Introduction

(Basic definitions, various types of process models and the corresponding type of resulting equations, Computational errors, conditioning and stability of algorithms, General process modeling, Modeling examples of lumped parameter and distributed parameter systems. Non-dimensionalization of model equations, Introduction to Fortran, IMSL and MATLAB programming.)

Numerical Analysis/Methods

- What is numerical analysis/method?
  - Analysis and design of algorithms for numerically solving mathematical problems in science and engineering
- Why do we care about numerical analysis?
  - Simulation of real-world phenomena and events
  - Virtual prototyping of engineering designs

Numerical Methods/Analysis

- What is numerical analysis/method?
  - Numerical methods are techniques by which mathematical problems are formulated so that they can be solved with arithmetic operations.
  - Numerical methods are about constructing and analyzing quantitative methods for the computation of solutions to mathematical problems.
  - Numerical methods are the means by which model equations are solved on the computer.

Numerical methods

- Numerical methods discretize and approximate
- In general, the precision is limited
- study of errors and their propagation is crucial
- often iterative methods are used (convergence!)
- Applications
  - Evaluation of functions
  - Interpolation
  - Optimization
  - Integration
  - solving differential equations

Basic Concept in Numerical Analysis

- All numerical methods involve approximations due to either limits in the algorithm or physical limits in the computer hardware. Errors associated with measurements or calculations can be characterized with reference to **accuracy and precision.**
- **Accuracy** refers to how closely a computed or measured value agree with the true value.
- **Precision** refers to how close measured or computed values agree with each other after repeated sampling.
- Other important concepts: (i) **convergence** and (ii) **stability**.
- **Convergence** of an iterative procedure is achieved when the desired accuracy criterion (or criteria) is satisfied.
- **Stability** is an important property of numerical methods specially for ODEs and PDEs.

Reasons to study numerical methods

- "Solve" problems with no analytic solution
  - Non-linear equations
  - Complex behaviours
- Understand these methods
  - Gain familiarity with common algorithms
  - Computing realities and calculations in principle
    - How they can be improved
    - How they can fail
  - Numerical methods shouldn't be used blindly

Reasons to study numerical methods

A few problems can be solved *exactly:*

Linear systems

$$\begin{aligned} x+y &= 1 \\ x-y &= 0 \Rightarrow x=y=1/2 \end{aligned}$$

Integrals of polynomials

$$I=\int_0^1 x^3 dx \Rightarrow I=1/4$$

Reasons to study numerical methods

Some problems cannot be solved *exactly:*

Non-linear equations

$$x^5+3x^4-7x^3+x^2+2x-2=0 \qquad \Rightarrow x=?$$

Differential equations

$$\begin{aligned} \dot{x} &= e^{t^2} \\ x(1) &= 0 \qquad \Rightarrow x(t)=? \end{aligned}$$

Reasons to study numerical methods

- "Two main objectives
  - **quantify errors**
    Approximation without error estimation is useless
  - **increase efficiency**
    Solutions which take years or need more resources that you have are useless

Applications of Numerical Methods

- Computer graphics—root finding, interpolation, curve fitting, optimization, ODE solver, PDE solver, finite element method
- Computer vision—optimization, curve fitting, linear equations.
- Machine learning—curve fitting, linear equations, function approximation
- Simulation for prototyping—ODE solver, PDE solver, optimization, numerical integration, interpolation, finite element method

Also:

- Different chemical engineering areas results in different types of mathematical problems, such as follows:

Applications of Numerical Methods

Types of Chemical Engineering Problems Listed by Area

AREA	MOST COMMON PROBLEM TYPE
MATERIAL AND ENERGY BALANCES	Systems of linear equations; sometimes systems of nonlinear algebraic equations.
HEAT TRANSFER	Boundary value problems, initial value problems.
MASS TRANSFER	Boundary value problems, initial value problems.
KINETICS	Systems of nonlinear algebraic equations, initial value problems, boundary value problems.
THERMODYNAMICS	Systems of nonlinear algebraic equations, initial value problems, integration, interpolation.
CONTROL	Initial value problems.
DESIGN	Optimization.

Analytical vs. Numerical Analysis

- Consider solving $x^2=2$
- Analytically, the root of the equation is determined.
- Numerically, the root of the equation will found using a computer program?
- Computer can only do arithmetic operations.
- Design a procedure consisting of only arithmetic operations to find the root.

Analytical vs. Numerical Analysis

Numerical	Analytical
approximate	exact
more intuitive	less intuitive
easily coded	not so easy
easy to get	not so easy

Analytical vs. Numerical Analysis

Example: Newton's 2nd law of Motion

- *"The time rate change of momentum of a body is equal to the resulting force acting on it."*

Formulated as **F = m.a**

F = net force acting on the body

m = mass of the object (kg)

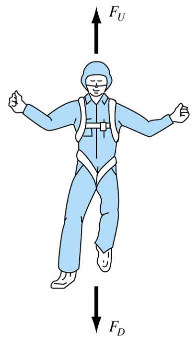
a = its acceleration (m/s^2)

Some complex models may require more sophisticated mathematical techniques than simple algebra

- Example, modeling of a falling parachutist:

F_U = Force due to air resistance = $-cv$ (***c = drag coefficient***)

F_D = Force due to gravity = mg



Analytical vs. Numerical Analysis

Example: Newton's 2nd law of Motion

F = m.a, a=dv/dt

$$\frac{dv}{dt} = \frac{F}{m}$$

$$F = F_D + F_U$$

$$F_D = mg$$

$$F_U = -cv$$

$$\frac{dv}{dt} = \frac{mg - cv}{m}$$

$$\frac{dv}{dt} = g - \frac{c}{m} v$$

- This is a first order ordinary **differential equation**. Can be solved for v (velocity).
- It can **not** be solved using algebraic manipulation
- Analytical Solution:

  If the parachutist is initially at rest (v=0 at t=0), using calculus dv/dt can be solved to give the result:

$$\underbrace{v(t)}_{\text{Dependent variable}} = \underbrace{\frac{gm}{c}}_{\text{Forcing function}}\left(1 - e^{-\overbrace{(c/m)}^{\text{Parameters}}\overbrace{t}^{\text{Independent variable}}}\right)$$

Analytical vs. Numerical Analysis

Example: Newton's 2nd law of Motion - analytical solution

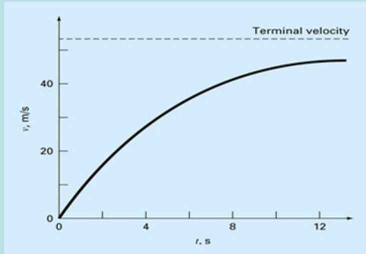
$$\frac{dv}{dt} = g - \frac{c}{m} v$$

$$v(t) = \frac{gm}{c}\left(1 - e^{-(c/m)t}\right)$$

If *v(t)* could not be solved **analytically**, then It will be solved by numerical methods.

$g = 9.8\ m/s^2$ $c = 12.5\ kg/s$ $m = 68.1\ kg$

t (sec.)	V (m/s)
0	0
2	16.40
4	27.77
8	41.10
10	44.87
12	47.49
∞	53.39



Analytical vs. Numerical Analysis

Example: Newton's 2nd law of Motion - numerical solution

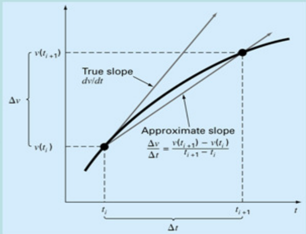
$$\frac{dv}{dt} \cong \frac{\Delta v}{\Delta t} = \frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i} \;\ldots\ldots\; \frac{dv}{dt} = \lim_{\Delta t \to 0} \frac{\Delta v}{\Delta t}$$

$$\frac{dv}{dt} = g - \frac{c}{m} v$$

$$\frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i} = g - \frac{c}{m} v(ti)$$

This equation can be rearranged to yield

$$v(t_{i+1}) = v(t_i) + [g - \frac{c}{m} v(t_i)](t_{i+1} - t_i)$$



t (sec.)	V (m/s)
0	0
2	19.60
4	32.00
8	44.82
10	47.97
12	49.96
∞	53.39

$\Delta t = 2$ sec

To minimize the error, use a smaller step size, Δt
No problem, if you use a computer!

Analytical vs. Numerical Analysis

Example: Newton's 2nd law of Motion – comparison: analytical vs. numerical

m=68.1 kg c=12.5 kg/s
g=9.8 m/s

t (sec.)	V (m/s)
0	0
2	16.40
4	27.77
8	41.10
10	44.87
12	47.49
∞	53.39

$\Delta t = 2$ sec

t (sec.)	V (m/s)
0	0
2	19.60
4	32.00
8	44.82
10	47.97
12	49.96
∞	53.39

$\Delta t = 0.5$ sec

t (sec.)	V (m/s)
0	0
2	17.06
4	28.67
8	41.94
10	45.60
12	48.09
∞	53.39

$\Delta t = 0.01$ sec

t (sec.)	V (m/s)
0	0
2	16.41
4	27.83
8	41.13
10	44.90
12	47.51
∞	53.39

$$v(t) = \frac{gm}{c}\left(1 - e^{-(c/m)t}\right)$$

$$v(t_i + 1) = v(t_i) + [g - \frac{c}{m} v(t_i)]\Delta t$$

If you want to minimize the error, use a smaller step size, Δt

Analytical vs. Numerical Analysis

Example: Newton's 2nd law of Motion – matlab code

```
• g=9.8;
• cd=12.5;
• m = 68.1;

• dt = input('time increment (s):');
• tf = input('final time (s):');

• ti=0;
• vi=0;

• while (1)

•    dvdt = g-(cd/m)*vi;
•    vi = vi + dvdt*dt;
•    ti = ti + dt;
•    if ti >= tf, break, end
• end

• disp('velocity (m/s):')
• disp(vi)
```

$$v(t_{i+1}) = v(t_i) + [g - \frac{c}{m} v(t_i)](t_{i+1} - t_i)$$

m=68.1 kg; c=12.5 kg/s; g=9.8 m/s

t (sec.)	V (m/s)
0	0
2	19.60
4	32.00
8	44.82
10	47.97
12	49.96
∞	53.39

What is this course about?

- This is not a course to teach you to code.
- This is a course to teach you computer algorithms for analyzing and solving science and engineering problems in numerical ways.
- Numerical analysis is the study of procedures for solving problems with a computer.
- Numerical analysis is always *numerical!*
- The analysis of errors in numerical methods is critically important

Modelling: The Basic Steps

Modelling: The Basic Steps

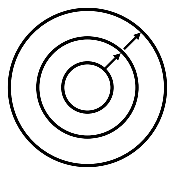
- Identify the problem
- Develop a conceptual model
- Develop a mathematical model
- Solve the equations
- Compare results with reality
- Improve the model if necessary
- Write a report

The Next Four Steps

- Solve the mathematical equations
- Does the solution make mathematical sense?
- Does the “correct solution” match reality?
- Write a report

Simple Model

An oil spill is circular in shape and is spreading out in still water.



Question:
If the radius increases at 0.1 ms^{-1}, at what **rate** is the area expanding at $r = 10$ m?

Simple Model

Question:
If the radius increases at 0.1 ms^{-1}, at what **rate** is the area expanding at r = 10 m?

This is known

This is to be found

Simple Model

Question:
If the radius increases at 0.1 ms^{-1}, at what **rate** is the area expanding at r = 10 m?

$$\frac{dr}{dt}$$

This is known

This is to be found

Simple Model

Question:
If the radius increases at 0.1 ms^{-1}, at what **rate** is the area expanding at r = 10 m?

$$\frac{dr}{dt}$$

This is known

$$\frac{dA}{dt}$$

This is to be found

Simple Model

What do you want?

What are you given?

$$\frac{dA}{dt} = \quad \frac{dr}{dt}$$

What do you need to balance this up?

Simple Model

What do you want?

What are you given?

$$\frac{dA}{dt} = \frac{dA}{dr}\frac{dr}{dt}$$

What do you need to balance this up?

Simple Model

How to find $\frac{dA}{dr}$?

need a formula connecting A & r

Simple Model

How to find $\frac{dA}{dr}$?

need a formula connecting A & r

$$A = \pi r^2$$

$$\frac{dA}{dr} = 2\pi r$$

Simple Model

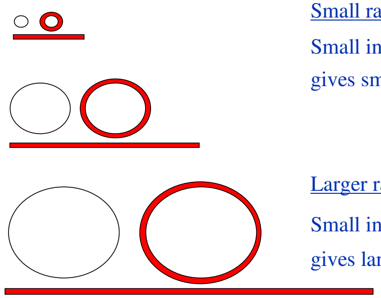
Question: If the radius increases at 0.1 ms^{-1}, at what **rate** is the area expanding at $r = 10$ m?

$$\begin{aligned} \frac{dA}{dt} &= \frac{dA}{dr}\frac{dr}{dt} \\ &= 2\pi r \frac{dr}{dt} \\ &= 2 \times \pi \times 10 \times 0.1 \\ &= 2\pi \\ &\approx 6.3 \text{ m}^2\text{s}^{-1} \end{aligned}$$

Note: It is common to leave the answer as this

Simple Model

What does $\frac{dA}{dr} = 2\pi r$ actually mean ?



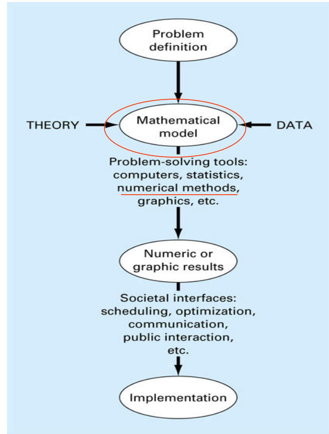
Small radius:

Small increase in radius gives small increase in area

Larger radius:

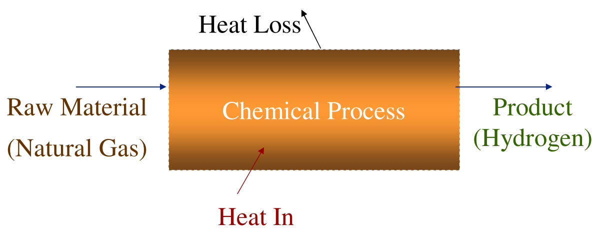
Small increase in radius gives larger increase in area

The Engineering Problem Solving Process



Chemical Process

- Chemical processing involves transformation of raw material and input energy into a finished or desired product



More details will be provided in class

Considerations in Chemical Processing

Several questions related to different aspect of chemical processing arise when we deal with chemical processing:

- Synthesis: What sequence of processes are required (mixer, heater, reactor, separator) ?
- Design: What type and size of equipment?
- Operation: What operating conditions will yield desirable product?
- Control: What process input can be manipulated ?
- Safety: *What If* a process unit fails?
- Environmental: How can we operate the system to minimize pollutants ?

Some or all of these questions can be answered with the help of process models

Model, Process Model & Chemical Process/System

Model

A mathematical or physical *system* obeying certain specified conditions, whose behavior is used to understand a physical, biological, or social system to which it is analogous to.

"*McGraw-Hill Dictionary of Scientific and Technical Terms*"

Process Model

A process model is a *set of equations* (+ necessary input data to solve the equations) that allows us to predict the behavior of a *chemical process* system

Chemical Process/System: A single or a combination of chemical unit operations that cause physical and/or chemical change in a substance or mixture of substances, e.g.

- Chemical reactor
- Heat exchanger
- Separator (distillation column)

Basic Approach to Process Modeling

Model Formulation

- Identify the underlying physics, chemistry or biology governing the process
- Describe physical-chemical relationships in terms of mathematical equations

Input Specification & Parameter Identification

- Specification of design variables
- Degree of freedom analysis
- Parameter identification/estimation

Model Validation

- Compare predictions (calculation results) with experimental results

Types of Process Models

- Fundamental Model
  - These models are based on known physical-chemical relationships
    - Conservation Equations
      - Mass Conservation
      - Energy Conservation
      - Species Balance
    - Constitutive Relationships
      - Ideal gas law
      - Reaction kinetics or rate law
      - Heat transfer rate
- Empirical Model:
  - These models are usually employed when the processes are too complex or poorly understood
    - Least-square fit of experimental data

General Classification of Chemical Engineering Systems

1. **According to the variation of state variables with time:**
   a. Steady state models
   b. Unsteady state models (dynamic models)
2. **According to the spatial variation of state variables:**
   a. Lumped models
   b. Distributed models
3. **According to the functional dependence of the rate-governing laws upon the state variables:**
   a. Linear models
   b. Nonlinear models
4. **According to the type of processes taking place with the boundaries of the system**
   a. Mass transfer b. Heat transfer
   c. Momentum transfer d. Chemical reaction
   e. Combination of any two or more of these processes

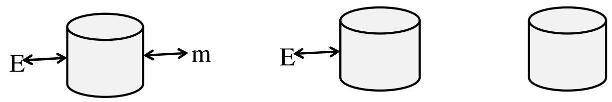
General Classification of Chemical Engineering Systems

5. **According to the number of phases in the system**
   a. Homogeneous models b. Heterogeneous models
6. **According to the number of stages in the system:**
   a. Single stage b. Multi stage
7. **According to the modes of operation of the system:**
   a. Batch b. Semi-batch (fed-batch) c. Continuous
8. **According to the system's thermal relation with the surroundings**
   a. Adiabatic b. Nonadiabatic
9. **According to the thermal characteristics of the system:**
   a. Isothermal b. Nonisothermal

General Classification of Chemical Engineering Systems

10. **According to system's thermodynamical characteristics**

a. Open b. Closed c. Isolated systems



Stationary nonequilibruim state (steady state) *Thermodynamic equilibrium with time* *Thermodynamic equilibrium with time*

Classification Based on Spatial Homogeneity

Lumped Parameter System

A system wherein *process variables* are <u>spatially homogeneous</u> (do not vary in spatial dimension) but may vary with time.

Distributed Parameter System

A system wherein *process variables* are <u>spatially heterogeneous</u> (vary with space) and may vary with time.

Classification Based on Temporal Variation

Steady-State System

Chemical processes that operate at steady-state conditions, i.e. the inputs and the outputs of the process(es) or process variables do not change with time.

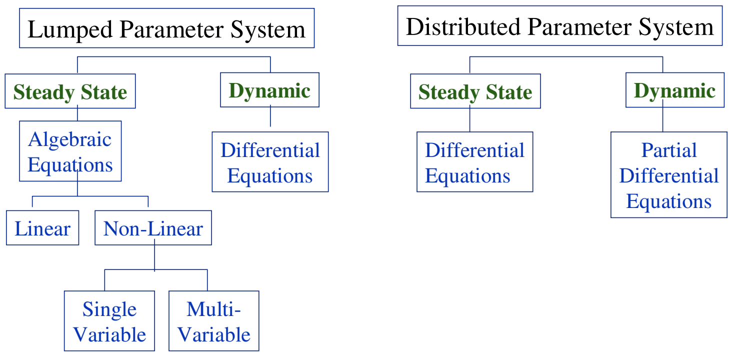
Dynamic System

Chemical processes for which inputs and the outputs of the process(es) change with time, i.e. they have a dynamic behavior.

- e.g. batch reactors for pharmaceutical chemicals

<u>Note</u>: Dynamic behavior can also be encountered during start-ups and shut-downs of processes or when certain inputs are changed either deliberately or accidentally.

Types of System and Resulting Equations



Process Modeling: General Discussion

- Mathematical equations constituting process models arise from the fundamental laws of mass, energy, and momentum conservation.
  - For systems undergoing changes in chemical composition, species balance equations must be included in the process model.
- For reliable outputs from a process model, we must ensure that the model constitutes "*correct equations*" describing the system; as well, we must be confident that we are "*solving the equations correctly*".

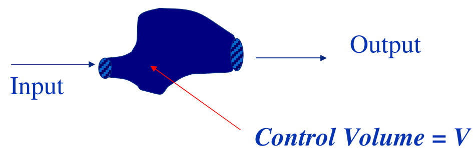
Differential and Integral Balance Equations

Differential Balance Equations
- Equations are derived by considering what is happening in a system at any instance in time. Each term of the equation is a RATE (rate of input, output etc.)

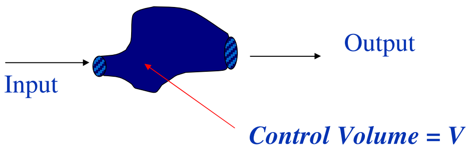
Integral Balance Equation
- Equations are derived by considering the state of a system at two distinct time. Each term of the equation is an AMOUNT of the balance quantity

Differential Balance Equation – General Form

Rate of *INPUT* + *Rate of* *GENERATION* − *Rate of* *OUTPUT* − *Rate of* *CONSUMPTION* = *Rate of* *ACCUMULATION*

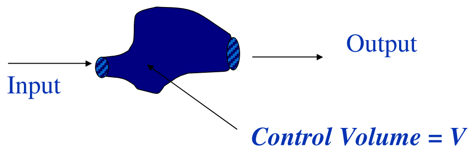


Mass Conservation: Material Balance Equation



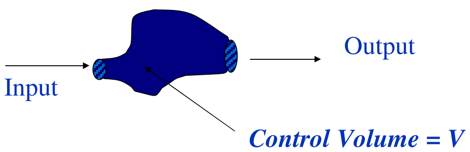
$$\begin{matrix}\text{Rate of} & & \text{Rate of} & & \text{Rate of}\\ \text{INPUT} & - & \text{OUTPUT} & = & \text{ACCUMULATION}\end{matrix}$$

Mass Conservation: Energy Balance Equation



$$\begin{matrix}\text{Rate of} & & \text{Rate of} & & \text{Rate of}\\ \text{INPUT} & - & \text{OUTPUT} & = & \text{ACCUMULATION}\end{matrix}$$

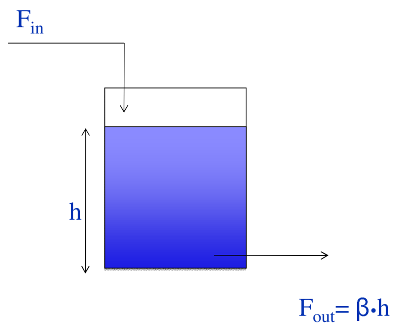
Mole Balance Equation



$$\begin{matrix}\text{Rate of} & & \text{Rate of} & & \text{Rate of} & & \text{Rate of} & & \text{Rate of}\\ \text{INPUT} & + & \text{GENERATION} & - & \text{OUTPUT} & - & \text{CONSUMPTION} & = & \text{ACCUMULATION}\end{matrix}$$

Question: Is mole balance equation a conservation equation ?

Transient Mass Balance: Storage Tank Example



Differential Energy Balance Equation

Recall that energy is one of the quantities that is always conserved. This leads to simple form of balance equation involving accumulation, input and output terms.

$$\frac{dE_{sys}}{dt} = \dot{E}_{in} - \dot{E}_{out} \qquad \textbf{(1)}$$

$\frac{dE_{sys}}{dt} =$ Rate of change of the energy stored in the system

$\dot{E}_{in} =$ Rate at which energy enters the system

$\dot{E}_{out} =$ Rate at which energy leaves the system

Each term is in Joules/seconds (= Watts) or in equivalent units

Differential Energy Balance Equation .... Cont.

Each term of the energy balance equation will be examined.

Energy content of the system

The total energy of the system, E_{sys}, is a sum of three forms of energy – (i) internal, (ii) kinetic and (iii) potential

$$E_{sys} = U_{sys} + K_{k,sys} + E_{p,sys} \qquad \textbf{(2)}$$

In terms of mass specific properties, we can write the above equation as follows

$$E_{sys} = m_{sys} \cdot (\bar{U}_{sys} + \bar{K}_{k,sys} + \bar{E}_{p,sys}) \qquad \textbf{(3)}$$

where, $\mathbf{m_{sys}}$ is the mass of material contained within a system at any time

Differential Energy Balance Equation .... Cont.

Rate of energy input to the system

The input rate of energy contains contribution from all three forms of energy + flow work + *heat input*:

$$\dot{E}_{in} = \dot{m}_{in}(\bar{H}_{in} + \frac{u^2_{in}}{2} + gz_{in}) + \dot{Q} \qquad \textbf{(4)}$$

where, the terms have usual meaning.

$$\dot{W}_{fl} = P\dot{V} = \dot{m}(P\bar{V}) \qquad \textbf{(5)}$$

It must be recognized that the flow work term has already been included in the above equation. For information sake, the flow work is given by the following equation

$$\dot{m} \cdot \bar{H} = \dot{m} \cdot (\bar{U} + P\bar{V}) \qquad \textbf{(6)}$$

which can then be combined with internal energy to yield:

Differential Energy Balance Equation .... Cont.

Rate of energy output from the system

The output rate of energy contains contribution from all three forms of energy + flow work + *shaft work done by the system*:

$$\dot{E}_{out} = \dot{m}_{out}(\bar{H}_{out} + \frac{u^2_{out}}{2} + gz_{out}) + W_s \qquad \textbf{(7)}$$

where, the terms have usual meaning.

The overall energy balance can then be written by combining equations (3), (4) and (7)

$$\frac{d[m_{sys} \cdot (\bar{U}_{sys} + \bar{K}_{k,sys} + \bar{E}_{p,sys})]}{dt} = \dot{m}_{in}(\bar{H}_{in} + \frac{u^2_{in}}{2} + gz_{in}) + \dot{Q} - \dot{m}_{out}(\bar{H}_{out} + \frac{u^2_{out}}{2} + gz_{out}) - W_s \qquad \textbf{(8)}$$

Differential Energy Balance Equation …. Cont.

- For most of the chemical processes, the kinetic and potential energy changes in the system and between the inlet and outlet streams are negligible
- That is,

$$\boxed{d\bar{E}_{sys} = d\bar{U}_{sys} + \cancel{d\bar{K}_{k,sys}} + \cancel{d\bar{E}_{p,sys}}} \qquad \textbf{(9)}$$

- and

$$\boxed{\dot{m}_{in}\left(\frac{u^2_{in}}{2}\right) - \dot{m}_{out}\left(\frac{u^2_{out}}{2}\right) = 0} \qquad \textbf{(10)}$$

$$\boxed{\dot{m}_{in}(gz_{in}) - \dot{m}_{out}(gz_{out}) = 0} \qquad \textbf{(11)}$$

Differential Energy Balance Equation …. Cont.

Substituting equations (9), (10), and (11) in equation (8),

$$\boxed{\frac{d[m_{sys}\cdot(\bar{U}_{sys})]}{dt} = \dot{m}_{in}(\bar{H}_{in}) + \dot{Q} - \dot{m}_{out}(\bar{H}_{out}) - W_s} \qquad \textbf{(12)}$$

Next, we evaluate the accumulation term or LHS of eq. (12). First, we express internal energy in terms of enthalpy and pressure

$$\boxed{\bar{U} = \bar{H} - \frac{P}{\rho}} \qquad \textbf{(13)}$$

Expanding LHS of equation (12)

$$\boxed{\frac{d[m_{sys}\cdot(\bar{H}_{sys} - \frac{P}{\rho})]}{dt} = (\bar{H}_{sys} - \frac{P}{\rho})\frac{dm_{sys}}{dt} + m_{sys}\frac{d(\bar{H}_{sys})}{dt} - m_{sys}\frac{d(P/\rho)}{dt}} \qquad \textbf{(14)}$$

Differential Energy Balance Equation …. Cont.

Simplification of eq. (14) below depends on what valid assumptions can made

$$\boxed{\frac{d[m_{sys}\cdot(\bar{H}_{sys} - \frac{P}{\rho})]}{dt} = (\bar{H}_{sys} - \frac{P}{\rho})\frac{dm_{sys}}{dt} + m_{sys}\frac{d(\bar{H}_{sys})}{dt} - m_{sys}\frac{d(P/\rho)}{dt}}$$

Differential Energy Balance Equation …. Cont.

Case1: If m_{sys}, P and ρ are constant, then

$$\boxed{\frac{d[m_{sys}\cdot(\bar{H}_{sys} - \frac{P}{\rho})]}{dt} = m_{sys}\frac{d(\bar{H}_{sys})}{dt}} \qquad \textbf{(15)}$$

The above assumption may hold true for constant pressure liquid-system (*ρ=constant*) for which the input mass flow rate is equal to output mass flow rate (*m_{sys}=constant*)

Applying eq. (15) in overall energy balance equation (12)

$$\boxed{m_{sys}\frac{d(\bar{H}_{out})}{dt} = \dot{m}_{in}(\bar{H}_{in}) + \dot{Q} - \dot{m}_{out}(\bar{H}_{out}) - W_s} \qquad \textbf{(16)}$$

Differential Energy Balance Equation .... Cont.

Case2: If m_{sys} is NOT constant but P and ρ are. Also, if the system is *a lumped-parameter system*

$$\frac{d[m_{sys}\cdot(\bar{H}_{sys}-\frac{P}{\rho})]}{dt} = (\bar{H}_{sys}-\frac{P}{\rho})\frac{dm_{sys}}{dt}+m_{sys}\frac{d(\bar{H}_{sys})}{dt}$$

For lumped-parameter system, because of the well-mixed assumption, we can define the properties of the fluid in the system to be equal to that of the outlet fluid stream, therefore

$$\frac{d[m_{sys}\cdot(\bar{H}_{out}-\frac{P}{\rho})]}{dt} = (\bar{H}_{out}-\frac{P}{\rho})\frac{dm_{sys}}{dt}+m_{sys}\frac{d(\bar{H}_{out})}{dt} \qquad \textbf{(17)}$$

Differential Energy Balance Equation .... Cont.

Applying eq. (17) in overall energy balance equation (12)

$$(\bar{H}_{out}-\frac{P}{\rho})\frac{dm_{sys}}{dt}+m_{sys}\frac{d(\bar{H}_{out})}{dt} = \dot{m}_{in}(\bar{H}_{in})+\dot{Q}-\dot{m}_{out}(\bar{H}_{out})-W_s \qquad \textbf{(18)}$$

From mass balance,

$$\frac{dm_{sys}}{dt} = \dot{m}_{in}-\dot{m}_{out} \qquad \textbf{(19)}$$

Substituting eq. (19) in (18),

$$(\bar{H}_{out}-\frac{P}{\rho})(\dot{m}_{in}-\dot{m}_{out})+m_{sys}\frac{d(\bar{H}_{out})}{dt} = \dot{m}_{in}(\bar{H}_{in})+\dot{Q}-\dot{m}_{out}(\bar{H}_{out})-W_s \qquad \textbf{(20)}$$

Differential Energy Balance Equation .... Cont.

Expanding eq. (20)

$$\bar{H}_{out}\dot{m}_{in}-\bar{H}_{out}\dot{m}_{out}-(\frac{P}{\rho})(\dot{m}_{in}-\dot{m}_{out})+m_{sys}\frac{d(\bar{H}_{out})}{dt} = \dot{m}_{in}(\bar{H}_{in})+\dot{Q}-\dot{m}_{out}(\bar{H}_{out})-W_s \qquad \textbf{(21)}$$

Rearranging,

$$m_{sys}\frac{d(\bar{H}_{out})}{dt} = \dot{m}_{in}(\bar{H}_{in}-\bar{H}_{out})+(\frac{P}{\rho})(\dot{m}_{in}-\dot{m}_{out})+\dot{Q}-W_s \qquad \textbf{(22)}$$

For liquids, further simplify

$$m_{sys}\cdot\bar{C}_p\cdot\frac{dT}{dt} = \dot{m}_{in}\cdot\bar{C}_p(T_{in}-T_{out})+(\frac{P}{\rho})(\dot{m}_{in}-\dot{m}_{out})+\dot{Q}-W_s \qquad \textbf{(23)}$$

Approximations and Round-Off Errors

Numerical errors

- Roundoff error: finite precision
  numerical calculations are almost always approximations
- Truncation error: a calculation has to stop
  Examples:
  - Approximation (e.g. finite Taylor series)
  - Discretization

  It is crucial to know when to stop (i.e. when a calculations is converged!). To check this, change parameters (e.g. step size, number of basis states) and check result.
- modeling error

Numerical errors

- Numerical methods yield ***approximate*** results that are close to the exact analytical solution.
- How confident we are in our approximate result ? In other words,
- Number of *significant figures* indicates **precision**. Significant digits of a number are those that can be used with *confidence,* e.g., the number of certain digits plus one estimated digit.

53,800 How many significant figures?

5.38 x 10^4 3

5.3800 x 10^4 5

Zeros are sometimes used to locate the decimal point not significant figures.

0.00001753 4

0.001753 4

Error Definitions

True error: E_t = True value – Approximation (+/-)

$$\textbf{True percent relative error:}\ \varepsilon_t = \left|\frac{\textbf{True value} - \textbf{Approximation}}{\textbf{True value}}\right| \times 100\%$$

Approximate Error

- For numerical methods, the true value will be known only when we deal with functions that can be solved *analytically*.
- In real world applications, we usually do not know the answer a priori.

Approximate Error = Current Approximation (i) – PreviousApproximation(i-1)

$$\textbf{Approximate Relative Error:}\ \varepsilon_a = \left|\frac{\textbf{Approximate error}}{\textbf{Approximation}}\right| \times 100\%$$

Truncation errors

- Truncation errors are problem specific. It results from using an approximation of the function instead of its true value.
- Often, every step involves an approximation, e.g. a finite Taylor series.
- The truncation errors accumulate.
- Often, truncation errors can be calculated.

Example

$$\sin(x) = \sum_{m=0}^{\infty} (-1)^m \frac{x^{2m+1}}{(2m+1)!}$$

$$\sin(x) \cong x - \frac{x^3}{3!}$$

$$E_t = \sin(0.5) - 0.5 - \frac{0.5^3}{6} = 2.59 \times 10^{-4}$$

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = \left(1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!}\right) + \sum_{n=4}^{\infty} \frac{x^n}{n!}$$

$$= p_3(x) + \sum_{n=4}^{\infty} \frac{x^n}{n!}$$

Roundoff errors

• Precision of representation of numbers is finite. Computer retains only a certain number of significant figures for each number it stores or uses.
 - errors accumulate

• a real number x can be represented as

$fl(x) = x\cdot(1+\varepsilon)$:   floating point computer representation

$|fl(x)-x| = \varepsilon x$ absolute error (often also Δx)

$|fl(x)-x|/x = \varepsilon$ relative error

Example: Consider 1 divided by 3. If computer retained 7 significant figures, the number it registers is

$$Round\ off\ error = 0.000000033\overline{3}\ or\ 0.33\overline{3}\times 10^{-7}$$

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Roundoff errors

Another example….

Consider the following quadratic equation

$$x^2 - 2.57\times10^3 x + 1 = 0$$

$$x = \frac{2.57\times10^3 \pm \sqrt{(2.57\times10^3)^2 - 4}}{2}$$

$$x = \frac{2.57\times10^3 \pm y}{2}$$

If $y = 2.56999922\times10^3 \Rightarrow x = 2.5699961\times10^3$

If $y = 2.5699992\times10^3 \Rightarrow x = 2.569996\times10^3$

If $y = 2.57\times10^3 \Rightarrow x = 2.57\times10^3$

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Error Analysis

A “numerical solution” is different from a “mathematical solution.” Numerical solutions are approximations to the exact solution.

How “good” a numerical solution is depends on how close it is to the exact solution and what is the error we are willing to tolerate.

If $\hat{p}$ is an approximation to p,

- ► the absolute error is $E_p = |p - \hat{p}|$
- ► the relative error is $R_p = \frac{|p-\hat{p}|}{|p|}$. It may be expressed as a percentage.
- ► the approximation has d significant digits if d is the largest integer such that $\frac{|p-\hat{p}|}{|p|} < 5\times10^{-d}$

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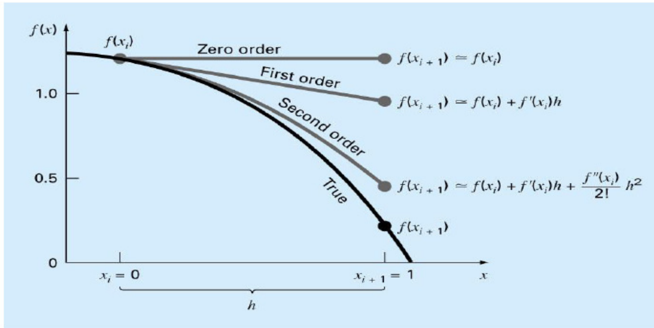
Sources Of Errors

- Truncation Error
- Round Off Errors
- Noise
- Human errors

Truncation Error

- In numerical analysis arise when approximations are used to estimate some quantity. Often a Taylor series is used to approximate a solution which is then truncated. The figure below shows a function f(xi) being approximated by a Taylor series that has been truncated at different levels. The more terms that are retained in the Taylor series the better the approximation and the smaller the truncation error.

Truncation Error



Taylor Series: Approximate the function $f(x) = 1.2 - 0.25x - 0.5x^2 - 0.15x^3 - 0.1x^4$ from $x_i = 0$ with $h = 1$ and predict $f(x)$ at $x_{i+1} = 1$.

Round Of Error

- **Rounding errors** originate from the fact that computers can only represent numbers using a fixed and limited number of significant figures. Thus, numbers such as or cannot be represented exactly in computer memory. The discrepancy introduced by this limitation is call round-off error. Even simple addition can result in round-off error. Often computers have the capacity to represent numbers in two different precisions, called **single** and **double** **precision.**
- A computer number has three parts
  - the sign (+ or -)
  - the fraction part (called the mantissa)
  - the exponent part
- There are three level of precision and these are the number of bits used for mantissa and exponent.

Round Of Error

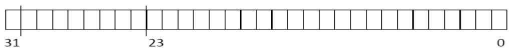
- A computer number has three parts
  - the sign (+ or -)
  - the fraction part (called the mantissa)
  - the exponent part
- There are three level of precision and these are the number of bits used for mantissa and exponent.

	Length	Sign	Mantissa	Exponent	Range
Single	32	1	23	8	$10^{\pm 38}$
Double	64	1	52	11	$10^{\pm 308}$
Extended	80	1	64	15	$10^{\pm 4931}$

Round Of Error

Single Precision

- In **single precision,** 23 bits out of a total of 32 bits are used to represent the significant digits in the number. Of the remaining bits, 8 are used to store the exponent and one bit is used to store the sign.
- Bit Organization in a Single Precision Number:



single precision numbers can range from $\pm 1.175494351\times10^{-38}$ to $\pm 3.4028235\times10^{38}$. In single precision, π can be represented as 3.141593.

Round Of Error

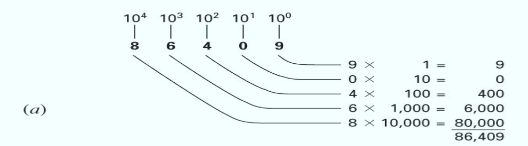
Double Precision

- Due to the limited number of significant digits in single precision, most modern computers use **double precision** which uses 64 bits with 52 digits used to represent the significant figures. This allows , for example, to be represented as 3.141592653589793, that is, 16 digits. The full range for number representation using double precision is $\pm 2.2250738585072020\times10^{-308}$ to $\pm 1.7976931348623157\times10^{308}$.
  - The use of double precision reduces the effects of rounding error and should be used whenever possible in numerical calculations.

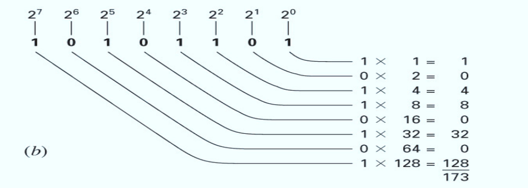
Round Of Error

Number Representation

86409
in Base-10



173
in Base-2



Noise

Noise: is the error in data. The numerical result must have the same number of significant digits as the original data (same *precision*).

Human error

- Mathematical equation/model.
- Computing tools/machines.
- Error in original data.
- Propagated error.

Notation and accuracy

Normalized decimal form of a number:

$$p = \pm 0.d_1 d_2 d_3 \cdots d_k d_{k+1} \cdots \times 10^n$$

Chopping off: $fl_{chop}(p) = \pm 0.d_1 d_2 d_3 \cdots d_k \times 10^n$

Rounding off: $fl_{round}(p) = \pm 0.d_1 d_2 d_3 \cdots r_k \times 10^n$ where $d_k d_{k+1} \cdots$ is rounded to the nearest integer.

Order of approximation

For two functions $f(h)$ and $g(h)$, we say that $f(h) = \mathcal{O}(g(h))$ if there is a positive constant C such that $|f(h)| \le C|g(h)|$ for sufficiently small h.

$$\frac{1}{1-h} = \mathcal{O}(1+h)$$

We say the function $p(h)$ approximates the function $f(h)$ with **order of approximation** $\mathcal{O}(h^n)$

$$f(h) = p(h) + \mathcal{O}(h^n)$$

Rate of Error Propagation

A numerical algorithm is **stable** if small initial errors produce results with small errors.

Suppose ε is the initial error and $\varepsilon(n)$ is the error after n steps. The growth of the error

- is linear if $|\varepsilon(n)| \approx n\varepsilon$
- is exponential if $|\varepsilon(n)| \approx K^n \varepsilon$. As $n \to \infty$
  - it grows without bound if $K > 1$
  - it decreases to zero if $0 < K < 1$