\underline{A}} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & k \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \\ &= \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} + ka_{31} & a_{22} + ka_{32} & a_{23} + ka_{33} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \end{aligned}$$

   multiplies third row of $\underline{\underline{A}}$ by k and adds it to the second row.

2.1.10 Determinant

- Determinant of square $(n \times n)$ matrix

$$\begin{aligned} \det(\underline{\underline{A}}) &= \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{vmatrix} \\ &= \sum (-1)^h \underbrace{(a_{1l_1} a_{2l_2} \cdots a_{nl_n})}_{\substack{n \text{ elements} \\ \text{from each row}}} \end{aligned}$$

- For the matrix

$$\underline{\underline{A}} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$

determinant is

$$\det(\underline{\underline{A}}) = (-1)^0 a_{11}a_{22} + (-1)^1 a_{12}a_{21}$$

2.1.11 Laplace's expansion

$$\det \underline{\underline{A}} = \sum_{j=1}^{n} a_{ij}\mathrm{cof}(a_{ij}) \text{ for } i = 1, 2, \ldots, n$$

or

$$\det \underline{\underline{A}} = \sum_{i=1}^{n} a_{ij}\mathrm{cof}(a_{ij}) \text{ for } j = 1, 2, \ldots, n$$

- compliment of a_{ij}
  - determinant formed by striking out i-th row and j-th column of an $n \times n$ matrix
  - determinant of $(n-1)$ order
  - Example. For the matrix

$$\underline{\underline{A}} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}$$

compliment of a_{22} is

$$\mathrm{comp}(a_{22}) = \begin{vmatrix} a_{11} & a_{13} & a_{14} \\ a_{31} & a_{33} & a_{34} \\ a_{41} & a_{43} & a_{44} \end{vmatrix}$$

- Minor of $\underline{\underline{A}}$ is formed by striking out rows and/or columns of $\underline{\underline{A}}$.
- cofactor of a_{ij}

$$\mathrm{cof}(a_{ij}) = (-1)^{i+j}\mathrm{comp}(a_{ij})$$

2.1.12 Properties of determinant

1. $\det(\underline{\underline{A}}) = \det(\underline{\underline{A}}^T)$
2. If all the elements of any row or column of $\underline{\underline{A}}$ are zero, $\det(\underline{\underline{A}}) = 0$.
3. If the elements of one row or one column of a matrix are multiplied by a constant c, then the determinant is multiplied by c.

   $$\det(c\underline{\underline{A}}) = c^n \det(\underline{\underline{A}})$$

4. The sign of determinant is changed if two columns or rows have their positions interchanged.
5. If $\underline{\underline{A}}$ and $\underline{\underline{B}}$ differ only in their kth columns, then

   $$\det(\underline{\underline{A}}) + \det(\underline{\underline{B}}) = \det(\underline{\underline{C}})$$

   where $\underline{\underline{C}}$ is $\underline{\underline{A}}$ with kth column replaced by sum of kth column of $\underline{\underline{A}}$ and $\underline{\underline{B}}$.

   $$\begin{aligned}\det(\underline{a}_1, \underline{a}_2, \ldots, \underline{a}_k, \ldots, \underline{a}_n) &+ \det(\underline{a}_1, \underline{a}_2, \ldots, \underline{b}_k, \ldots, \underline{a}_n) \\ &= \det(\underline{a}_1, \underline{a}_2, \ldots, \underline{a}_k + \underline{b}_k, \ldots, \underline{a}_n)\end{aligned}$$

6. If $\underline{\underline{A}}$ has two identical rows or columns, $\det(\underline{\underline{A}}) = 0$.
   - If any row (or column) of a matrix is a multiple of any other row (or column), then its determinant is zero.
7. The value of a determinant is unchanged if a multiple of one row (or column) is added to another row (or column).

   $$\det\begin{bmatrix} a_{11} & \cdots & a_{1j} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nj} & \cdots & a_{nn}\end{bmatrix} = \det\begin{bmatrix} a_{11} & \cdots & a_{1j} + ca_{1q} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nj} + ca_{nq} & \cdots & a_{nn}\end{bmatrix}$$

8. $\det \underline{\underline{A}}\,\underline{\underline{B}} = \det \underline{\underline{A}} \det \underline{\underline{B}}$

2.1.13 Inverse of $\underline{\underline{A}}$

$$\underline{\underline{A}}^{-1}\underline{\underline{A}} = \underline{\underline{I}}$$

- Cofactor matrix $\underline{\underline{C}}$.

$$\underline{\underline{C}} = \begin{bmatrix} \mathrm{cof}(a_{11}) & \mathrm{cof}(a_{12}) & \cdots & \mathrm{cof}(a_{1n}) \\ \mathrm{cof}(a_{21}) & \mathrm{cof}(a_{22}) & \cdots & \mathrm{cof}(a_{2n}) \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{cof}(a_{n1}) & \mathrm{cof}(a_{n2}) & \cdots & \mathrm{cof}(a_{nn}) \end{bmatrix}$$

- Adjoint matrix of $\underline{\underline{A}}$.

$$\mathrm{adj}(\underline{\underline{A}}) \equiv \underline{\underline{C}}^T$$

We multiply $\underline{\underline{A}}$ and $\mathrm{adj}(\underline{\underline{A}})$,

$$\underline{\underline{A}}\,\mathrm{adj}(\underline{\underline{A}}) = \underline{\underline{B}}$$

where

$$b_{ij} = \sum_{k=1}^{n} a_{ik}\mathrm{cof}(a_{jk})$$

Elements b_{ii} (diagonal)

$$b_{ii} = \sum_{k=1}^{n} a_{ik}\mathrm{cof}(a_{ik}) = \det(\underline{\underline{A}})$$

Elements b_{ij} $(i \neq j)$ (off-diagonal)

Laplace's expansion of matrix
j-th row replaced by i-th row

⇓

i-th row appears twice

⇓

0

This leads to

$$\underline{\underline{A}}\,\mathrm{adj}(\underline{\underline{A}}) = \det(\underline{\underline{A}})\,\underline{\underline{I}}$$

By dividing both sides by $\det(\underline{\underline{A}})$ (for $\det(\underline{\underline{A}}) \neq 0$),

$$\frac{\underline{\underline{A}}\,\mathrm{adj}(\underline{\underline{A}})}{\det(\underline{\underline{A}})} = \underline{\underline{I}}$$

From $\underline{\underline{AA}}^{-1} = \underline{\underline{I}}$,

$$\underline{\underline{A}}^{-1} = \frac{\mathrm{adj}(\underline{\underline{A}})}{\det(\underline{\underline{A}})}$$