CHEMICAL PROCESS CALCULATIONS

(Introduction to engineering calculations)

Lecture #2: August 08, 2022

Introduction

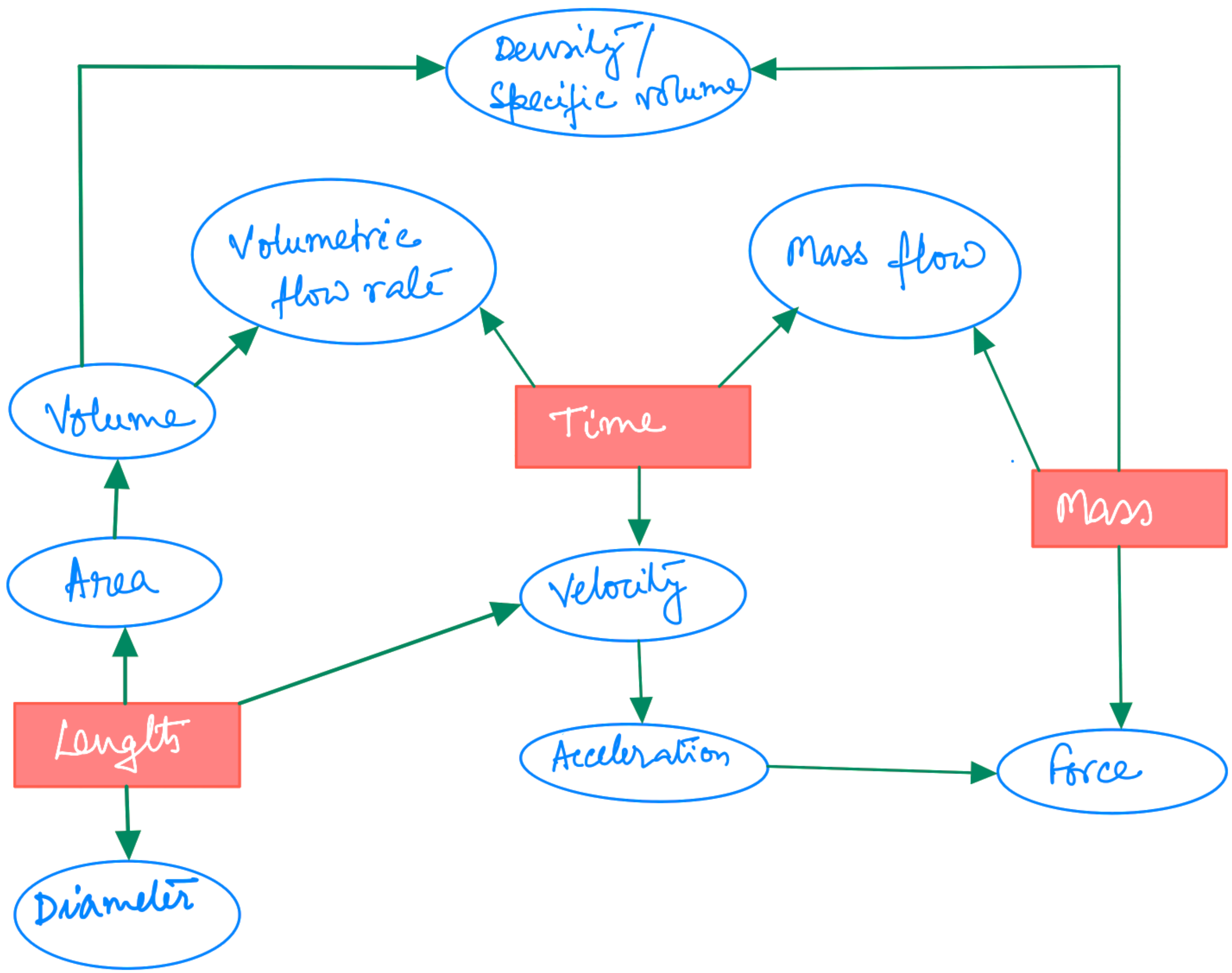
- Dealing with processes that are designed to convert raw materials into desired products

- Dimensions, units, and their conversion
- Processes and process variables
- Material balances
- Energy balances

Dimensions & Units

- Dimension – a measurable property
  - Basic (length, time, mass, temperature, molar amount)
  - Derived (velocity, density, pressure, flow rate, etc.)
- Unit – means of expressing dimensions
  - m – length, s – time, g – mass, K – temperature
  - Base units
  - Multiple units
  - Derived units

Basic and derived dimensions



Basic and derived dimensions

Basic		
Dimension	Unit	Symbol
Length	meter	m
Mass	kilogram	kg
Moles	gram-mole	mol or g-mole
Time	second	s
Temperature	kelvin	K
Electric current	ampere	A
Light intensity	candela	cd

Derived Units			
Dimension	Unit	Symbol	Equivalent
Volume	liter	L	$0.001\ m^3$
Force	newton	N	$1\ kg\ m/s^2$
Pressure	pascal	Pa	$1\ N/m^2$
Energy	joule	J	1 N m
Power	watt	W	1 J/s

Multiple Unit	
tera (T) = 10^{12}	nano (n) = 10^{-9}
giga (G) = 10^{9}	micro (µ) = 10^{-6}
mega (M) = 10^{6}	milli (m) = 10^{-3}
kilo (k) = 10^{3}	centi (c) = 10^{-2}

Significant Figures and Precision

- Limit to the accuracy in measured and/or calculated quantity
- All nonzero digits are significant
  - 321 (3)
  - 4.321 (4)
  - 8.7654321 (8)
- Zeroes in between nonzero digits are significant
  - 102 (3)
  - 102.03 (5)
  - 12030 (4)

Significant Figures and Precision

- Zeroes after non-zeroes & after the decimal place are significant
  - 1.00 (3)
  - 12.3004000 (9)
  - 1.2000 (5)
- No. < 1, zeroes after the decimal point but before non-zeroes are *insignificant*
  - 0.001 (1)
  - 0.010 (2)
  - 0.001020 (4)
  - 0.00102 (3)

Significant Figures and Precision

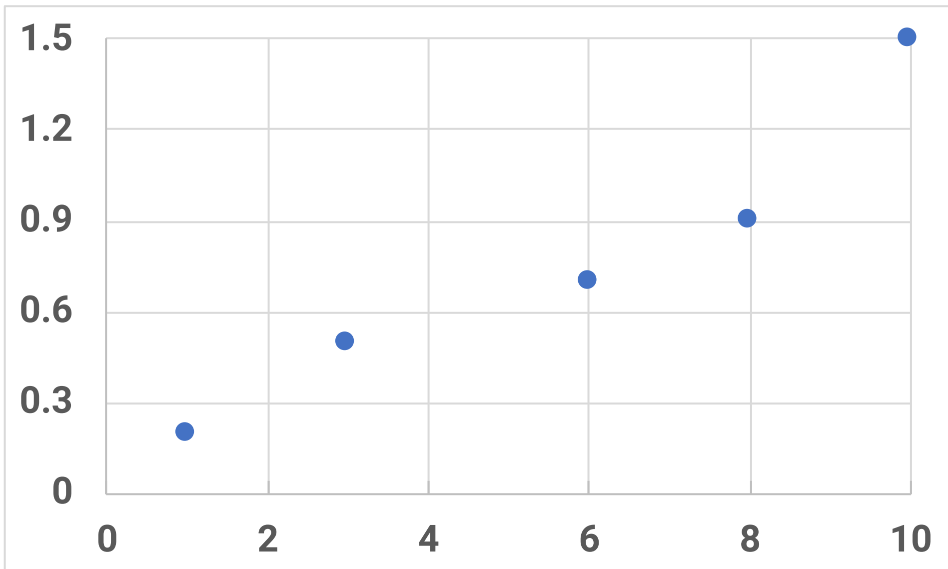
- Multiplication and/or Division
  - rounding off to the lowest number of involved significant figures
  - 1.23 (3) x 9.8 (2) = 12.054 (5) ⇒ 12 (2)
  - 9.8 (2) ÷ 1.23 (3) = 7.97 (3) ⇒ 8.0 (2)
  - 19.96 (4) x 8.0 (2) = 159.68 (5) ⇒ 1.6×10^2 (2)
  - $(2.5 \times 10^{-4}) \times (0.123 \times 10^7) \div 1.25 = 0.246 \times 10^3 \Rightarrow 0.25 \times 10^3 = 25$
- Addition and/or Subtraction
  - rounding off to the lowest number of involved decimal places
  - 1.2345 + 6.789 = 8.0235 ⇒ 8.024
  - 12 - 0.1 = 11.9 ⇒ 12

Dimensional homogeneity

- Valid equation must be dimensionally homogeneous
  - u_2 (m/s) = u_1 (m/s) + g (m/s^2) t (s)
  - homogeneous and consistent
- Dimensionally homogeneous equation may not necessarily be always valid
- D (m) = 55 t (min) + 1.22
- Dimensionless quantity

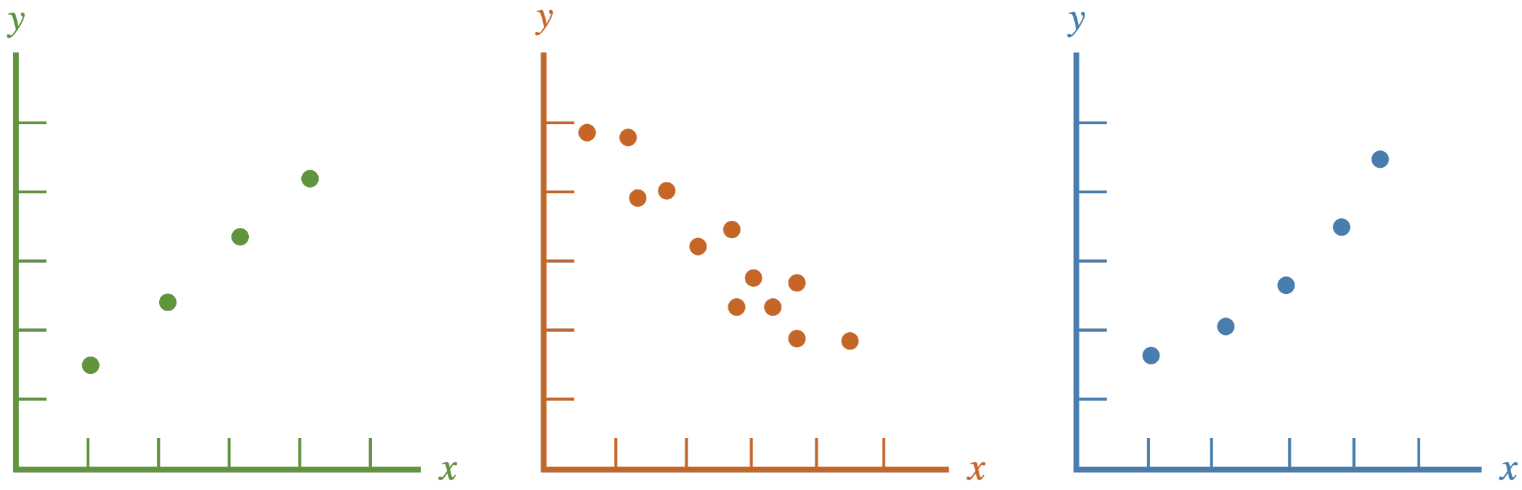
Data representation & analysis

x	1	3	6	8	10
y	0.2	0.5	0.7	0.9	1.5



interpolation / extrapolation

Data representation & analysis



$$y = y_1 + \frac{x - x_1}{x_2 - x_1}(y_2 - y_1)$$

Two-point linear interpolation

Data representation & analysis

$y = 5x + 4$

$y = 5(x-2)^2 - 25$

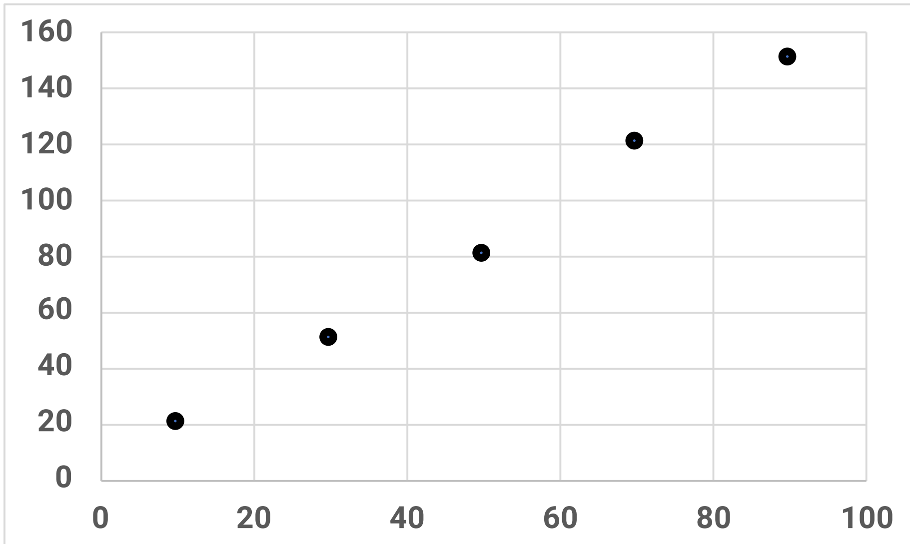
$y = 5 \times 10^6 \sin x / (x^2 + 2)$

$y = ax + b$

$a = \dfrac{y_2 - y_1}{x_2 - x_1}$ $\quad b = \begin{cases} y_1 - ax_1 \\ y_2 - ax_2 \end{cases}$

Data representation & analysis

10	20
30	50
50	80
70	120
90	150



$$y = mx + c$$

$$m = \frac{y_2 - y_1}{x_2 - x_1} = \frac{150 - 20}{90 - 10} = 1.625$$

$$c = y_1 - mx_1 = 20 - 1.625 \times 10 = 3.75$$

$$y = 1.625x + 3.75$$

$$y_2 = 1.625 \times 90 + 3.75 = 150$$

Nonlinear data

$$y = mx^2 + c$$

$$y^2 = \frac{m}{x} + c$$

$$\frac{1}{y} = m\left(x + 3\right) + c$$

$$\sin y = m\left(x^2 - 4\right)$$

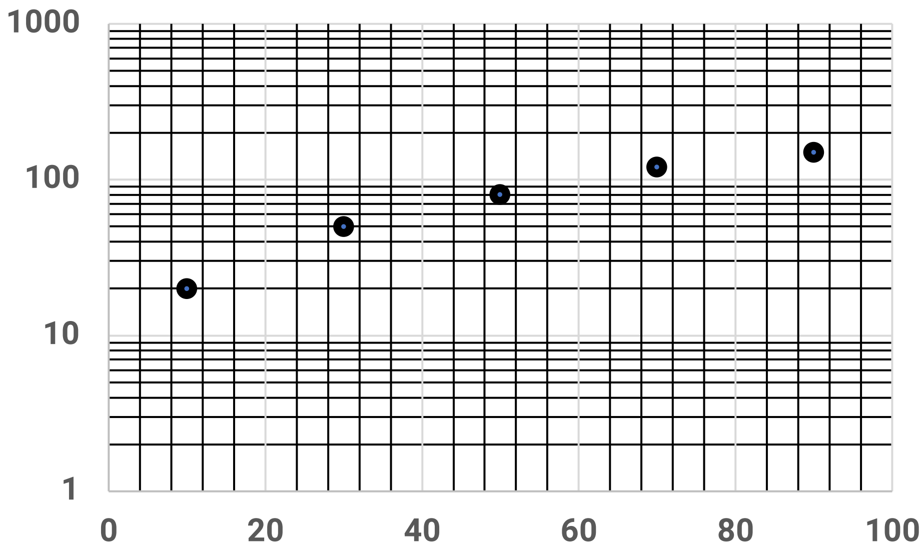
$$y = \frac{1}{m_1 x - c}$$

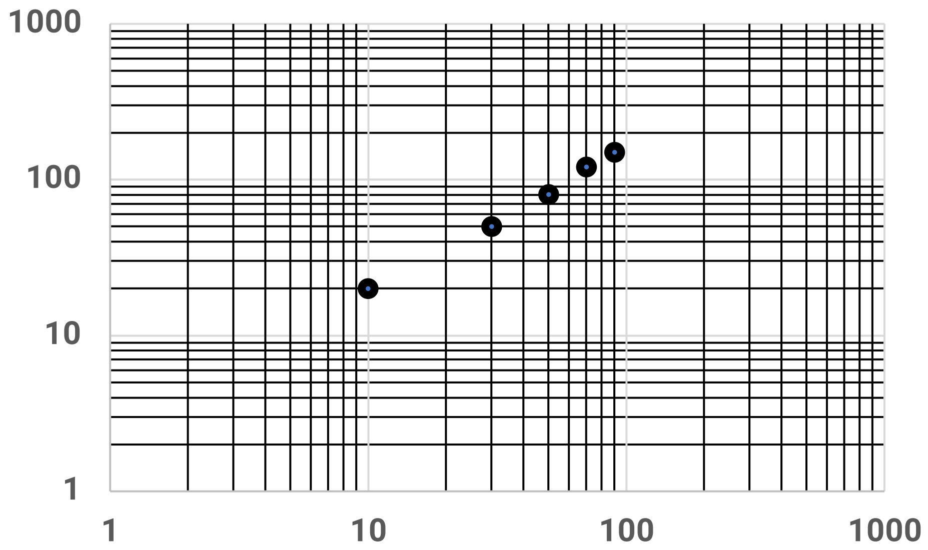
$$\Rightarrow \frac{1}{y} = m_1 x - c$$

$$y = 1 + x\left(mx^2 + c\right)^{1/2}$$

$$\Rightarrow \frac{\left(y-1\right)^2}{x^2} = mx^2 + c$$

Nonlinear data





Validating results

- back-substitution
- order-of-magnitude estimation
- test of reasonableness

Texts

- **BASIC PRINCIPLES AND CALCULATIONS IN CHEMICAL ENGINEERING**
  - David M. Himmelblau and James B. Riggs
  - Prentice Hall
- **ELEMENTARY PRINCIPLES OF CHEMICAL PROCESSES**
  - Richard M. Felder and Ronald W. Rousseau
  - John Wiley & Sons, Inc.