Math Tools

Tools of the Trade

Equations for Early IPOL 8512 Calculations

$$\text{Surface area of sphere} = 4\pi r^2 = 4\pi (d/2)^2 = \pi d^2$$

$$\text{volume of a sphere} = \frac{4}{3}\pi r^3$$

$$\text{circumference} = \pi \bullet \text{diameter} \quad \text{or} \quad c = \pi d$$

$$\text{volume of a regular solid} = \text{area of the base} \times \text{height}$$

$$V = A \times h$$

$$V_{cyl} = A_{base} \times h = \pi r^2 \times h = \pi \left(\frac{d}{2}\right)^2 \times h = \frac{\pi d^2 h}{4}$$

$$\text{time} = \frac{\text{quantity of resource}}{\text{rate of consumption}}$$

$$\text{flow in} = \text{flow out} = \frac{\text{stock}}{\text{residence time}} = F_{in} = F_{out} = \frac{M}{T}$$

Other Equations

Area of square = (length of side)^2

Circumference of circle of radius r = $2\pi r$

Area circle of radius r = πr^2

Area triangle = ½(base × height)

Surface area cube = 6(length side)^2

Volume cube = (length side)^3

$a^x \bullet a^y = a^{x+y}$

$a^x \div a^y = a^{x-y}$

$(a^x)^y = a^{x \bullet y}$

$$a^{-b} = \frac{1}{a^b}$$

Ideal Gas Equation Derivation

$P \propto n$ if T and V are constant

$P \propto T$ if n and V are constant

$P \propto \frac{1}{V}$ if n and T are constant

or $P \propto \frac{nT}{V}$

so $P =$ (a constant) $\frac{nT}{V}$

$\boldsymbol{PV = nRT}$ $\quad \frac{0.082058 \text{ L} \bullet \text{atm}}{\text{K} \bullet \text{mol}}$ or $\frac{8.3145 \text{ L} \bullet \text{kPa}}{\text{K} \bullet \text{mol}}$

Standard Temperature and Pressure

- **Standard Temperature and Pressure (STP)** = the standard sets of conditions for experimental measurements established to allow comparisons to be made between different sets of data. (There are no universally accepted standards.)
  - International Union of Pure and Applied Chemistry (IUPAC) uses 273.15 K (0 °C, 32 °F) and 100 kPa (14.504 psi, 0.986 atm, 1 bar)
  - An unofficial, but commonly used standard is **standard ambient temperature and pressure** (**SATP**) of 298.15 K (25 °C, 77 °F) and 100 kPa (14.504 psi, 0.986 atm). This is the most useful set of values for us.
  - National Institute of Standards and Technology (NIST) uses 20 °C (293.15 K, 68 °F) and 101.325 kPa (14.696 psi, 1 atm)

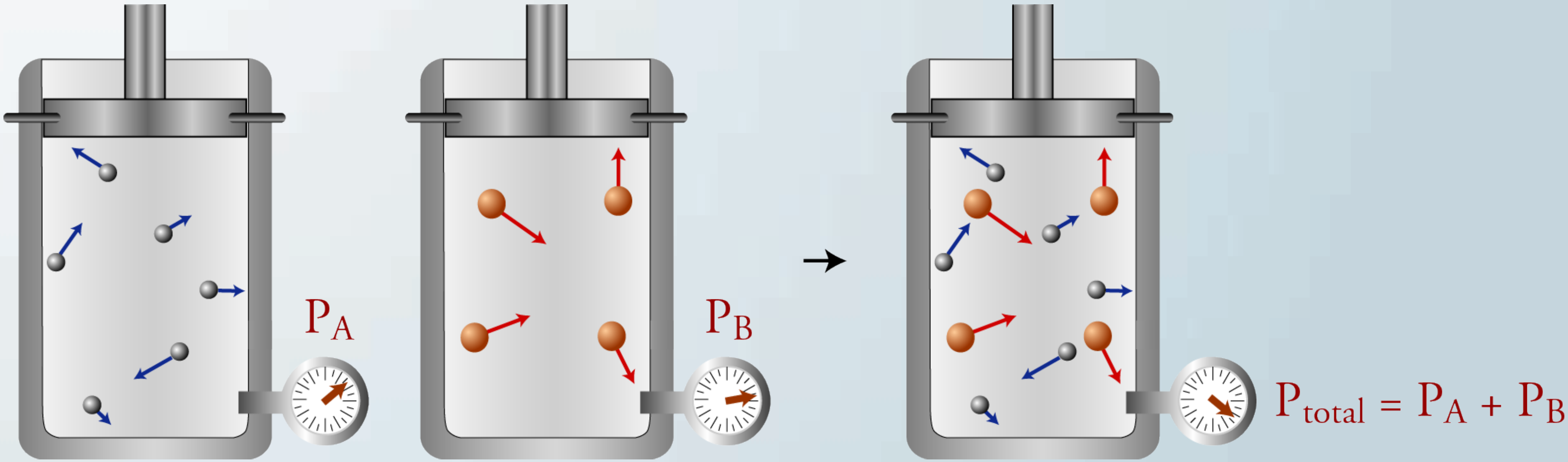
Molar Volume at SATP

- You will find the following derived conversion factor useful for converting between volume and moles of gas.

$$PV = nRT$$

$$\frac{V}{n} = \frac{RT}{P} = \frac{\left(\frac{8.3145\ \text{L} \cdot \cancel{\text{kPa}}}{\cancel{\text{K}} \cdot \text{mol}}\right)(298.15\ \cancel{\text{K}})}{100\ \cancel{\text{kPa}}} = \left(\frac{24.790\ \text{L}}{1\ \text{mol}}\right)_{\text{SATP}}$$

Dalton's Law of Partial Pressures



$$P_{\text{total}} = \Sigma P_{\text{partial}} \quad \text{or} \quad P_{\text{total}} = (\Sigma n_{\text{each gas}})\frac{RT}{V}$$

Partial Pressures and Constant T and P

$$V_A = n_A \frac{RT_A}{P_A} \qquad V_t = n_t \frac{RT_t}{P_t}$$

$$\frac{V_A}{V_t} = \frac{n_A \dfrac{RT_A}{P_A}}{n_t \dfrac{RT_t}{P_t}}$$

for gases at the same T and P

$$\frac{V_A}{V_t} = \frac{n_A \dfrac{RT}{P}}{n_t \dfrac{RT}{P}} = \frac{n_A}{n_t}$$

Partial Pressures and Constant T and V

$$P_A = n_A \frac{RT_A}{V_A} \qquad P_t = n_t \frac{RT_t}{V_t}$$

$$\frac{P_A}{P_t} = \frac{n_A \frac{RT_A}{V_A}}{n_t \frac{RT_t}{V_t}}$$

for gases at the same T and V

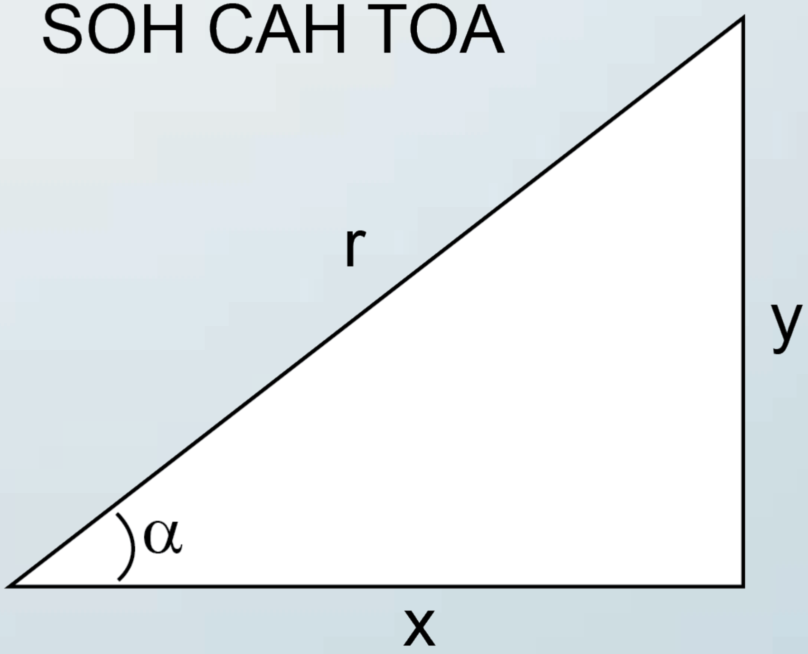
$$\frac{P_A}{P_t} = \frac{n_A \frac{RT}{V}}{n_t \frac{RT}{V}} = \frac{n_A}{n_t} = \text{mole fraction} = X_A$$

$$P_A = X_A P_t$$

A Little Trig Stuff

- One of the following relationships and your calculator will help you to do one of the homework problems.

SOH CAH TOA



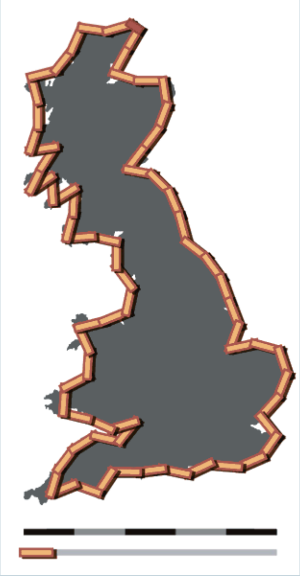
$$\sin \alpha = \frac{\text{opposite}}{\text{hypotenuse}} = \frac{y}{r}$$

$$\cos \alpha = \frac{\text{adjacent}}{\text{hypotenuse}} = \frac{x}{r}$$

$$\tan \alpha = \frac{\text{opposite}}{\text{adjacent}} = \frac{y}{x}$$

Fractal Units and Lengths of Uneven Surfaces

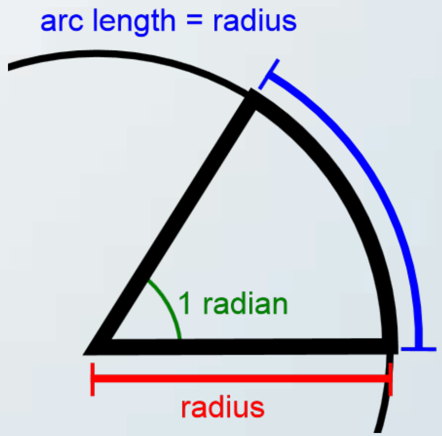
- If the coastline of Britain is measured using the fractal unit of 200 km, then the value derived for the length of the coastline is 2400 km (approx.).



- If we use the fractal unit of 50 km, the value derived for the length of the coastline is 3400 km (1000 km more).

Angles - Radians and Degrees

- A radian is the ratio between the length of an arc and its radius. It is normally described in terms of pi (π) and as a unitless quantity.



- A complete circle has an arc length of $2\pi r$ (its circumference), so a complete circle is 2π radians.

$$\text{Radian} = \frac{\text{length of arc}}{\text{radius}} = \frac{2\Pi r}{r} = 2\Pi$$

- A complete circle is 360°, 360° is 2π radians, leading to the following conversion factor.

$$\frac{360^o}{2\Pi} = \frac{180^o}{\Pi}$$

Linear Equation

- A common form of a linear equation in the two variables x and y is

  y = mx + b

  y = (slope)x + (y-intercept)

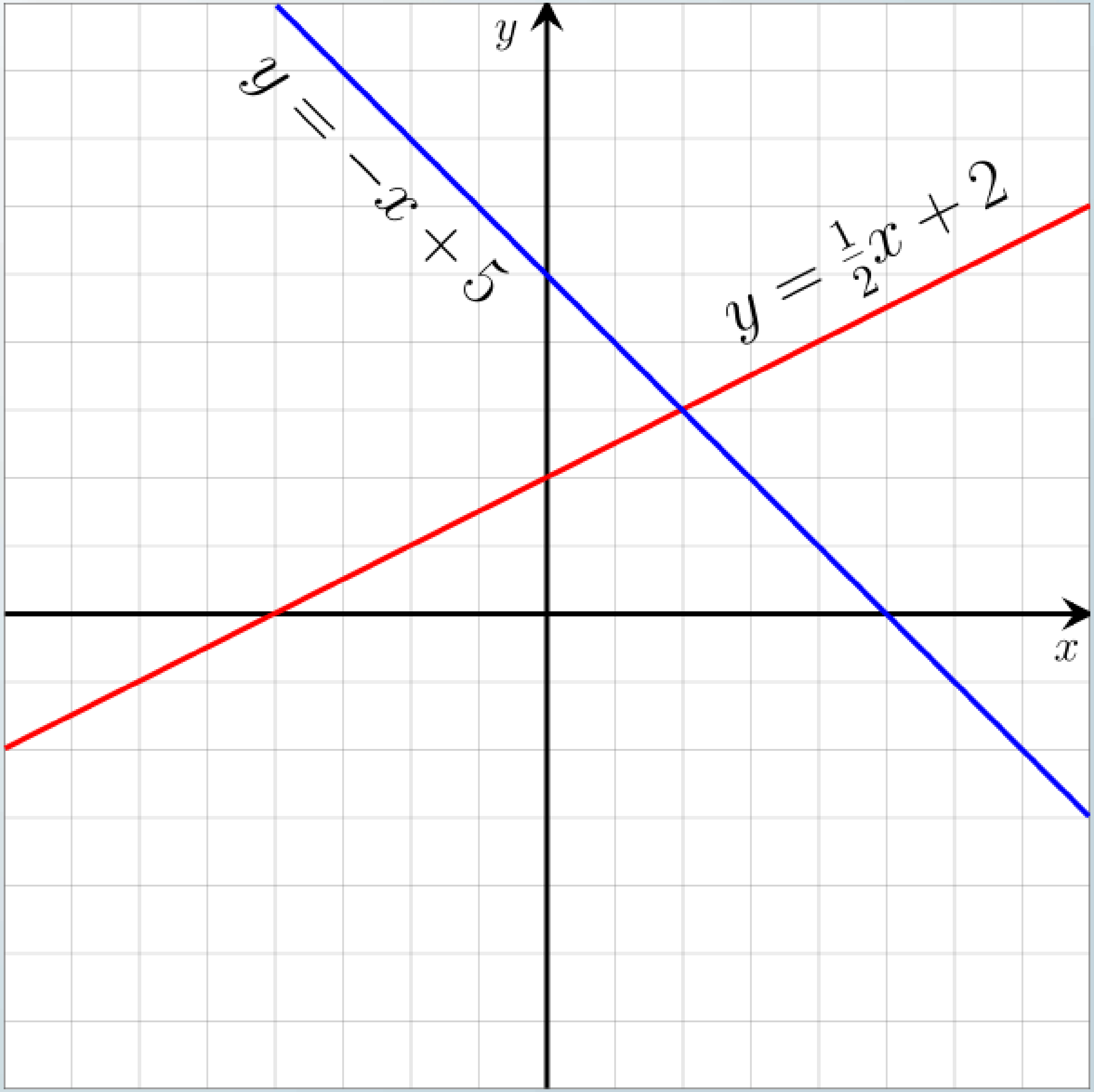
- The origin of the name "linear" comes from the fact that the set of solutions of such an equation forms a straight line in the plane.

  m = slope = $\Delta y/\Delta x$,

  b = y-intercept

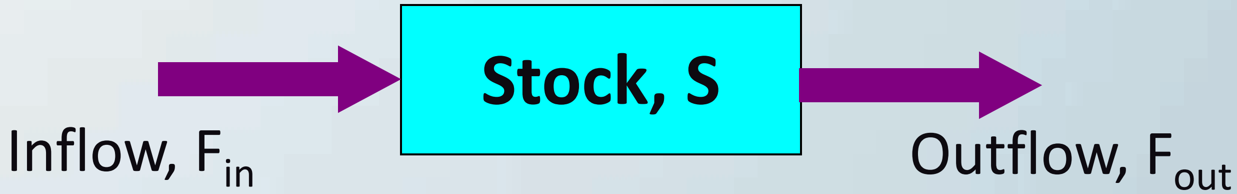
  = the point at which the line crosses the y-axis.

Linear Equation Examples



Box Models

- We make a simple model of a system by representing the reservoirs with a "box" and the transport/transformation with arrows.
- We usually assume the box is well-mixed, and we usually are not concerned with internal details.



- *Stock* = the amount of stuff (matter, energy, electric charge, chemical species, organisms, pollutants, etc.) in the reservoir
- *Flows* = the amount of stuff flowing into and out of the reservoir as a function of time

Why Use Box Models?

To understand or predict:

- Concentrations of pollutants in various environmental reservoirs as a function of time: e.g. water pollution, outdoor/ indoor air pollution
- Concentrations of toxic substance in organs after inhalation or ingestion; setting standards for toxic exposure or intake
- Population dynamics, predator-prey and food-chain models, fisheries, wildlife management
- Biogeochemical cycles and climate dynamics (nutrients, energy, air, trace gases, water)

How Box Models Work

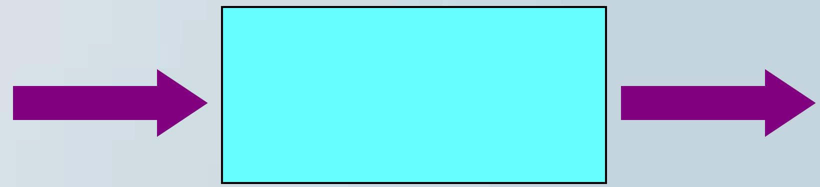
Basic rule of box models:

change in stock over time = inflow – outflow

$\Delta S/\Delta t = F_{in} - F_{out}$

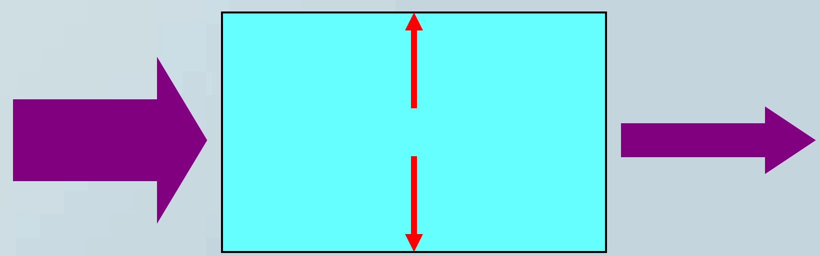
Situation 1: Equilibrium

$F_{in} = F_{out}$ $\Delta S/\Delta t = 0$

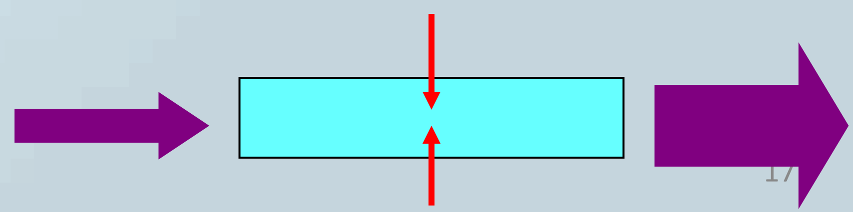


Situation 2: Non-equilibrium

$F_{in} > F_{out}$ $\Delta S/\Delta t > 0$



$F_{in} < F_{out}$ $\Delta S/\Delta t < 0$



Steady-State Calculations

$$\text{Flow in} = F_{in} = \frac{\text{amount into system}}{\text{time}}$$

$$\text{Flow out} = F_{out} = \frac{\text{amount out of system}}{\text{time}}$$

$$\text{Stock} = M$$

$$\text{Residence time} = T$$

$$F_{in} = F_{out} = \frac{M}{T}$$

Two Ways to Do Steady-State Calculations

What is the residence time in days of H_2O in Earth's atmosphere?

- Equation-based
- Unit Analysis

From COW appendix,

- the precipitation rate is 5.18×10^{14} m^3/yr.
- the amount of water in the atmosphere is 1.3×10^{13} m^3.

Steady-State Calculations

That is the residence time of H_2O in Earth's atmosphere?

$$F_w = \frac{M_w}{T_w}$$

$$T_w = \frac{M_w}{F_w} = \frac{1.3 \times 10^{13}\ \mathrm{m}^3}{5.18 \times 10^{14}\ \mathrm{m}^3/\mathrm{yr}} = \mathbf{0.025\ yr}\left(\frac{365\ \mathrm{day}}{1\ \mathrm{yr}}\right) = \mathbf{9.1\ days}$$

or

$$?\ \mathrm{day} = 1.3 \times 10^{13}\ \cancel{\mathrm{m}^3}\left(\frac{1\ \cancel{\mathrm{yr}}}{5.18 \times 10^{14}\ \cancel{\mathrm{m}^3}}\right)\left(\frac{365\ \mathrm{day}}{1\ \cancel{\mathrm{yr}}}\right) = \mathbf{9.1\ days}$$

Box Models for Different Situations

- What is the basic math behind box models?
- What kinds of box model are frequently used in environmental science?
- How can the following situations be analyzed mathematically with box models?
  - population growth
  - radioactive decay
  - greenhouse gas emissions
  - depletion of oil stocks
  - pollution building up in a lake

General Solution to Box Models

1. Draw box model, label stocks and flows
2. Set up differential equation for each box expressing the rate of change of the stock

$$\frac{dS}{dt} = F_{in} - F_{out}$$

3. Solve for S(t) by integrating the differential equation, or in lieu of integrating, use the pre-integrated solutions given in class for S(t). The trick here is to recognize which type of box model calls for which type of solution.

Equations for Different Situations

- Steady State

$$S(t) = S_0$$

- F_{in} - F_{out} = constant

$$S(t) = S_0 + \Delta Ft$$

- Exponential Growth of Stocks

$$S(t) = S_0 e^{rt}$$

- Exponential decline (decay) of Stocks

$$S(t) = S_0 e^{-rt}$$

Equations for Different Situations

- One flow constant and the other proportional to stock (e.g. constant inflow, and an outflow proportional to stock)

$$S(t) = \frac{(rS_0 - F_0)}{r} e^{-rt} + \frac{F_0}{r}$$

- Exponential increase in inflow

$$S(t) = S_0 + \frac{F_0}{r}(e^{rt} - 1)$$

- Exponential increase in outflow

$$S(t) = S_0 - \frac{F_0}{r}(e^{rt} - 1)$$

Case A: Stock is in Steady State

$F_{in} = F_{out} = F$

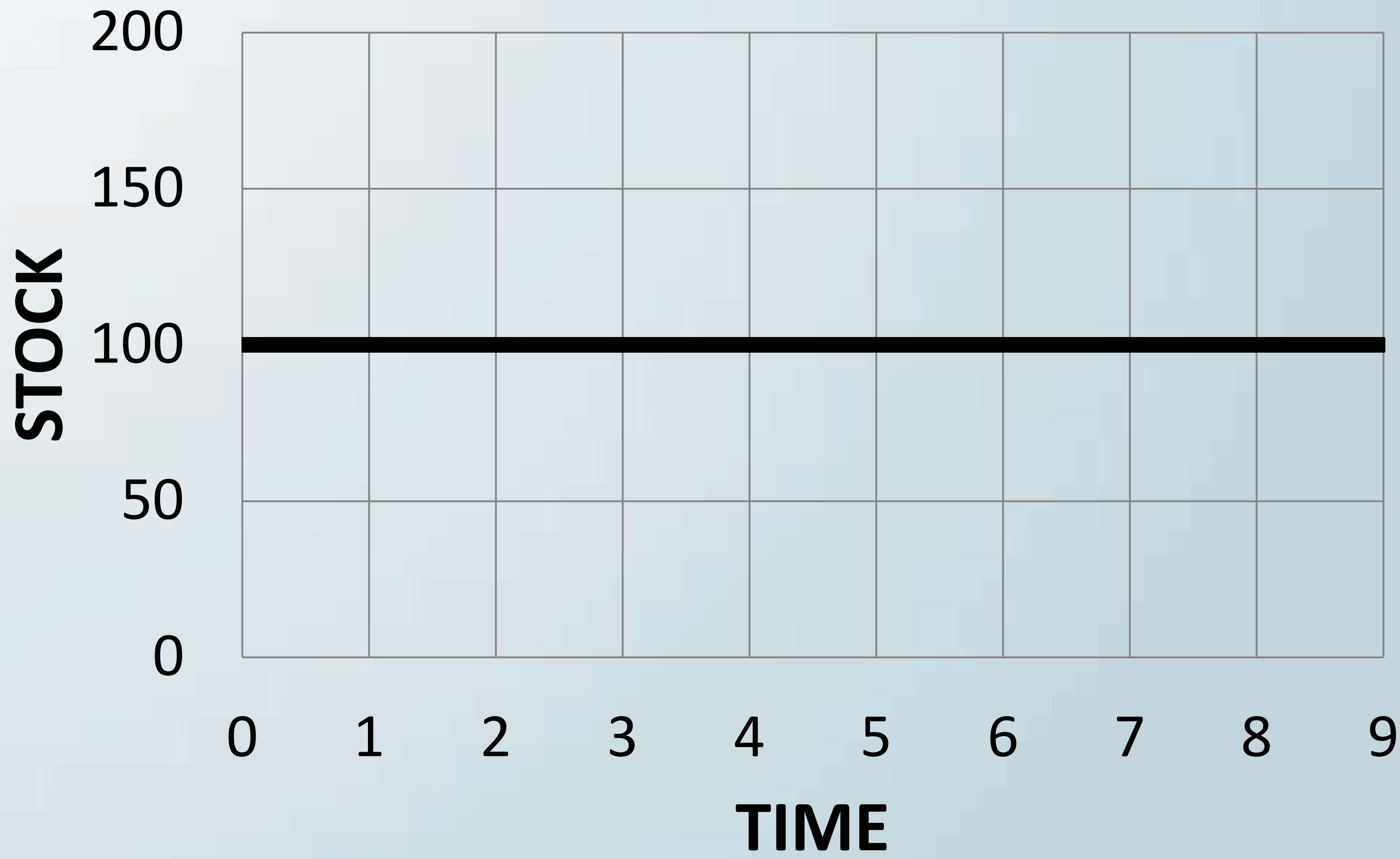
$$\frac{dS}{dt} = F_{in} - F_{out} = F - F = 0$$

$\mathbf{S(t) = S_0}$ (i.e. no change from initial value)

Residence time T is defined for steady state:

$T = S/F$

Stock is in Steady State: S(t) = S0



Case B: F_{in} - F_{out} = constant

- If stock is not in steady state, then we must solve the differential equation:

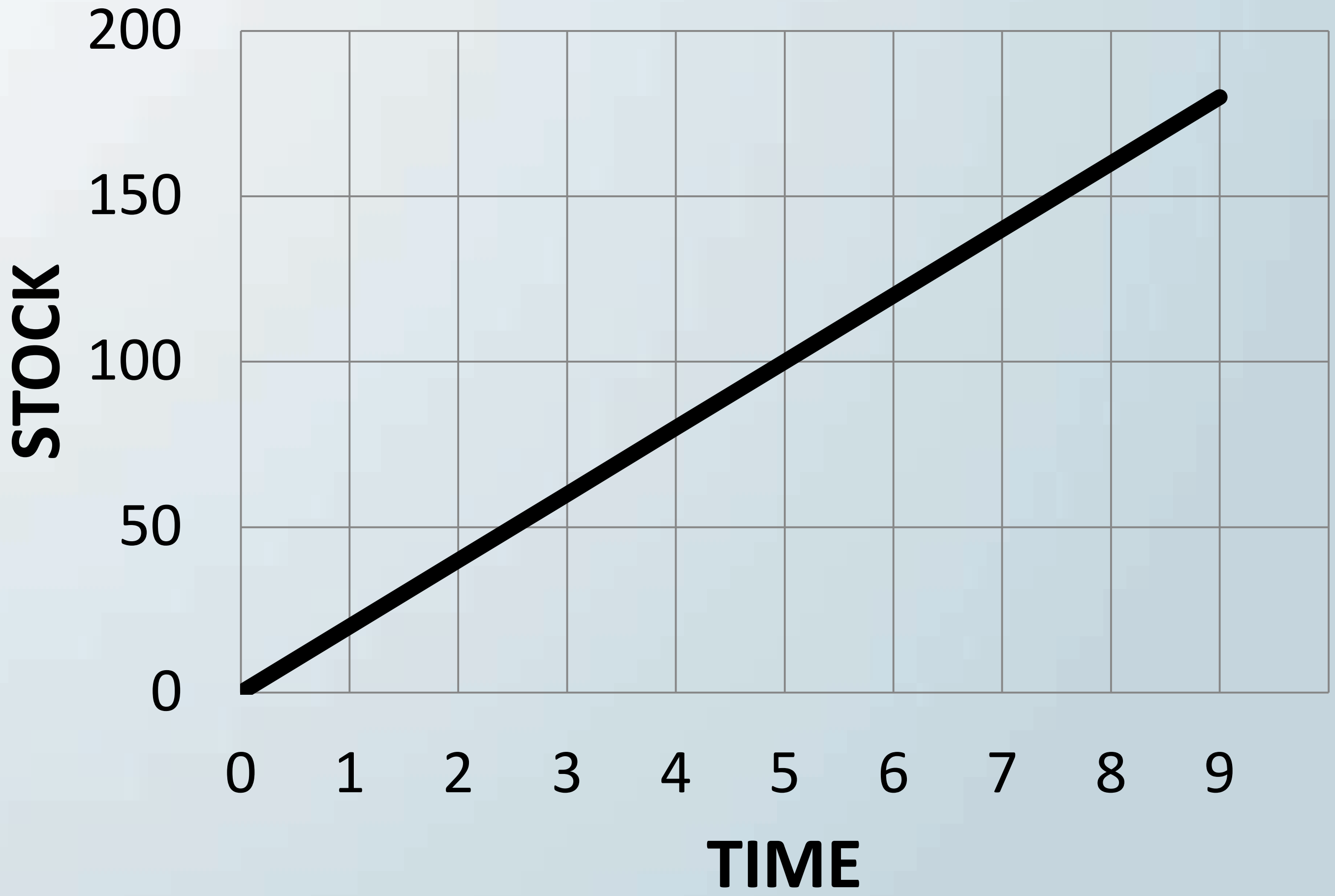
$$\frac{dS}{dt} = F_{in}(t) - F_{out}(t)$$

- Simplest case is when the difference between F_{in} and F_{out} is constant:

$$\frac{dS}{dt} = F_{in}(t) - F_{out}(t) = \Delta F \qquad dS = \Delta F dt$$

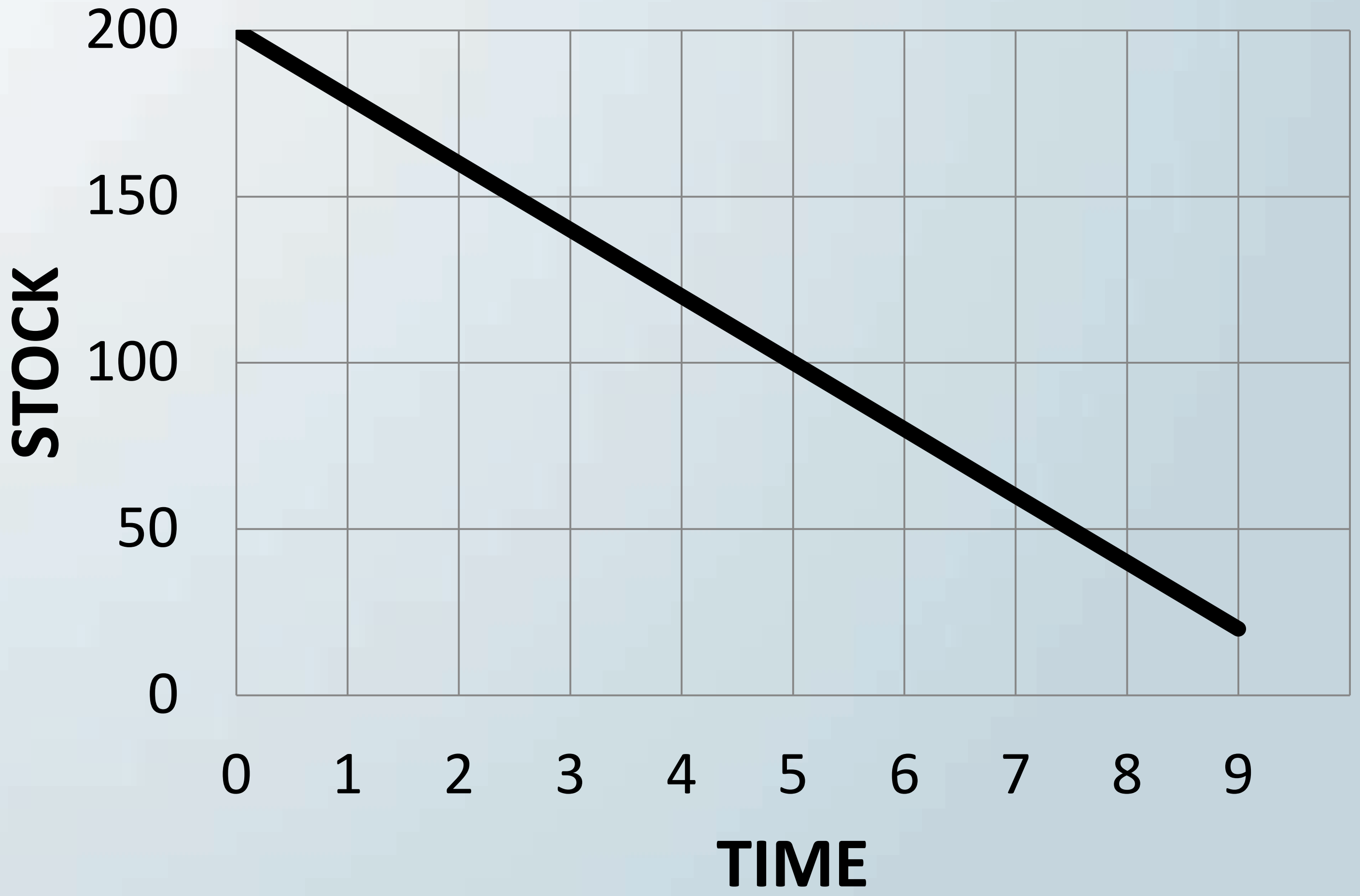
$$\int_{S(0)}^{S(t)} dS = \Delta F \int_0^t dt \qquad \boxed{S(t) = S_0 + \Delta F t}$$

$F_{in} - F_{out} = \text{constant}: S(t) = S_0 + \Delta F t$



Ex. $S_0 = 0$, $\Delta F = 20$

$F_{in} - F_{out}$ = constant: $S(t) = S_0 + \Delta F t$



Ex. $S_0 = 200$, $\Delta F = -20$

Exponential Growth – Fixed Percentage per Year

- Exponential growth when the increase in some quantity is proportional to the amount currently present
- If fixed percentage per year.

$N_1 = N_0(1 + r)$ $N_2 = N_1(1 + r)$ $N_3 = N_0(1 + r)$ etc.

or $\boldsymbol{N(t) = N_0(1 + r)^t}$

$N(t)$ = amount at time t

N_0 = initial amount

r = rate

t = time

Exponential Growth – Smooth, Continuous

- If we assume that the rate of change is smooth and continuous.

$$\frac{dN}{dt} = rN$$

- Leads to

$$N(t) = N_0 e^{rt}$$

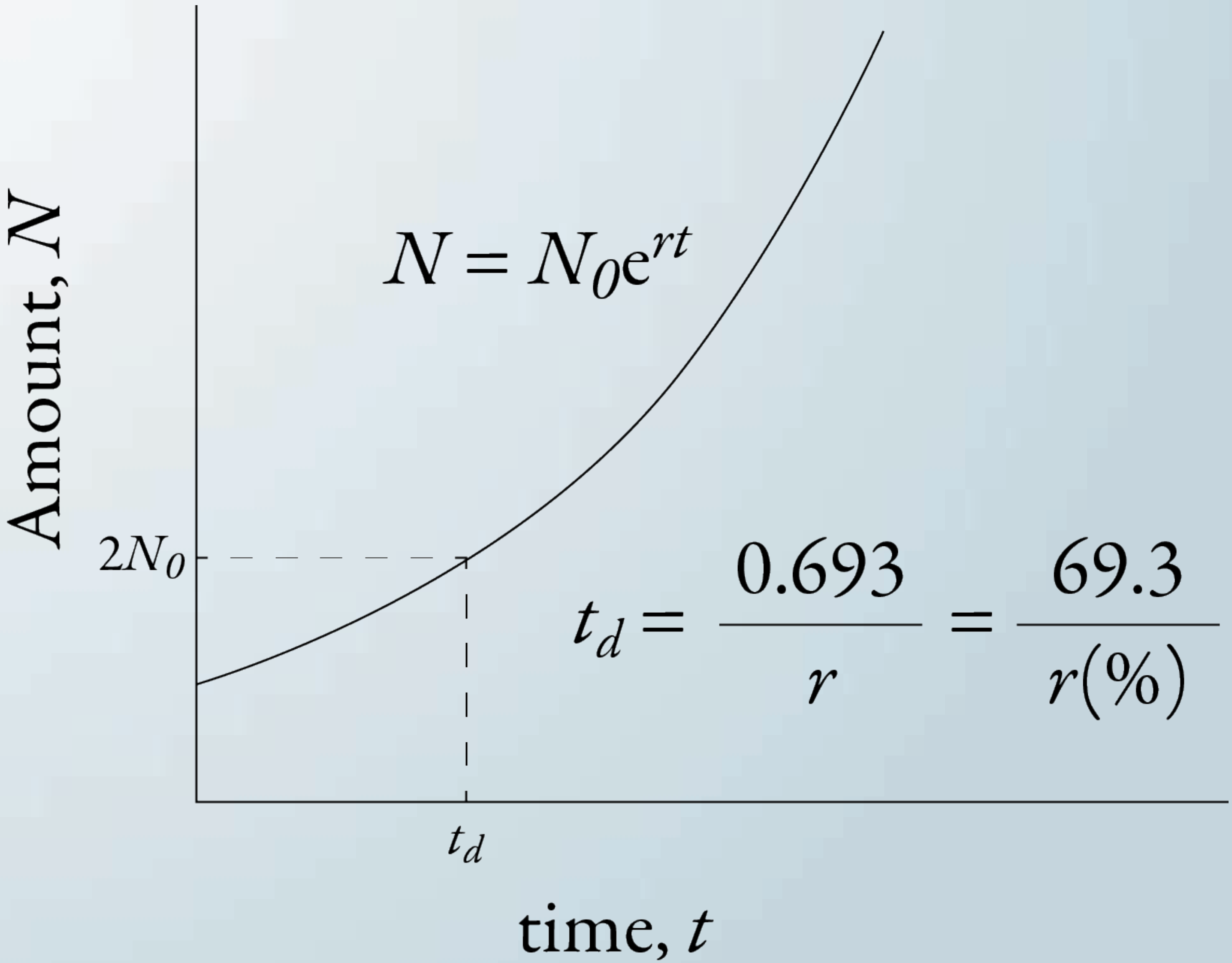
$N(t)$ = amount at time t

N_0 = initial amount

r = rate

t = time

Exponential Growth



$$t_d = \frac{0.693}{r} = \frac{69.3}{r(\%)}$$

Logarithms

- The logarithm of a number is the exponent by which a fixed number, the base, has to be raised to produce that number. The log base *a* of a number *y* is the power of *a* that yields *y*.

$\log_a y = \log_a a^x = x$ e.g $\log_{10} 1000 = \log_{10} 10^3 = 3$

$\log_{10}$ is commonly described as just log.

Log_e is commonly described as ln.

$e = 2.71828182845904523536028747135266249775 72...$

$\log_a a = 1$ e.g. $\log 10 = \log 10^1 = 1$ or $\ln e = \ln e^1 = 1$

$\text{Log}_a (b \bullet c) = \log_a b + \log_a c$

$\text{Log}_a (b \div c) = \log_a b - \log_a c$

$\text{Log}_a b^c = c \log_a b$ e.g. $\ln 2^{-3} = -3 \ln 2$

Exponential Growth

$$N(t) = N(0)e^{rt}$$

$N(t)$ = number at time t

$N(0)$ = initial number

r = rate of change

$$\ln[N(t)] = \ln[N(0)] + \ln(e^{rt})$$

$$\ln[N(t)] = \ln[N(0)] + rt$$

Doubling Time

$N(t)$ = amount time t N_0 = amount at time 0 t = time

r = rate Rate has units of 1/time,

e.g. a rate of change of 12% per year corresponds to 0.12/yr

$$N(t) = N_0 e^{rt}$$

for doubling $N(t) = 2N_0$

so $2N_0 = N_0 e^{rt_d}$

$$2 = e^{rt_d}$$

$$\ln 2 = \ln (e^{rt_d})$$

$$\ln 2 = rt_d \ln e$$

$$\ln 2 = rt_d$$

$$\frac{\ln 2}{r} = t_d = \frac{\mathbf{0.693}}{r}$$

For x doublings, $N(t) = 2^x N_0$

Case C. Exponential Growth of Stocks

- Type 1: Inflow is directly proportional to the stock: $F_{in} = rS$ $\quad (F_{out} = 0)$

$$\frac{dS}{dt} = rS \qquad \frac{dS}{S} = r\,dt \qquad \int_{S_0}^{S_t} \frac{dS}{S} = r\int_0^t dt$$

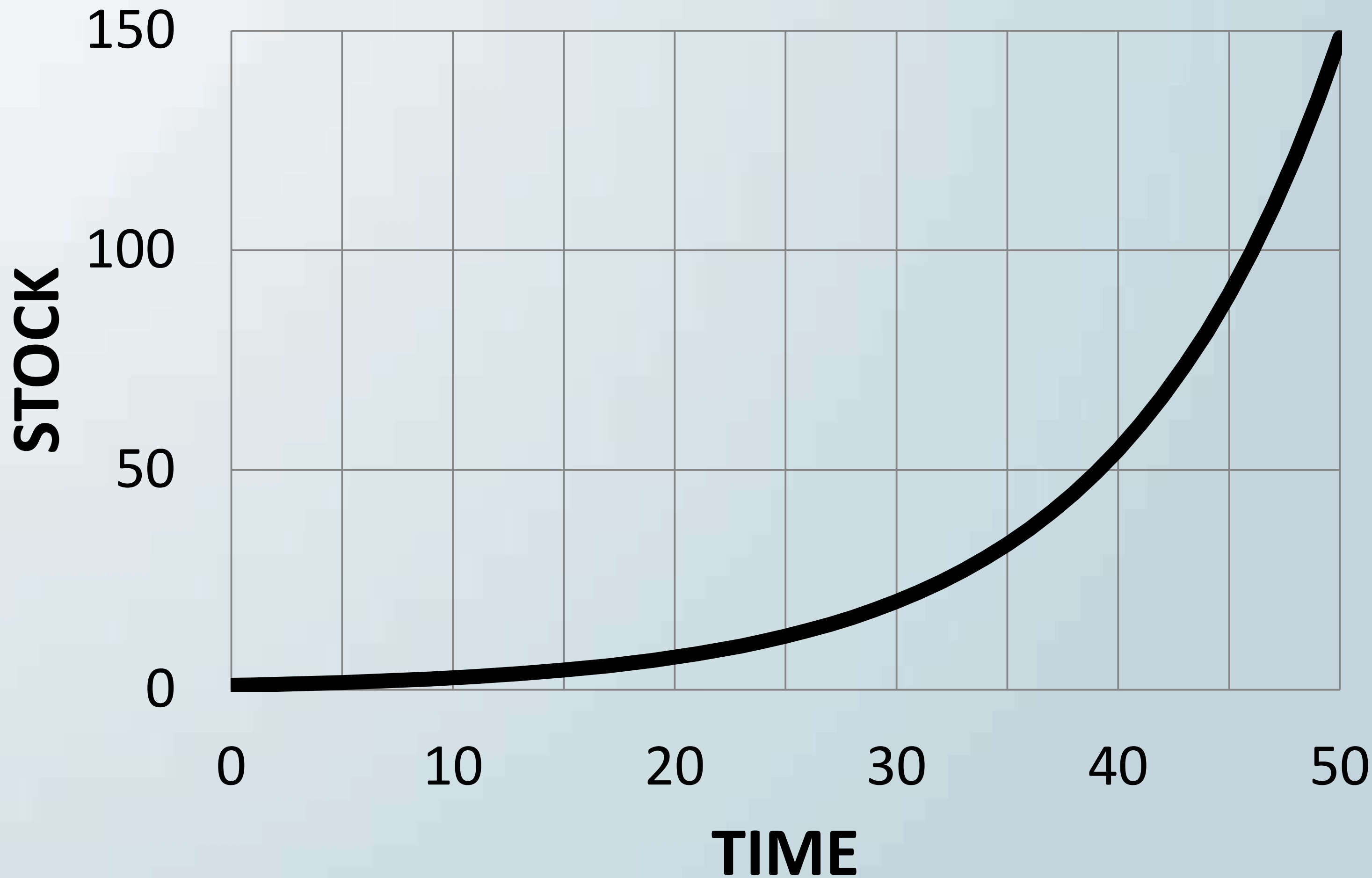
$$\ln(S_t) - \ln(S_0) = \ln\left(\frac{S_t}{S_0}\right) = rt \qquad \boxed{S(t) = S_0\, e^{rt}}$$

- Ex. If you put $100 in an account with a 0.84% annual percentage rate, how much money will you have after 10 years?

If you put \$100 in an account with an interest rate of 0.84%, how much money will you have after 10 years?

$$S(t) = S_0 e^{rt} = \$100\ e^{(0.0084\ 1/\text{yr}\ 10\ \text{yr})} = \$108.76$$

Exponential Growth of Stocks: $S(t) = S_0 e^{rt}$



Ex. S_0=1, r=0.1/y

Exponential Decline and Half-Life

$N(t)$ = amount time t N_0 = amount at time 0 t = time

k = rate k has units of 1/time,

$$N(t) = N_0 e^{-kt}$$

When half gone $N(t) = 1/2 N_0$

so $1/2 N_0 = N_0 e^{-kt_{1/2}}$

$2^{-1} = e^{-kt_{1/2}}$

$\ln 2^{-1} = \ln(e^{-kt_{1/2}})$

$-\ln 2 = -kt_{1/2} \ln e$

$\ln 2 = kt_{1/2}$

$$\frac{\ln 2}{k} = t_{1/2} = \frac{\mathbf{0.693}}{k}$$

Exponential Decline of Stocks

- Outflow is proportional to stock.

  $F = -rS$

  $$S = S_0e^{-rt}$$

- Ex. Iodine-131 has a half-life of 8.0197 days. If we start with 37 GBq (or 1 curie) of I-131, how much is left after 14 days?
- The **becquerel** (symbol **Bq**) (pronounced: 'be-kə-rel) is the SI-derived unit of radioactivity. One Bq is defined as the activity of a quantity of radioactive material in which one nucleus decays per second. The Bq unit is therefore equivalent to an inverse second, s^{-1}.
- The curie is a common non-SI unit. It is is now defined as 37 GBq.

Iodine-131 has a half-life of 8.0197 days. If we start with 37 GBq (or 1 curie) of I-131, how much is left after 14 days?

$$t_{1/2} = \frac{0.693}{k} \qquad k = \frac{0.693}{t_{1/2}} = \frac{0.693}{8.0197\ \text{day}} = 0.0864\ \text{day}^{-1}$$

$$S(t) = S_o\, e^{-kt} = 37\ \text{GBq}\, e^{-0.0864\ 1/\text{day}(14\ \text{day})} = \mathbf{11\ GBq}$$