Jordan University
Faculty of Engineering & Technology
Chemical Engineering Department
Chemical Engineering Principles I

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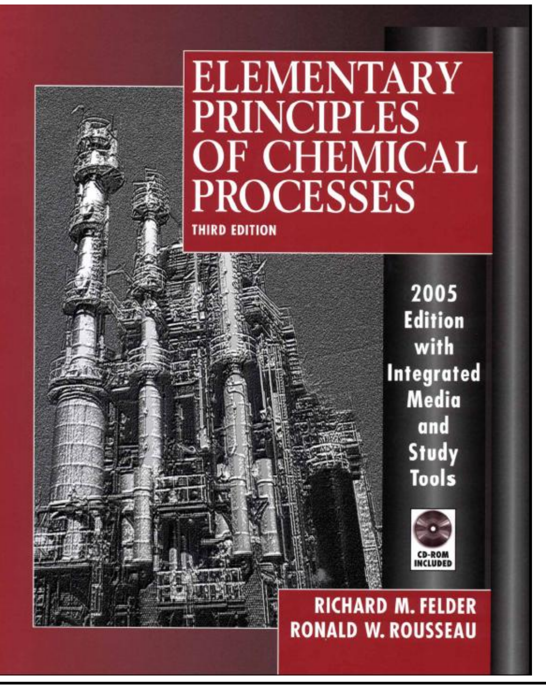
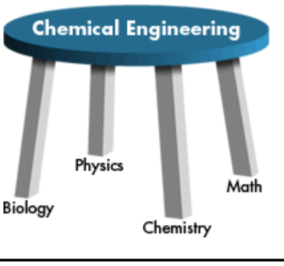
Textbook:

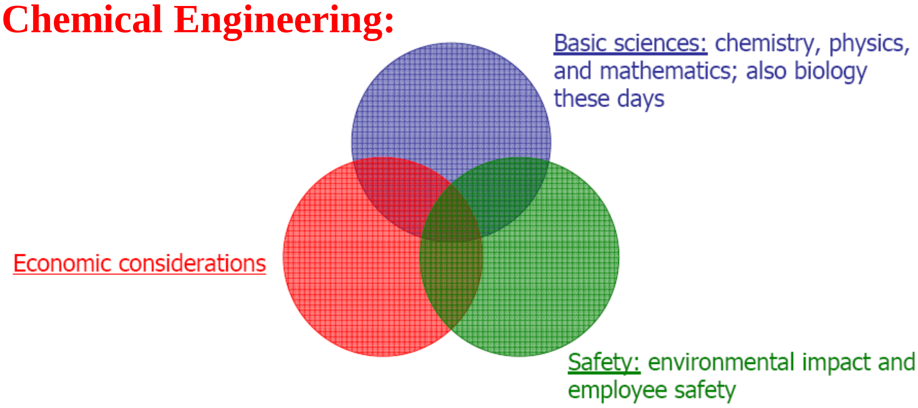


Background: What is Chemical Engineering?

- **Chemical engineer:** The engineer who creates processes based upon physical/chemical/biological changes. These processes may yield marketable products, e.g., gasoline, and penicilin, or non-commercial products, like clean air and water.
- **Chemical Engineering** combines the principles of mathematics, physics, chemistry and biology with engineering practices in order to improve the human environment.

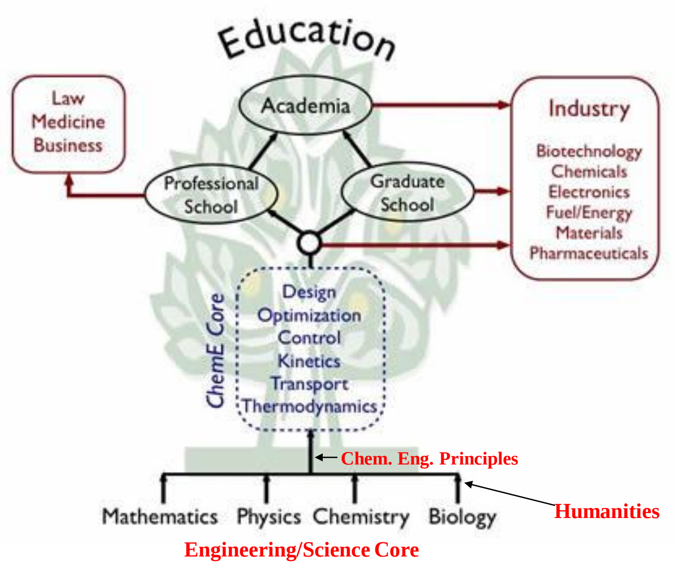


Chemical Engineering:



- **Main difference between Chemical Engineering and Chemistry:**
  - **Chemical Engineering** focuses on the large(industrial) scale.
  - **Chemistry** focuses on the lab (small) scale.

Chemical Engineering Curriculum



- Chemical engineers as a profession, is barely 100 years old. It started at **the interface of chemistry and mechanical engineering**. **The principal goal** then was to **commercialize chemical reactions developed on a chemist's bench**.
- **Top 10 chemical engineering achievements** (list compiled in 1983 in celebration of the 75th anniversary of the AIChE):

  1. Synthetic rubber
  2. Antibiotics
  3. Polymers or "plastics"
  4. Synthetic fibers
  5. Cryogenic separation of air
  6. Catalytic cracking of crude oil
  7. Separation of nuclear isotopes
  8. Pollution control
  9. Fertilizers, especially ammonia
  10. Biomedical engineering

- Contemporary chemical engineering encompasses:

  1. Production of novel materials
  2. Biotechnology
  3. Waste treatment
  4. Pollution control
  5. Energy
  6. Process control

- **Where do the chemical engineers work?**
  - 45% do ``traditional'' ChE: chemical, petroleum, plastic, paper, consumer goods
  - 35% do ``new'' ChE: environment, consulting, microelectronics, biotechnology, materials
  - 10% go to ChE graduate school
  - 10% go to other graduate school (law, medicine, business)

Chapter 2 :

** Dimensions; units and Conversion factors :

* Dimension : quantity that can be calculated or measured.

measured such as : Length, mass, time, ... etc.

Calculated such as : velocity = $\frac{\text{Length}}{\text{time}}$

$$\text{Volume} = (\text{Length})^3$$

$$\text{Density} = \frac{\text{Mass}}{(\text{Length})^3}$$

⋮

etc

* All quantities of interest (in this course) can be expressed in terms of :

Mass (M)

Length (L)

time (t)

Temperature (T)

Moles (mole)

Electric current (A)

Light intensity (cd) → candela

* A quantity consists of its <u>numerical value</u> and its <u>units</u>

** Different systems of units :

1. International system of units : (SI units)

- Base (Fundamental) units :

$$\left.\begin{array}{l}\text{Length } [=]\ m \\ \text{Mass } [=]\ kg \\ \text{time } [=]\ s\end{array}\right\} \text{MKS system}$$

Temperature [=] °C or K

absolute temp. — Kelvin

and gmole for amount of species

- Derived (secondary) units :

Examples: Volume [=] m^3

Velocity [=] m/s

Force [=] $kg.\frac{m}{s^2} \equiv N$

Energy or work [=] $N.m \equiv J$

Power [=] $\frac{J}{s} \equiv$ watt

pressure [=] $\frac{N}{m^2} \equiv pa$

Viscosity [=] $\frac{kg}{m.s} \equiv pa.s \equiv \frac{N}{m^2}.s$

2. CGS system of units

- Base units : cm; g, s, °C or K, gmole

- Derived units :

Examples : force [=] $g.\frac{cm}{s^2} \equiv$ dyne

pressure [=] $\frac{dyne}{cm^2}$

work or Energy [=] dyne.cm $\equiv$ erg

viscosity [=] $\frac{g}{cm.s} \equiv$ poise

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3. British system of units or American Engineering system (AEs) or British gravitational (BG)

- Base units : ft ; slug or lbm , s , °F ; °R ; lbmmole

Degrees Fahrenheit (°F)

°R: absolute temp. → Degrees Rankine

lb_m: pound-mass

- Derived units :

1 slug = 32.2 lbm

Examples : pressure [=] lbf / ft²

force [=] slug. $\frac{ft}{s^2}$ ≡ lb_f

Energy or work [=] lbf. ft

power [=] $\frac{lb_f . ft}{s}$

* Prefixes : they are attached to some units to indicate scale or magnitude

Examples :

peta	(P)	10^{15}		deka		10^{1}
tera	(T)	10^{12}		deci	(d)	10^{-1}
giga	(G)	10^{9}		centi	(c)	10^{-2}
mega	(M)	10^{6}		milli	(m)	10^{-3}
kilo	(k)	10^{3}		micro	(μ)	10^{-6}
				nano	(n)	10^{-9}
				pico		10^{-12}
				femto		10^{-15}
				atto		10^{-18}

* Conversion factor : ratio of a quantity to its equivalent in different unit (= 1)

Ex : 1 m = 100 cm

Keep a copy of conversion factors table with you

Ex: $1\ m = 100\ cm \Rightarrow \frac{1\ m}{100\ cm} = \frac{100\ cm}{1\ m} = 1$

$1\ ft = 12\ in \Rightarrow \frac{1\ ft}{12\ in} = \frac{12\ in}{1\ ft} = 1$

* Rule for conversion: to convert a quantity from one set of units to another; start with this quantity and multiply by the suitable conversion factor to replace old unit with new one.

Ex: Convert a distance of 150 ft to its equivalent in cm:

pick up from conversion factor table the suitable conversion factor:

$1\ ft = 30.48\ cm$

$$\frac{150\ ft}{} \left| \frac{30.48\ cm}{1\ ft} \right. = 4572\ cm$$

Ex: Convert $g = 9.81\ \frac{m}{s^2}$ to its equivalent in AES of units $\rightarrow \frac{ft}{s^2}$

$$g = \frac{9.81\ m}{s^2} \left| \frac{1\ ft}{0.3048\ m} \right. = 32.2\ \frac{ft}{s^2}$$

Ex: Convert $0.02562\ \frac{g \cdot in}{min^2}$ to its equivalent in $\frac{ton \cdot mile}{wk^2}$

pick up from conversion table: $5 \times 10^{-4}\ ton = 453.593\ g$

$1\ ft = 12\ in$

$3.2808\ ft = 0.0006214\ mile$

and we know: $1\ wk = 7\ day$; $1\ day = 24\ hr$; $1\ hr = 60\ min$

$$\frac{0.02562\ \cancel{g} \cdot \cancel{in}}{\cancel{min^2}} \left| \frac{5 \times 10^{-4}\ ton}{453.593\ \cancel{g}} \right| \frac{\cancel{1\ ft}}{12\ \cancel{in}} \left| \frac{0.0006214\ mile}{3.2808\ \cancel{ft}} \right| \frac{(60\ \cancel{min})^2}{(1\ \cancel{hr})^2} \left| \frac{(24\ \cancel{hr})^2}{(1\ \cancel{day})^2} \right| \frac{(7\ \cancel{day})^2}{(1\ wk)^2} = 4.53 \times 10^{-5}\ \frac{ton \cdot mile}{wk^2}$$

* some focus on force :

let us take gravitational force (weight) : W

$W = mg$

In SI : $1\ N = 1\ Kg \cdot \frac{m}{s^2}$

In AES : $1\ lb_f = 1\ slug \frac{ft}{s^2}$

$1\ slug = 32.2\ lbm$

$\therefore 1 lb_f = 32.2\ lbm \frac{ft}{s^2}$

$32.2 \frac{lb_m \cdot ft}{lb_f \cdot ft} = 1 = g_c \leftarrow$

$g = 9.81 \frac{m}{s^2}$
$= 32.2 \frac{ft}{s^2}$

g_c : gravitational conversion factor

Thus the weight can be rewritten as : $W = \frac{mg}{g_c}$

This is for cases in which the mass is given in lb_m

In SI units a unit for force is defined in a way similar to AES units $\Rightarrow$ it is Kg_f : Kilogram force

$1\ Kg_f = 9.81\ Kg \frac{m}{s^2} = 9.81\ N$

$g_c = \frac{9.81\ kg \cdot m}{Kg_f \cdot s^2}$: for SI units

Ex: a body of a mass of 10 lb_m. what is its weight in lb_f

$W = \frac{mg}{g_c} = (10)\frac{(32.2)}{32.2} = 10\ lb_f$

Ex: a body of a mass of 10 kg. what is its weight in Kg_f

$W = \frac{mg}{g_c} = (10)\frac{(9.81)}{(9.81)} = 10\ Kg_f$

** some rules on units and dimensions :

- Dimensional Consistency (homogeneity) :

Every valid eq. must be dimensionally Consistent ; that is all additive terms on both sides of eq. must have the same dimension.

Ex : $E = \frac{1}{2} m u^2 + mgz$

Energy [=] J — Kinetic energy — Potential energy: $kg \cdot \frac{m}{s^2} m = N \cdot m = J$

$kg \cdot \frac{m^2}{s^2} = \frac{kg \cdot m}{s^2} \cdot m = N \cdot m = J$

∴ OK there is consistency in dimensions.

Ex : $u(t) = 3t^2 - 2t + 7$ where $u(t)$ is velocity in m/s and t is time in s

what are the units of 3, 2, and 7

$3 \frac{m}{s^3}$; $2 \frac{m}{s^2}$; $7 \frac{m}{s}$

Check : $\frac{m}{s} [=] 3 \frac{m}{s^3} s^2 - 2 \frac{m}{s^2} s + 7 \frac{m}{s}$

$\frac{m}{s} [=] 3 \frac{m}{s} - 2 \frac{m}{s} + 7 \frac{m}{s}$ ✓

- you can multiply or divide quantities of different dimensions :

Ex : 1 m divided by 2 s yields 0.5 m/s

1 kg multiplied by $9.81 \frac{m}{s^2}$ yields $9.81 \frac{kg \cdot m}{s^2}$

- you can only add or subtract quantities of the same dimensions :

Ex : $3\,ft \cancel{+ 5} \, kg = \propto$

Ex: $3\,m - 1\,ft =$ yes it is okay but first make the units of length to be homogeneous

- $3m - \dfrac{1\,ft \mid 0.3048\,m}{\mid 1\,ft} = \dots\ m$

  or $\dfrac{3m \mid 1\,ft}{\mid 0.3048\,m} - 1 = \dots\ ft$

- Coefficients in physical laws do NOT have units:

  Ex: $KE = \frac{1}{2} m u^2$

  $\frac{1}{2}$ is unitless

- Exponents are dimensionless:

  Ex: $K.E = \frac{1}{2} m u^{2}$ → is dimensionless

- Transcendental function and arguments of these functions must be dimensionless.

  Transcendental functions: Exponential, Logarithmic, Trigonometric ← sin, cos, tan ... etc

$f(x)$ ← argumet is dinensionless

$\underbrace{e}$ → Dimensionless

$$\underbrace{\log(\overbrace{f(x)}^{\text{Dimensionless}})}_{\text{Dimensionless}}$$

The same for example: $\ln(f(x))$, $\tan(f(x))$, --- etc

Ex: The reaction rate constant of some reaction depends upon temperature in the following manner:

$$K = 1.2 \times 10^{-5} \, e^{\left(\frac{-2\times10^{+4}}{1.987T}\right)}$$

where K is the rxn constant in $\frac{mol}{cm^3 . s}$ and T is temperature in kelvin K and the quantity 2×10^{4} has a unit of $\frac{cal}{mol}$

what are the units of 1.2×10^{-5} and 1.987

$e^{\left(\frac{-2\times10^{+4}}{1.987T}\right)}$ must be Dimensionless $\Rightarrow$ 1.2×10^{-5} has the same unit as K $\therefore 1.2\times10^{-5} \frac{mol}{cm^3 . s}$

The argument which is $\frac{-2\times10^{4}}{1.987T(K)}$ must be also dimensionless

$$\Rightarrow \frac{-2\times10^{+4}\,cal}{mol} \Big| \frac{}{T(K)} \Big| \frac{mol.K}{1.987\,cal} \; [=] \; \text{Dimensionless}$$

$\therefore 1.987 \frac{cal}{mol.K}$

Ex: Reynolds number is defined as:

$$Re = \frac{\rho u D}{\mu}$$

where ρ is density
u is velocity
D is diameter
μ is viscosity

what is the unit of Re

Let us try SI units:

$$Re \,[=]\, \frac{\cancel{kg}}{\cancel{m^3}} \Big| \frac{\cancel{m}}{\cancel{s}} \Big| \frac{\cancel{m}}{} \Big| \frac{\cancel{m.s}}{\cancel{kg}} = \text{Dimensionless}$$

Ex: Consider the eq. $D(t) = 3t + 4$

D is distance in ft and t is time in s

(a) what are the units of 3 and 4

(b) Rewrite the eq. to have D in m and t in min.

(a) $3 \frac{ft}{s}$; $4\ ft$

(b) $t(s) = \dfrac{t(min) \mid 60\ s}{\mid 1\ min} = 60\ t(min)$

$D(ft) = \dfrac{D(m) \mid 1\ ft}{\mid 0.3048\ m} = \dfrac{D(m)}{0.3048}$

substitute now in the original eq.:

$$\frac{D(m)}{0.3048} = (3)\left(60\, t(min)\right) + 4$$

$\therefore\quad D(m) = 54.86t + 1.22$

Exercise : what is the unit of 1.22 ?

Verify the validity of the eq. by taking some numerical example.

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** Data; data presentation; and data analysis:

* Significant figures: The number of digits from the first non-zero digit on the left to either:
  (a) the last digit (zero or non-zero) on the right if there is a decimal point.
  (b) the last non-zero digit if there is no decimal point.

Ex:

1137	:	# of s.f = 4
1100	:	2 sf
0.041	:	2 sf
100.003	:	6 s.f.
200.00	:	5 s.f.

* scientific notation:
  → for very large or small numbers: They expressed as a product of numbers between 0.1 and 10 and a power of 10

  Ex: $320,000 = 3.2 \times 10^5$

Remark: When you use scientific notation you must maintain the same # of s.f.

Ex: $0.0003100 = 3.100 \times 10^{-4}$

not 3.1×10^{-4}

Ex: Assume that the distance d is a function of time t according to:

$$d = 16.2 - 16.2\, e^{-0.021 t}$$

where d is in μm and t is in s

Convert the eq. to have d in inches (in) and t in min

$$d(\mu m) = d(in) \left|\frac{2.54\ cm}{1\ in}\right|\frac{1\ m}{100\ cm}\left|\frac{10^6\ \mu m}{1\ m}\right. = 25400\, d(in)$$

$$t(s) = t(min)\left|\frac{60\ s}{1\ min}\right. = 60\, t(min)$$

$$25400\, d(in) = 16.2 - 16.2\, e^{(-0.021)(60\, t(min))}$$

$$d(in) = 6.38 \times 10^{-4} - 6.38 \times 10^{-4}\, e^{-1.26\, t(min)}$$

* Addition or substraction :

Rule : note the decimal position of the last (i.e. rightmost) significant digit ; the position farthest to the left decide the s.f. in the answer.

Ex: $1.0000 + 0.036 + 1.22 = 1.256 = 1.26$

Ex: $2.75 \times 10^6 + 3.400 \times 10^4 =$

$2.75 \times 10^6 + 0.03400 \times 10^6 = 2.784 \times 10^6$

$= 2.78 \times 10^6$

Ex: $565 + 64 = 5.65 \times 10^2 + 0.64 \times 10^2 = 6.29 \times 10^2$

$= 629$

Ex: $1530 - 2.56 = 1.53 \times 10^3 - 0.00256 \times 10^3$

$= 1.52744 \times 10^3$

$= 1.53 \times 10^3 = 1530$

Exception to the rule of s.f. : Counted quantities and integers Contain ∞ number of s.f.

Ex: 1000 students : ∞ s.f.

Why this exception? Because the # of s.f. indicates the precision in the numerical value of the quantity

Ex: $6.2 \Rightarrow$ Range $= 6.15 - 6.25$

$6.20 \Rightarrow$ Range $= 6.195 - 6.205$

* Arithmetic operations with significant figures:

* Multiplication or division:

Rule: s.f. in the answer = smallest # of s.f. in quantities being multiplied or divided

4 s.f. Rounding-off

Ex: $\dfrac{573.5}{254} = 2.2578 = 2.26$ (3 s.f.)

3 s.f

(The answer must have 3 s.f.)

Rounding-off

Ex: $(33.5)\,(2.5) = 83.75 = 84$

3 s.f. 2 s.f.

Remark: If the digit being rounded-off is 5; the convention is to make the last digit of the rounded off number is even.

Ex: $1.235 = 1.24$

$1.245 = 1.24$

** Uncertainty and propagation of uncertainty:

Ex: Measured temperature = 321 °C with uncertainty ± 0.5

How to estimate the uncertainty of a calculated quantity in terms of measured quantities?

assume that a calculated quantity y is a function of several measured quantities: $x_1, x_2, \ldots, x_n$ having uncertainty $u_1, u_2, \ldots, u_n$; respectively.

From mathematics; a first order Taylor series expansion yields:

$$y(x_1 + u_1, x_2 + u_2, \ldots, x_n + u_n) \cong y(x_1, x_2, \ldots, x_n) + \frac{\partial y}{\partial x_1} u_1 + \frac{\partial y}{\partial x_2} u_2 + \cdots + \frac{\partial y}{\partial x_n} u_n$$

If the individual uncertainties are statistically independent, the uncertainty of y is

$$y(x_1 + u_1, u_2 + x_2, \ldots, x_n + u_n) - y(x_1, x_2, \ldots x_n) = \frac{\partial y}{\partial x_1} u_1 + \frac{\partial y}{\partial x_2} u_2 + \cdots + \frac{\partial y}{\partial x_n} u_n$$

and a root-mean-squared (RMS) value of the uncertainty of y; u_y can be calculated as:

$$u_y = \sqrt{\left(\frac{\partial y}{\partial x_1} u_1\right)^2 + \left(\frac{\partial y}{\partial x_2} u_2\right)^2 + \cdots + \left(\frac{\partial y}{\partial x_n} u_n\right)^2}$$

Ex : Determine the RMS uncertainty of a cylinder's density, ρ, using the following measured values:

Mass ; $M = 1.669 \pm 0.01$ kg

D ; Diameter $= 0.050 \pm 0.001$ m

Length ; $L = 0.100 \pm 0.001$ m

$$\rho = \frac{M}{V} \qquad V = \frac{\pi D^2}{4} L$$

$$\rho = \frac{4M}{\pi D^2 L} = \frac{(4)(1.669)}{\pi (0.05)^2 (0.1)} = 8500.1 \ \frac{kg}{m^3} \pm ? \ \frac{kg}{m^3}$$

$u_m = 0.01$ kg $\qquad u_D = 0.001$ m $\qquad u_L = 0.001$ m

$$u_\rho = \sqrt{\left(\frac{\partial \rho}{\partial M} u_m\right)^2 + \left(\frac{\partial \rho}{\partial L} u_L\right)^2 + \left(\frac{\partial \rho}{\partial D} u_D\right)^2}$$

$$\frac{\partial \rho}{\partial M} = \frac{4}{\pi D^2 L} = \frac{\rho}{M} \quad ; \quad \frac{\partial \rho}{\partial L} = \frac{-4M(\pi D^2)}{(\pi D^2 L)^2} = \frac{-4M}{\pi D^2 L^2} = \frac{-\rho}{L} = \frac{-\rho}{L}$$

$$\frac{\partial \rho}{\partial D} = \frac{-4M(2\pi D L)}{(\pi D^2 L)^2} = \frac{-8M}{\pi D^3 L} = \frac{(-2)}{D} \frac{4M}{\pi D^2 L} = \frac{-2\rho}{D}$$

$$u_\rho = \sqrt{\left(\frac{-\rho}{L} u_L\right)^2 + \left(\frac{\rho}{M} u_M\right)^2 + \left(\frac{-2\rho}{D} u_D\right)^2}$$

$$= \sqrt{\left(\frac{8500.1}{0.1}(0.001)\right)^2 + \left(\frac{8500.1}{1.669}(0.01)\right)^2 + \left(\frac{-2 * 8500.1}{0.05}(0.001)\right)^2}$$

$$= 354 \ \frac{kg}{m^3} \Rightarrow \rho = (8500.1 \pm 354) \ \frac{kg}{m^3}$$

** process data representation and analysis :

* The operation of chemical plant is based on the measurements of process variables such as : Temperature ; T , pressure ; P , flowrates , Concentration ,... etc .

* Estimation of data using Linear interpolation or extrapolation :

Interpolation : estimation of y at x value located within the range of x

x	y
13	0.5
17	0.6
20	$\boxed{?}$
24	0.75

or estimation of x at y value located within the range of y

x	y
13	0.5
$\boxed{?}$	0.4
15	0.9
25	1.2

Extrapolation : estimation of y at x value located outside the range x or estimation of x at y value located outside of the range y.

x	y
300	7
400	13
600	$\boxed{?}$

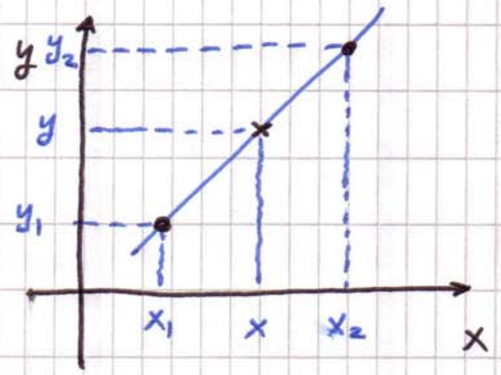
x	y
3.7	0.3
4.0	0.1
?	0.05

How to perform interpolation or extrapolation?

Linear interpolation/extrapolation relationship:

$$\frac{y-y_1}{x-x_1} = \frac{y_2-y_1}{x_2-x_1} \quad \text{or} \quad \frac{x-x_1}{y-y_1} = \frac{x_2-x_1}{y_2-y_1}$$

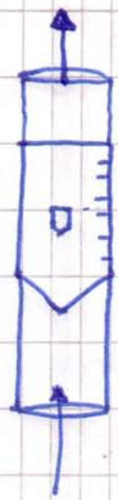
* for linear interpolation we need two points: (x_1, y_1) and (x_2, y_2)



from Geometrical point view: slope between (x_1,y_1) and (x_2,y_2) is the same as between (x,y) and (x_1,y_1) or (x_2,y_2).

Ex: Having the following calibration data of rotameter:

(R) Rotameter reading	(F) flowrate; L/min
10	20
30	52.1
50	84.6



(a) Find the flowrate when the rotameter reading is 16

(b) 〃 〃 〃 〃 〃 〃 〃 〃 38

(c) 〃 〃 〃 〃 〃 〃 〃 〃 70

"flowmeter"

(d) what is the expected Rotameter reading if the flow rate is 60 L/min ?

(a) at $R = 16$ $F = ?$

R	F
$R_1 = 10$	$20 = F_1$
$R = 16$	$? = F$
$R_2 = 30$	$52.1 = F_2$

$$\frac{F_2 - F_1}{R_2 - R_1} = \frac{F - F_1}{R - R_1}$$

$$\frac{52.1 - 20}{30 - 10} = \frac{F - 20}{16 - 10}$$

$\therefore F = 29.63$ L/min

" Interpolation "

(b) at $R = 38$ $F = ?$

R	F
$R_1 = 30$	$52.1 = F_1$
$R = 38$	$? = F$
$R_2 = 50$	$84.6 = F_2$

$$\frac{F_2 - F_1}{R_2 - R_1} = \frac{F - F_1}{R - R_1}$$

$$\frac{84.6 - 52.1}{50 - 30} = \frac{F - 52.1}{38 - 30}$$

" Interpolation "

$\therefore F = 65.1$ L/min

(c) at $R = 70$ $F = ?$

R	F
$R_2 = 30$	$52.1 = F_2$
$R_1 = 50$	$84.6 = F_1$
$R = 70$	$? = F$

$$\frac{F_2 - F_1}{R_2 - R_1} = \frac{F - F_1}{R - R_1}$$

$$\frac{84.6 - 52.1}{50 - 30} = \frac{F - 84.6}{70 - 50}$$

" Extrapolation "

$\therefore F = 117.1$ L/min

(d) at $F = 60$ L/min $R = ?$

R	F
$R_1 = 30$	$52.1 = F_1$
$R = ?$	$60 = F$
$R_2 = 50$	$84.6 = F_2$

$$\frac{R_2 - R_1}{F_2 - F_1} = \frac{R - R_1}{F - F_1}$$

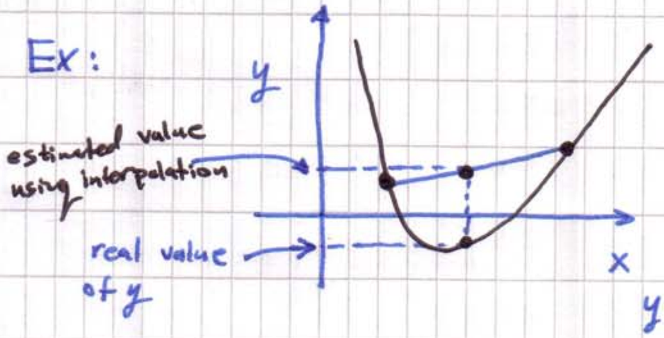
$$\frac{50 - 30}{84.6 - 52.1} = \frac{R - 30}{60 - 52.1}$$

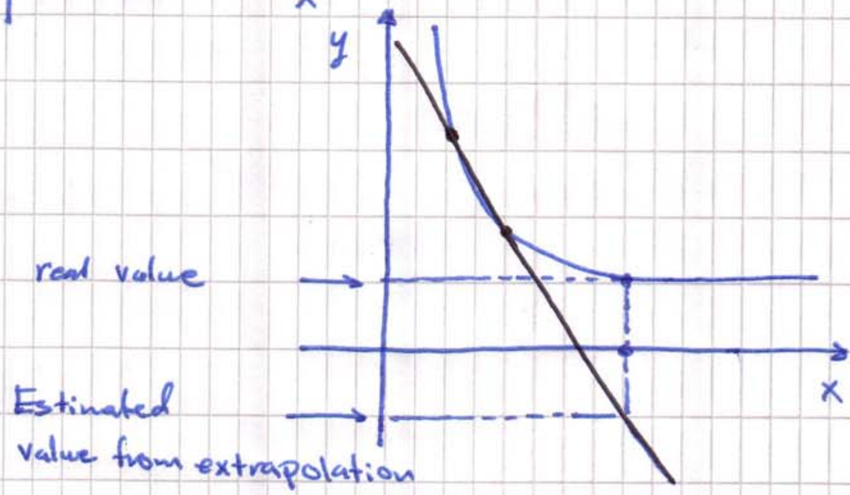
$\therefore R = 34.9$

" Interpolation "

* Remark : sometimes Linear interpolation or extrapolation is Risky and lead to incorrect estimation of data that are correlated according to highly nonlinear functions

Ex:





How to estimate data for such situations ?

perform $\boxed{\text{curve fitting}}$: Finding the best function y(x) that fit the data with small errors.

* Sometimes ; it is possible to measure process variables directly, but more often we must relate one variable to another that is easier to measure ⇒ This is called (Calibration experiment) from which we can develop one eq. relating one variable with another.

** Curve fitting :

Suppose we have data for y (dependent variable) versus x (independent variable) and we wish to derive a mathematical expression for $y(x)$.

→ The general strategy :

- ∆ plot y vs x on a normal rectangular paper (linear scale on both x and y-axes)

- ∆ If straight-line trend appears then :

$$y = ax + b$$

$$a = \text{slope} = \frac{y_2 - y_1}{x_2 - x_1}$$

$$b = \text{Intercept} = y_1 - a x_1$$

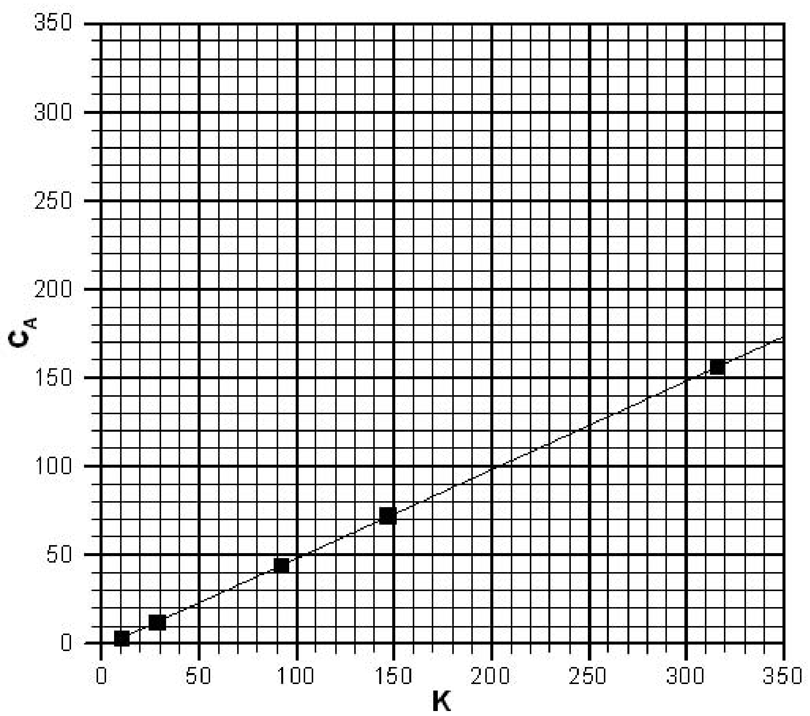
where (x_1, y_1) and (x_2, y_2) are two point that must coincide on the line.

- ∆ Else :
  - Guess a function for $y(x)$ that fit the data correctly (see function library)
  - Linearize this function : figure out what yield a straight line plot if the guess is correct
  - plot it and see if it works
  - If it works find the constants of the function

Ex: A conductivity meter is used to measure the concentration of solute, A, in an aqueous solution. Use the following experimental data to derive an expression for $C_A(K)$

K: Electrical conductivity; (μS/cm) (S = Siemen)	C_A: Solute Concentration; mg/L
10.0	3.000
28.5	12.00
92.0	44.00
147	72.00
316	156.0

plot C_A vs K ⇒ Calibration plot



∴ straight-line plot : $C_A = aK + b$

pick up two points ~~on~~ coincide on the line :

$(K_1, C_{A1}) = (50, 23)$

$(K_2, C_{A2}) = (300, 148)$

$$a = \text{slope} = \frac{C_{A2} - C_{A1}}{K_2 - K_1} = \frac{148 - 23}{300 - 50} = 0.5 .$$

$$C_A = 0.5K + b$$

To find b: $C_{A1} = 0.5K_1 + b$

$$23 = (0.5)(50) + b \Rightarrow b = -2$$

$\therefore$ $\boxed{C_A = 0.5K - 2}$

- Two aqueous solutions are drawn from two process vessels and analyzed. Their electrical conductivity are found to be $K = 200$ μs/cm and $K = 550$ μs/cm. Estimate salt concentrations in both vessels.

$$C_A(200) = (0.5)(200) - 2 = 98 \text{ mg/L}$$

$$C_A(550) = (0.5)(550) - 2 = 273 \text{ mg/L}$$

since the relationship is linear, you can get the same results using Linear interpolation for $K = 200$ and linear extrapolation for $K = 550$.

Ex: Linearize the following equations to get a straight line plot and how would you determine the constants a and b:

(a) $y = a\sqrt{x} + b$

let $t = \sqrt{x} \Rightarrow y = at + b$

$$a = \frac{y_2 - y_1}{t_2 - t_1} \quad ; \quad b = y_1 - at_1$$

$$= \frac{y_2 - y_1}{\sqrt{x_2} - \sqrt{x_1}} \quad ; \quad b = y_1 - a\sqrt{x_1}$$

(b) $y^2 = \frac{a}{x} + b$

let $z = y^2 \quad t = \frac{1}{x} \Rightarrow z = at + b$

$$a = \frac{z_2 - z_1}{t_2 - t_1} \quad ; \quad b = z_1 - at_1$$

$$= \frac{y_2^2 - y_1^2}{\frac{1}{x_2} - \frac{1}{x_1}} \quad ; \quad b = y_1^2 - a\frac{1}{x_1}$$

(c) $y = \frac{ax}{b+x}$

take the reciprocal of both sides:

$$\frac{1}{y} = \frac{b+x}{ax} = \frac{b}{a}\frac{1}{x} + \frac{1}{a}$$

let $z = \frac{1}{y} \quad t = \frac{1}{x} \Rightarrow z = \frac{b}{a}t + \frac{1}{a}$

$$\frac{b}{a} = \frac{z_2 - z_1}{t_2 - t_1} = \frac{\frac{1}{y_2} - \frac{1}{y_1}}{\frac{1}{x_2} - \frac{1}{x_1}} \quad ; \quad \frac{1}{a} = z_1 - \frac{b}{a}t_1$$

(d) $\sin y = ax + by$

Divide equation by x :

$$\frac{\sin y}{x} = a + b\frac{y}{x}$$

Let $\frac{\sin y}{x} = z \qquad t = \frac{y}{x}$

$$z = a + bt$$

$$b = \frac{z_2 - z_1}{t_2 - t_1} = \frac{\frac{\sin y_2}{x_2} - \frac{\sin y_1}{x_1}}{\frac{y_2}{x_2} - \frac{y_1}{x_1}}$$

$$a = z_1 - bt_1 = \frac{\sin y_1}{x_1} - b\frac{y_1}{x_1}$$

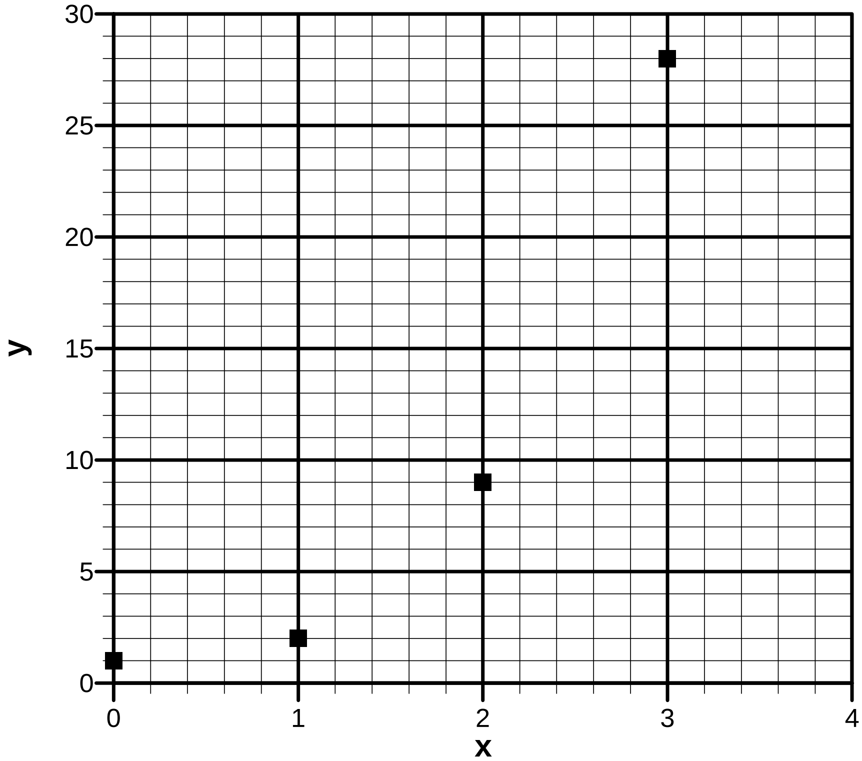
Ex: Given the following (x,y) data :

x	y
0	1
1	2
2	9
3	28

Find the best expression to relate x with y ?

$y(x) = ?$

– plot y versus x on a normal rectangular paper to see if straight line trend appears or not



∴ The trend is not linear

- Guess another function:

Let us try $y = ax^3 + b$

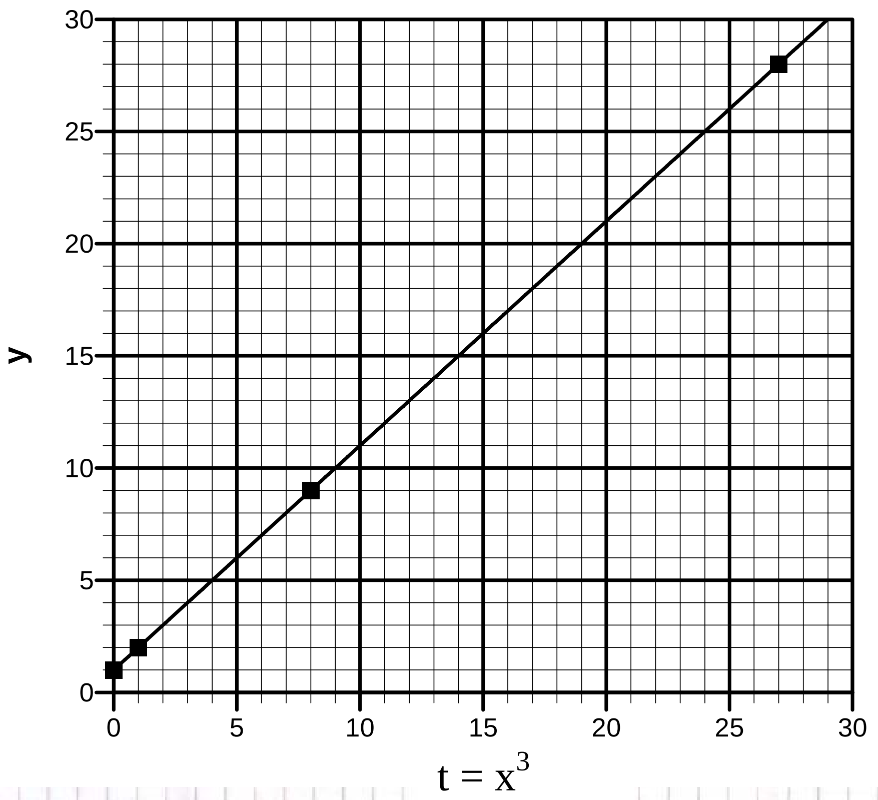
- linearize it:

let $x^3 = t \Rightarrow y = at + b$

x	y	$t = x^3$
0	1	0
1	2	1
2	9	8
3	28	27

- plot it to see if it works:

plot y versus $t = x^3$



So straight line plot $y = ax^3 + b$ work

- Determine the Constant a and b :

Choose two points that Coincide on the y vs t plot :

$(t_1, y_1) = (5, 6)$

$(t_2, y_2) = (25, 26)$

$y = at + b$

$$a = \frac{y_2 - y_1}{t_2 - t_1} = \frac{26 - 6}{25 - 5} = \frac{20}{20} = 1$$

$y = at + b = t + b$

$b = y_1 - t_1 = 6 - 5 = 1$

$\therefore \; y = t + 1 = x^3 + 1$

: Check the validity of expression by trying some data points

$y(0) = 1$ ✓

$y(2) = 8$ ✓

$y(3) = 28$ ✓

** Focusing on exponential and power law functions :

It is found that chemical process variables are often related with expressions of the form:

$y = a e^{bx}$ " Exponential functions "

$y = a x^{b}$ " Power law functions "

* Exponential functions :

How to linerize : $y = a e^{bx}$ $e = 2.71828$

take ln of both sides : $\ln y = \ln a + b x$

let $z = \ln y$

$\Rightarrow z = \underbrace{\ln a}_{\text{Intercept}} + \underbrace{b}_{\text{slope}} x$

plot $z = \ln y$ vs x to find a and b

x	y	$z = \ln y$
⋮	⋮	⋮

Note that $z = \ln y$ must be plot against x on normal rectangular paper.

* use of logarithmic scale (log-scale) to avoid generating $\ln y$ data column:

$$y = a e^{bx}$$

$$\ln y = \ln a + bx$$

we can transform $\ln y$ to $\log y$ using:

$$\log y = \frac{\ln y}{\ln 10}$$

$$\boxed{\ln 10 = 2.3025}$$

or $\ln y = \ln 10 \log y$

and $\ln a = \ln 10 \log a$

Thus $\ln 10 \log y = \ln 10 \log a + bx$

Dividing by $\ln 10$ gives:

$$\log y = \log a + \frac{b}{\ln 10} x$$

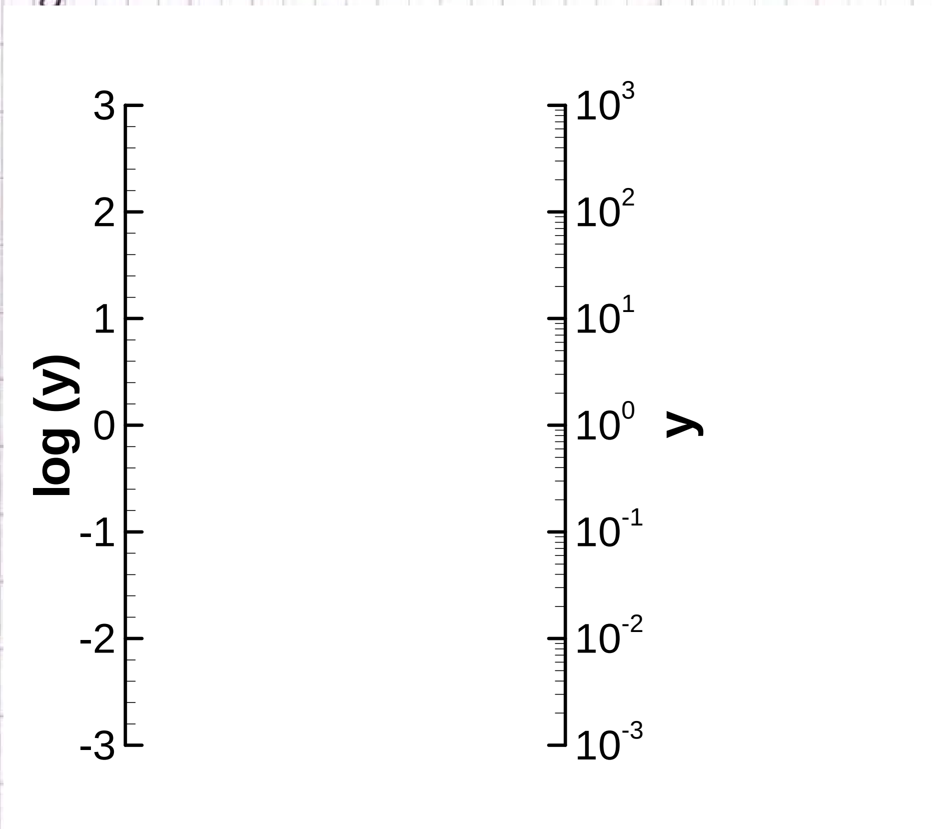
If $\log y$ is plotted on linear uniform scale against x on a linear uniform scale, then

$$\text{slope} = \frac{\log y_2 - \log y_1}{x_2 - x_1} = \frac{\log(y_2/y_1)}{x_2 - x_1} = \frac{b}{\ln 10}$$

$b = (\ln 10)(\text{slope value})$

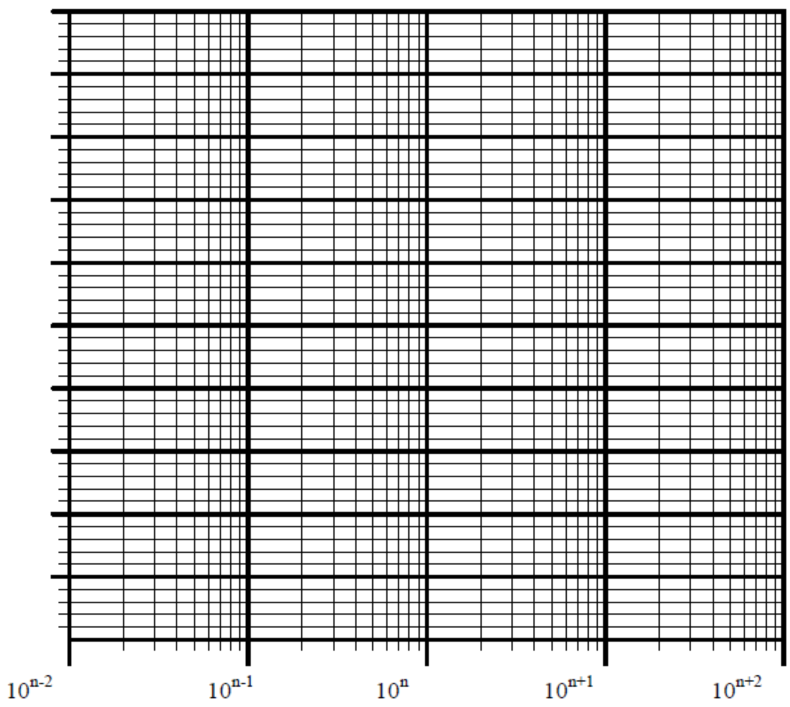
$$\text{Intercept} = \log y_1 - \frac{b}{\ln 10} x_1 = \log a \Rightarrow a = 10^{(\text{Intercept value})}$$

* How log-scale is built?



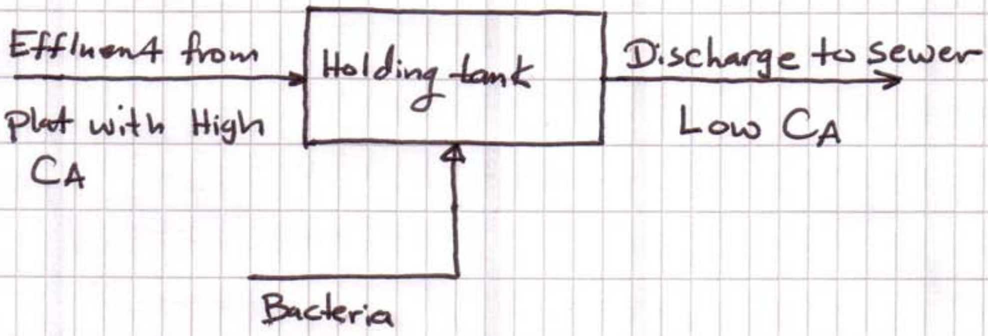
Thus, and to avoid generating log y data column, now, you can plot y (without taking log) on log scale and x on linear scale to fit exponential function

Semilog paper



Where **n** is an integer; its value depends on the range of the data

Ex: A toxic waste product from a chemical process, A, is treated in a holding tank with a bacterial agent that causes it to decompose:

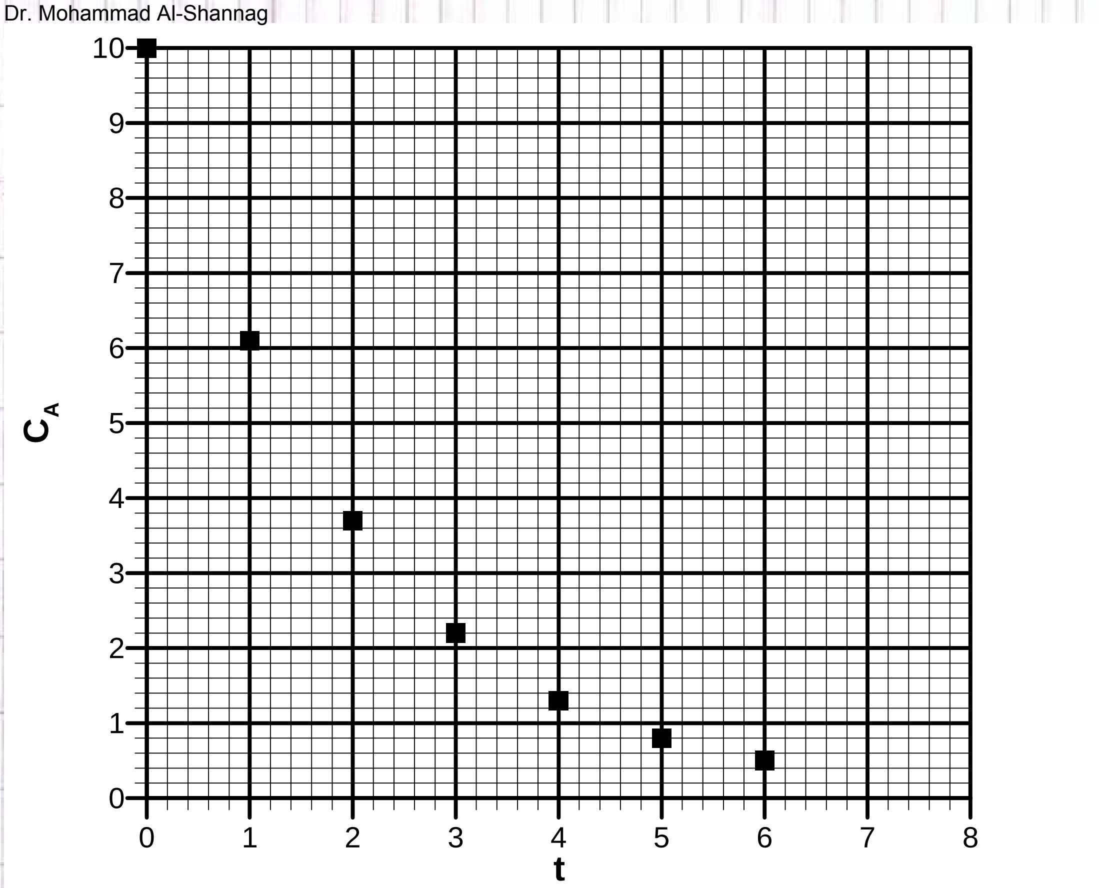


samples are frequently drawn from the reactor and analyzed for C_A leading to the following experimental data:

t(min)	C_A; mol A/L
0	10.0
1	6.20
3	2.20
4	1.30
5	0.80
6	0.50

we want to determine an expression for $C_A(t)$ so we can determine the holding time required for C_A to fall below its safe value of 0.001 mol/L.

- plot C_A versus t to explore the trend:



As can be shown in the above figure, the data are not correlated in a linear manner. However, the curve looks like an exponential decay; so let us try:

$$C_A = a\,e^{bt}$$ (the value of b must be negative since C_A decreases with t)

- Linearize the selected function:

$$\ln C_A = \ln a + bt$$

$$\ln 10 \log C_A = \ln 10 \log a + bt$$

and $$\log C_A = \log a + \frac{b}{\ln 10}\,t$$

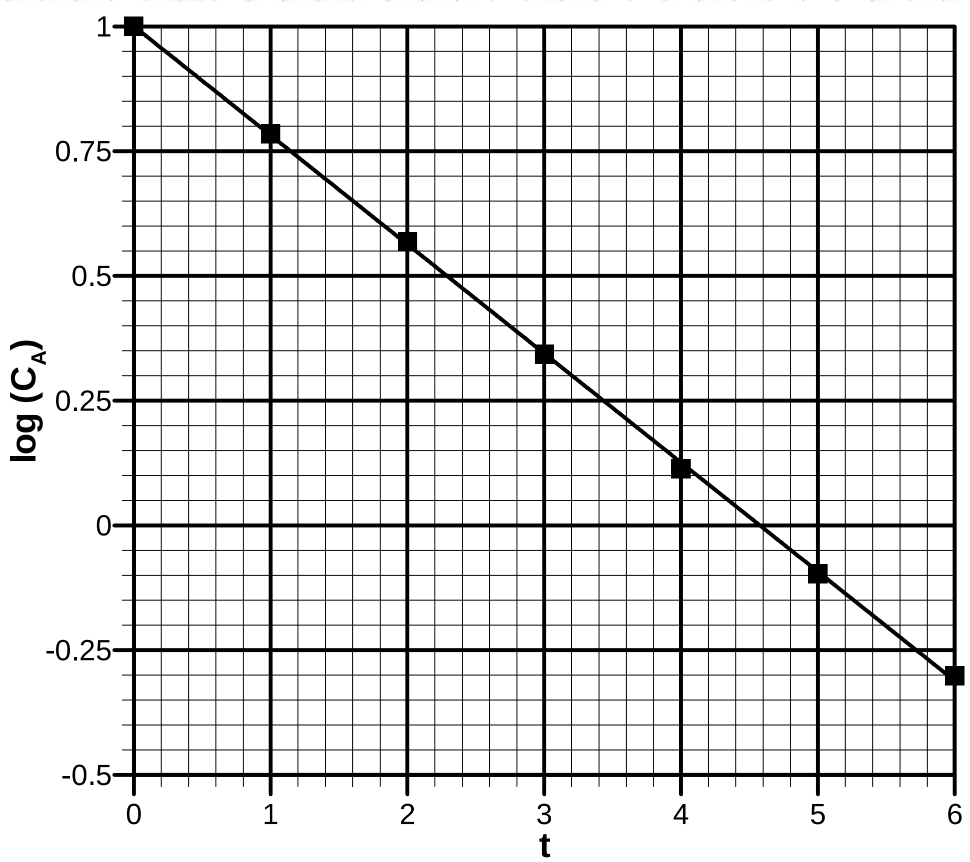
- use either rectangular uniform paper or semi-log paper to see if the selected function works:

* Rectangular paper plot :

plot $\log C_A$ on a linear scale versus t on a linear scale :

we need to generate $\log C_A$ column

t, min	C_A, mol/L	$\log C_A$
0	10.0	1
1	6.20	0.7924
3	2.20	0.3424
4	1.30	0.1134
5	0.80	−0.0969
6	0.50	−0.3010



Note that the plot is linear ⇒ $C_A = a\,e^{bt}$ is Correct choice

Pick up two points that coincide on the line:

$(t_1, \log C_{A1}) = (0, 1)$

$(t_2, \log C_{A2}) = (4.6, 0)$

$$\text{slope} = \frac{b}{\ln 10} = \frac{\log C_{A2} - \log C_{A1}}{t_2 - t_1} = \frac{\log(C_{A2}/C_{A1})}{t_2 - t_1}$$

$$= \frac{0-1}{4.6-0} = \frac{-1}{4.6}$$

$$\Rightarrow \boxed{b = -0.501}$$ -ve value obtained as expected

$$\text{Intercept} = \log a = \log C_{A_1} - \frac{b}{\ln 10} t_1$$

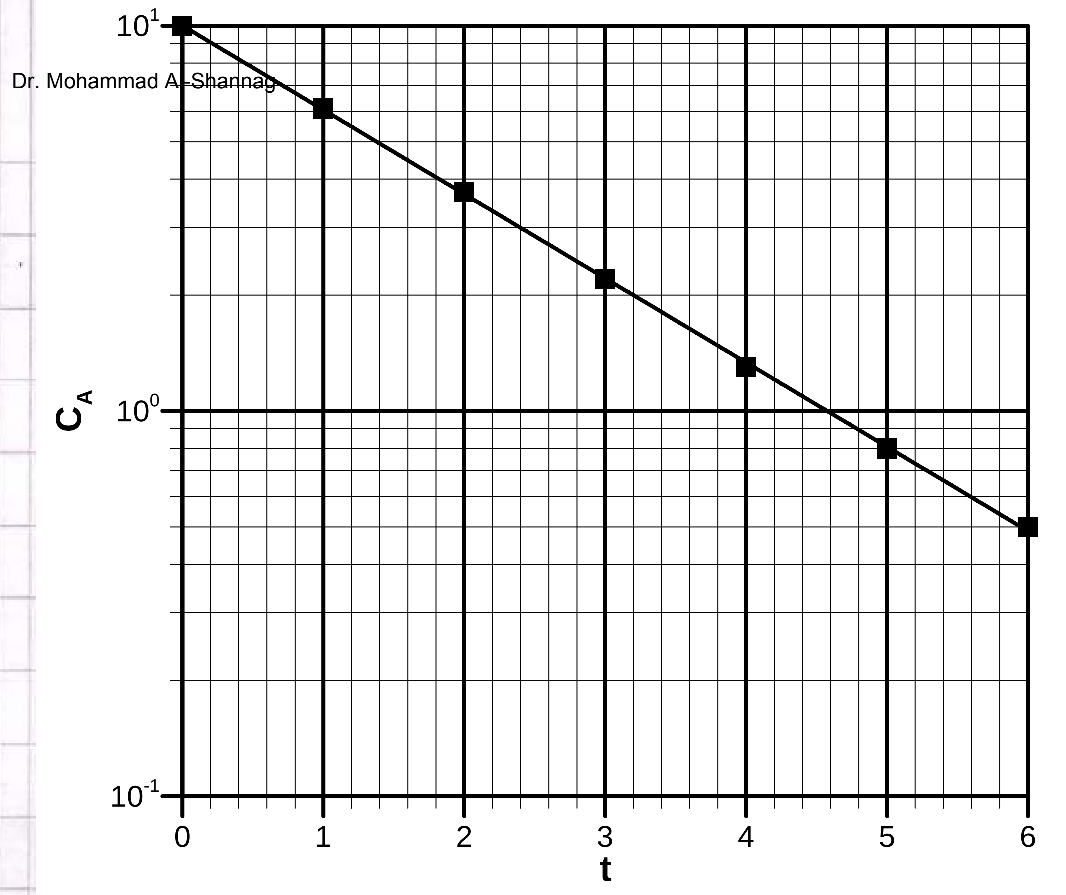
$$= 1 - \frac{-0.501}{\ln 10}(0) = 1$$

$$\Rightarrow a = 10^1 = 10 \qquad \boxed{a = 10}$$

$$\therefore \boxed{C_A = 10\, e^{-0.501t}}$$

* or we can use semi-log paper without the need of Calculating $\log C_A$ data column:

on a semi-log paper plot C_A on log-scale versus t on linear scale:



as shown in the figure a linear plot is obtained which indicates that the exponential function works well.

To find the constants a and b pick up two points that coincide on the line:

$$(t_1, C_{A1}) = (2.4, 3)$$
$$(t_2, C_{A2}) = (5.6, 0.6)$$

$$\text{slope} = \frac{\log C_{A2} - \log C_{A1}}{t_2 - t_1} = \frac{\log(C_{A2}/C_{A1})}{t_2 - t_1}$$

$$= \frac{\log(0.6/3)}{5.6 - 2.4} = \frac{b}{\ln 10}$$

$$\Rightarrow \boxed{b = -0.503}$$

$$\text{Intercept} = \log a = \log C_{A1} - \frac{b}{\ln 10} t_1 = \log 3 - \frac{-0.503}{\ln 10} = 1.0$$

$$\Rightarrow a = 10^1 = 10$$

$$\therefore C_A = 10\, e^{-0.503 t}$$

Now let us answer the second part of this example:
How long will it take for C_A to drop to 0.001 mol/L

$$C_A = 10\, e^{-0.501 t}$$

$$0.001 = 10\, e^{-0.501 t}$$

$$\ln(0.001) = \ln 10 - 0.501 t$$

$$\Rightarrow \quad t = \frac{\ln(10/0.001)}{0.502}$$

$$= 18.3 \text{ min}$$

Try to use linear extrapolation to find t at $C_A = 0.001$ without this nonlinear curve fitting:

t	C_A
$t_2 = 5$	$0.8 = C_{A2}$
$t_1 = 6$	$0.5 = C_{A1}$
$t = ?$	$0.001 = C_A$

$$\frac{t_2 - t_1}{C_{A2} - C_{A1}} = \frac{t - t_1}{C_A - C_{A1}}$$

$$\frac{5-6}{0.8-0.5} = \frac{t-6}{0.001-0.5}$$

$$\Rightarrow \quad t = 7.66 \text{ min}$$

as you see Large difference between two methods.
so if you use linear extrapolation the C_A will not reach safe value.

Conclusion: Extrapolation / Interpolation sometimes is risky.

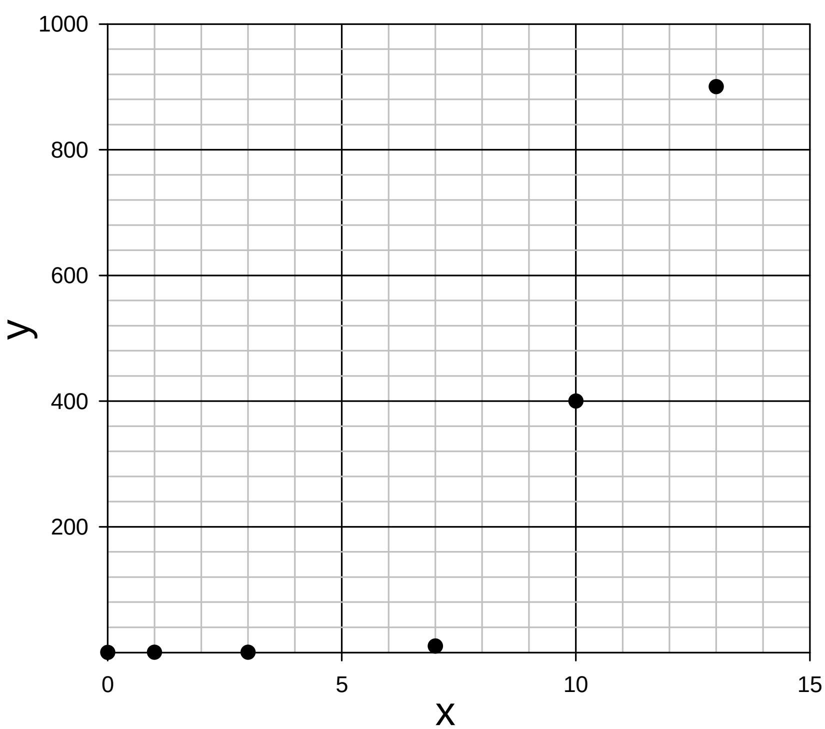
* Another advantage of Log scale :

* When variations in x or y values in some field are much greater than another field within the data ranges, log scale represents these variations in a manner much better than normal scale.

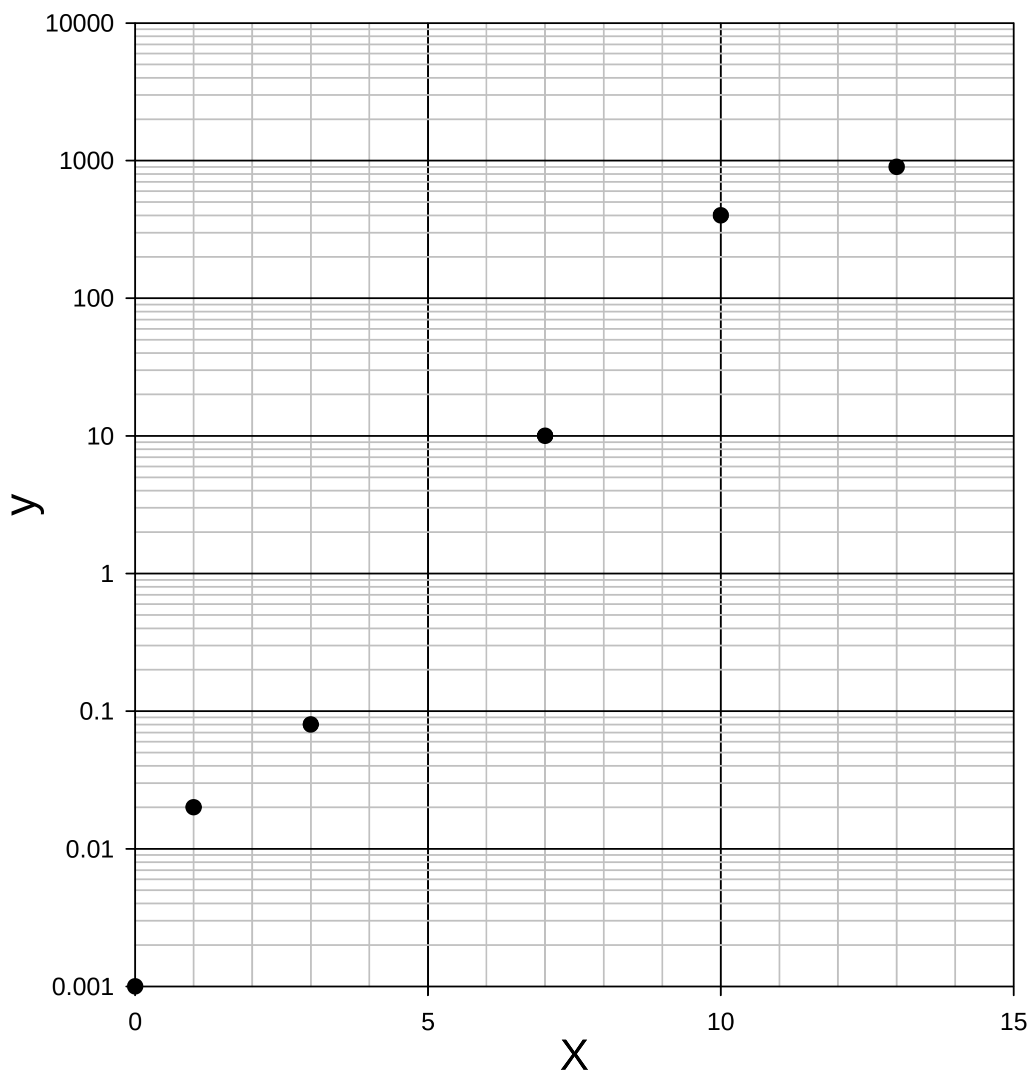
Ex: represent on a graph the variation of y with x for the following data:

x	y
0	0.001
1	0.02
3	0.08
7	10.0
10	400
13	900

Graph on rectangular paper:



Since variation at the begining of y range is much smaller than that at the end of y range it is better to use log scale for y and keep normal scale for x since variations in x values are not so large:



* power law functions:

$$y = a x^b$$

To Linearize take log of both sides:

$$\log y = \log a + b \log x$$

$$\Rightarrow \text{slope} = b = \frac{\log y_2 - \log y_1}{\log x_2 - \log x_1} = \frac{\log(y_2/y_1)}{\log(x_2/x_1)}$$

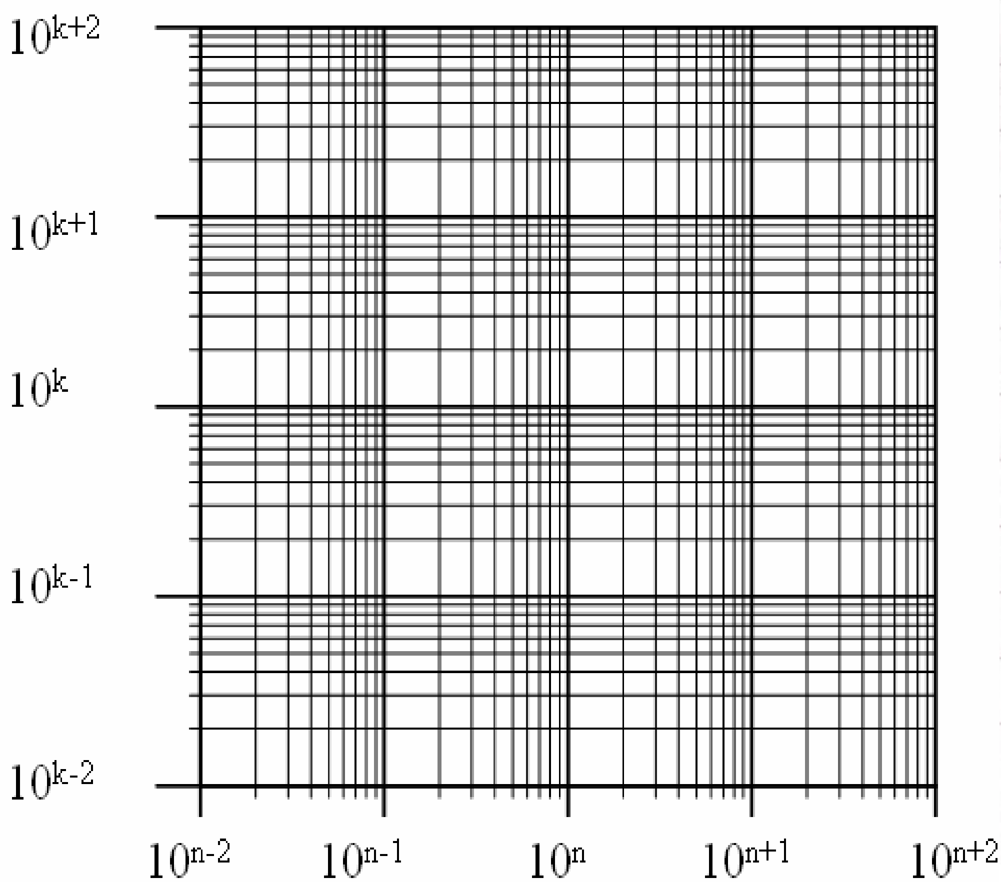
$$\text{Intercept} = \log a = \log y_1 - b \log x_1$$

$\Rightarrow$ To find the slope and intercept:

Δ plot: $\log y$ versus $\log x$ on rectangular paper

or Δ plot: y versus x on log-log paper:

log-log paper



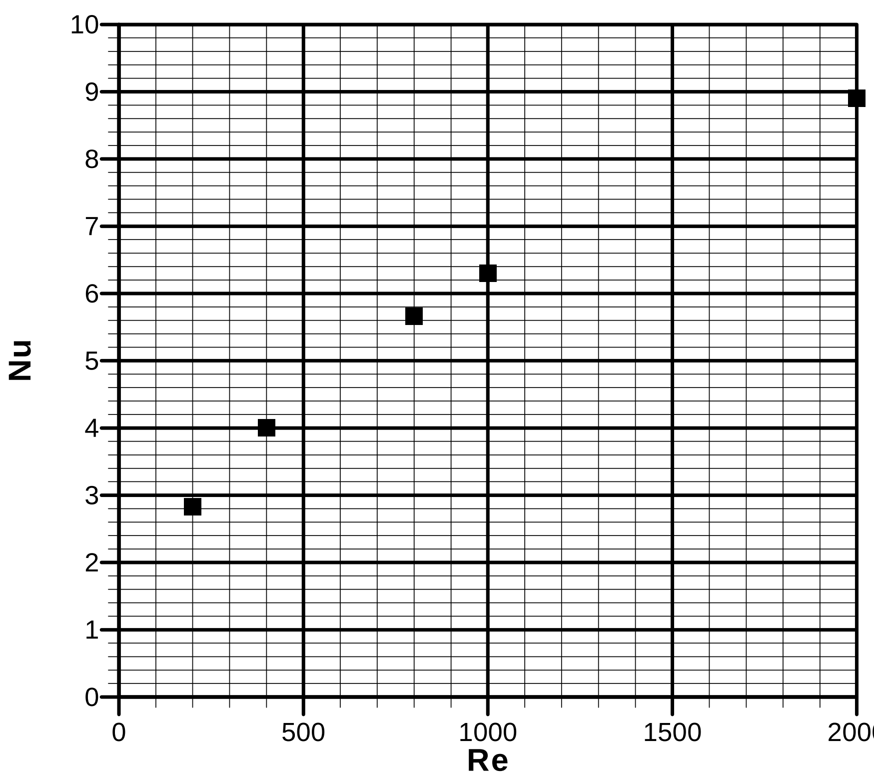
Where **n** and **j** are integers; their values depends on the range of the data

Ex : It is found from some measurements that Nusselt number varies with Reynolds number according to the following data :

Reynolds number; Re	Nusselt number, Nu
200	2.83
400	4.00
800	5.66
1000	6.30
2000	8.90

Derive an expression for Nu(Re)

⇒ plot Nu versus Re to explore suitable function:



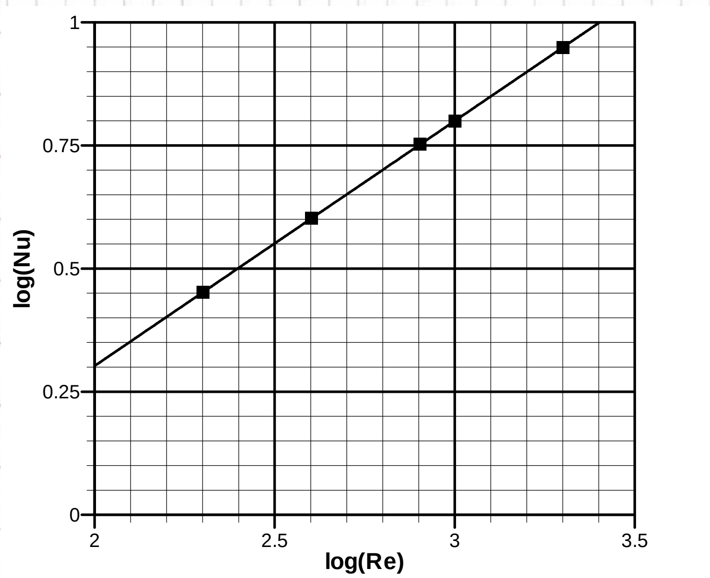
It is Not linear trend ; it looks like power law function let us try power law function:

$$Nu = a\ Re^{b}$$

Linearize $\Rightarrow$ $\log Nu = \log a + b \log Re$

To see if power law relation works well; plot $\log Nu$ vs. $\log Re$ on rectangular paper or Nu vs Re on log-log paper:

* Rectangular paper:



it gives linear plot $\Rightarrow$ $Nu = a Re^{b}$ works well

pick up two points that coincide on the line:

$(\log Re_1, \log Nu_1) = (2.4, 0.5)$

$(\log Re_2, \log Nu_2) = (3.1, 0.85)$

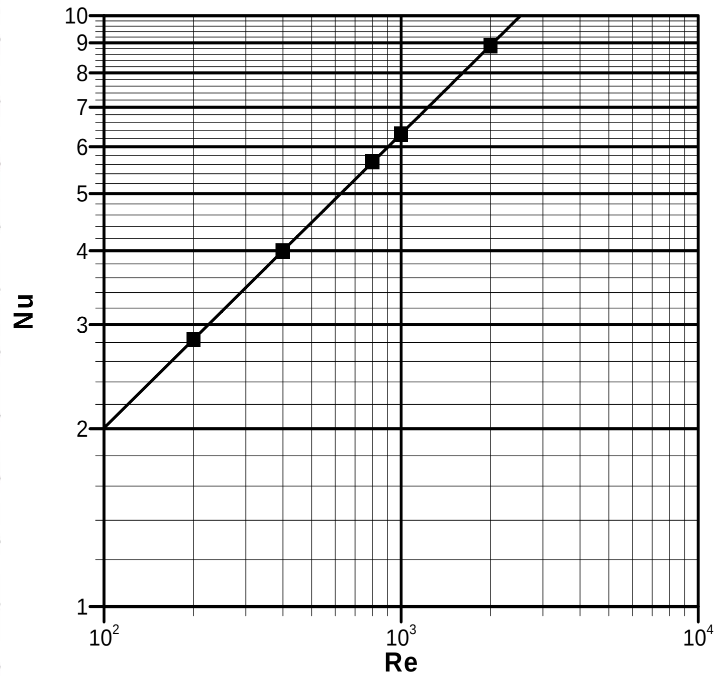
$$\text{slope} = b = \frac{\log Nu_2 - \log Nu_1}{\log Re_2 - \log Re_1} = \frac{0.85 - 0.5}{3.1 - 2.4} = 0.5$$

$$\text{Intercept} = \log a = \log Nu_1 - b \log Re_1 = 0.5 - (0.5)(2.4) = -0.7$$

$\Rightarrow a = 10^{-0.7} = 0.2$

$$\Rightarrow \boxed{Nu = 0.2\ Re^{0.5}}$$

* log-log paper:



It gives linear plot $\Rightarrow$ power law relation works well

Pick up two points that coincide on the line

$(Re_1, Nu_1) = (100, 2) \qquad (Re_2, Nu_2) = (400, 4)$

$$\text{slope} = b = \frac{\log Nu_2 - \log Nu_1}{\log Re_2 - \log Re_1} = \frac{\log(Nu_2 / Nu_1)}{\log(Re_2 / Re_1)} = \frac{\log(4/2)}{\log(400/100)}$$

$$= \frac{\log 2}{\log 4} = 0.5$$

$$\text{Intercept} = \log a = \log Nu_1 - b \log Re_1 = \log 2 - (0.5)\log 100$$

$$= -0.69897 \Rightarrow a = 10^{-0.69897} = 0.2$$

$$\Rightarrow \boxed{Nu = 0.2\ Re^{0.5}}$$

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* Remark : when you use log scale do NOT tak the log of the data Correspons to that scale:
Remember that plotting log(value) on normal scale is equivalent to plotting value on log scale.

Ex: A plot of F versus t yields a line that passes through the two points : $(t_1, F_1) = (15, 0.298)$ and $(t_2, F_2) = (30, 0.0527)$ on :
(a) semilog paper (b) log-log paper.

for each case calculate the eq. that relates F and t:

(a) semilog paper ⇒ log F or ln F vs t give the linear plot ⇒

$$F = a e^{bt}$$

$$\ln F = \ln a + bt$$

$$b = \text{slope} = \frac{\ln F_2 - \ln F_1}{t_2 - t_1} = \frac{\ln(F_2/F_1)}{t_2 - t_1} = \frac{\ln(0.0527/0.298)}{30 - 15}$$

$$\boxed{b = -0.1155}$$

$$\text{Intercept} = \ln a = \ln F_1 - b t_1 = \ln 0.298 - (-0.1155)(15)$$

$$= 0.52184$$

$$\Rightarrow a = e^{0.52184} = 1.685$$

So The equation is :

$$\boxed{F = 1.685\, e^{-0.1155t}}$$

(b) log-log paper $\Rightarrow$ $\log F$ versus $\log t$ is linear

$\Rightarrow$ Power law: $F = a\,t^{b}$

$$\log F = \log a + b \log t$$

$$b = \frac{\log F_2 - \log F_1}{\log t_2 - \log t_1} = \frac{\log(F_2/F_1)}{\log(t_2/t_1)}$$

$$= \frac{\log(0.0527/0.298)}{\log(30/15)}$$

$$= -2.5$$

$$\log a = \log F_1 - b \log t_1 = \log 0.298 - (-2.5)\log(15)$$

$$= 2.41444 \quad \Rightarrow \quad a = 10^{2.41444} = 259.7$$

$\therefore$ The relation is: $F = 259.7\ t^{-2.5}$