Units, Unit Conversions, and Other Tools for Calculations

http://preparatorychemistry.com/Bishop_Book_atoms_1.pdf

http://preparatorychemistry.com/Bishop_Book_atoms_2.pdf

http://preparatorychemistry.com/Appendix_A_atoms.pdf

http://preparatorychemistry.com/Appendix_B_atoms.pdf

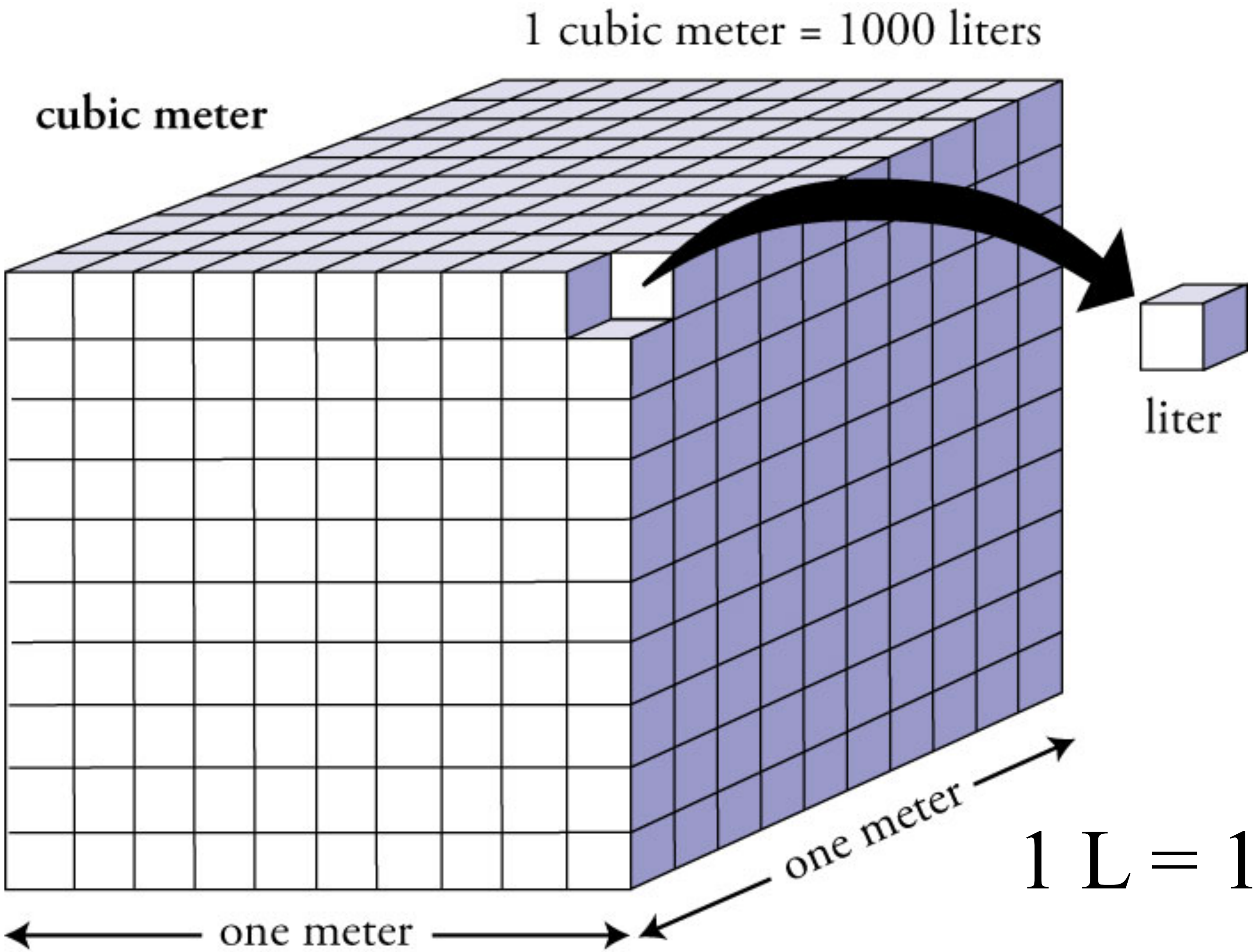
Values from Measurements

- A ***value*** is a quantitative description that includes both a unit and a number.
- For *100 meters*, the *meter* is a unit by which distance is measured, and the *100* is the number of units contained in the measured distance.
- ***Units*** are quantities defined by standards that people agree to use to compare one event or object to another.

Base Units for the International System of Measurement

- **Length meter, m**, the distance that light travels in a vacuum in 1/299,792,458 of a second
- **mass kilogram, kg**, the mass of a platinum-iridium alloy cylinder in a vault in France
- **time second, s**, the duration of 9,192,631,770 periods of the radiation emitted in a specified transition between energy levels of cesium-133
- **temperature kelvin, K**, 1/273.16 of the temperature difference between absolute zero and the triple point temperature of water
- **Amount of substance mole, mol**, the amount of substance that contains the same number of chemical units as there are atoms in 12 g of carbon-12.
- **Electric current ampere, A**, the amount of electric charge passing a point in an electric circuit per unit time with 6.241×10^{18} electrons, or one coulomb per second constituting one ampere.
- **Luminous intensity candela, Cd**, the luminous intensity of a source that emits monochromatic radiation of frequency 540×10^{12} hertz and that has a radiant intensity of $1/683$ watt per steradian.

Derived Unit



$$1\ \mathrm{L} = 10^{-3}\ \mathrm{m}^3$$

$$10^3\ \mathrm{L} = 1\ \mathrm{m}^3$$

Other Derived Units

Force	newton, N = kg·m/s^2
Energy or Work	joule, J = N·m
Power	watt, W = J/s
Gas pressure	pascal, Pa = N/m^2
Radiation exposure	sievert, Sv = J/kg

4-5 Sv exposure leads to 50% chance of death

Metric Prefixes

Prefix	Abbreviation	Number
exa	E	10^{18}
peta	P	10^{15}
tera	T	10^{12}
giga	**G**	**10^{9} or 1,000,000,000**
mega	**M**	**10^{6} or 1,000,000**
kilo	**k**	**10^{3} or 1000**
centi	**c**	**10^{-2} or 0.01**
milli	**m**	**10^{-3} or 0.001**
micro	**μ**	**10^{-6} or 0.000001**
nano	**n**	**10^{-9} or 0.000000001**
pico	p	10^{-12}
femto	f	10^{-15}
atto	a	10^{-18}

Scientific (Exponential) Notation

- Numbers expressed in scientific notation have the following form.

Exponent, a positive or negative integer

$$a \times 10^b$$

Coefficient, a number with one nonzero digit to the left of the decimal point

Exponential term

Scientific Notation (Example)

- 5.5×10^{21} carbon atoms in a 0.55 carat diamond.
  - 5.5 is the coefficient
  - 10^{21} is the exponential term
  - The ^{21} is the exponent.
- The coefficient should have just one nonzero digit to the left of the decimal point.

Uncertainty

- The coefficient reflects the number's uncertainty.
- It is common to assume that coefficient is plus or minus one in the last position reported unless otherwise stated.
- Using this guideline, 5.5×10^{21} carbon atoms in a 0.55 carat diamond suggests that there are from 5.4×10^{21} to 5.6×10^{21} carbon atoms in the stone.

Size (Magnitude) of Number

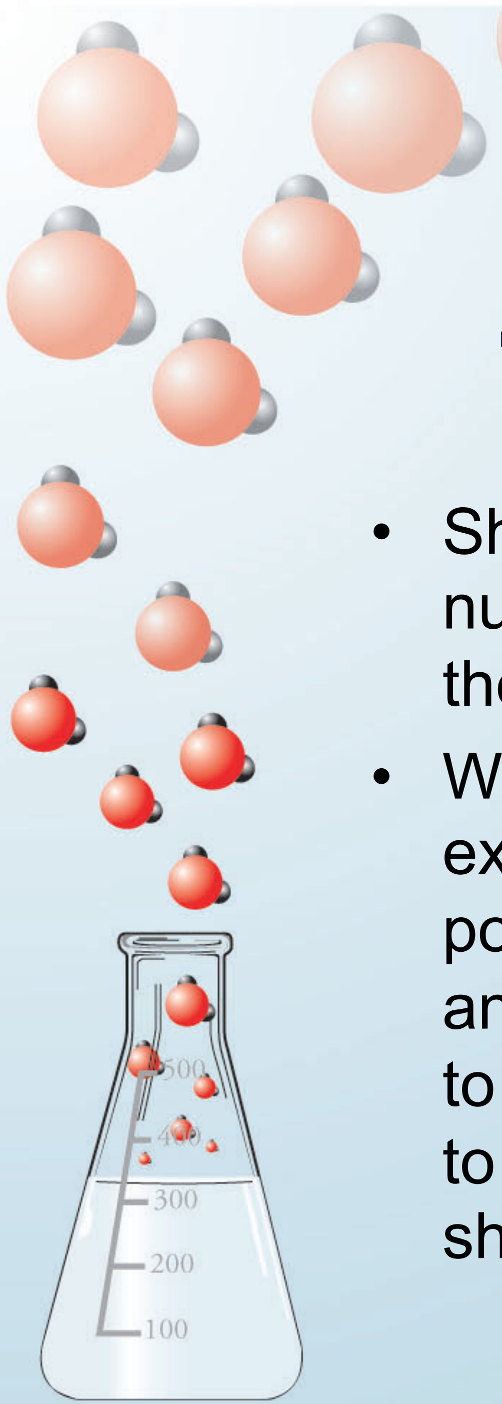
- The exponential term shows the size or magnitude of the number.
- Positive exponents are used for large numbers. For example, the moon orbits the sun at 2.2×10^4 or 22,000 mi/hr.

$$2.2 \times 10^4 = 2.2 \times 10 \times 10 \times 10 \times 10 = 22{,}000$$

Size (Magnitude) of Number

- Negative exponents are used for small numbers. For example, A red blood cell has a diameter of about 5.6×10^{-4} or 0.00056 inches.

$$5.6 \times 10^{-4} = 5.6 \times \frac{1}{10^4} = \frac{5.6}{10 \times 10 \times 10 \times 10} = 0.00056$$



From Decimal Number to Scientific Notation

- Shift the decimal point until there is one nonzero number to the left of the decimal point, counting the number of positions the decimal point moves.
- Write the resulting coefficient times an exponential term in which the exponent is positive if the decimal point was moved to the left and negative if the decimal position was moved to the right. The number in the exponent is equal to the number of positions the decimal point was shifted.

From Decimal Number to Scientific Notation (Examples)

- For example, when 22,000 is converted to scientific notation, the decimal point is shifted four positions to the left so the exponential term has an exponent of 4.

$$22{,}000 = 2.2 \times 10^{4}$$

- When 0.00056 is converted to scientific notation, the decimal point is shifted four positions to the right so the exponential term has an exponent of -4.

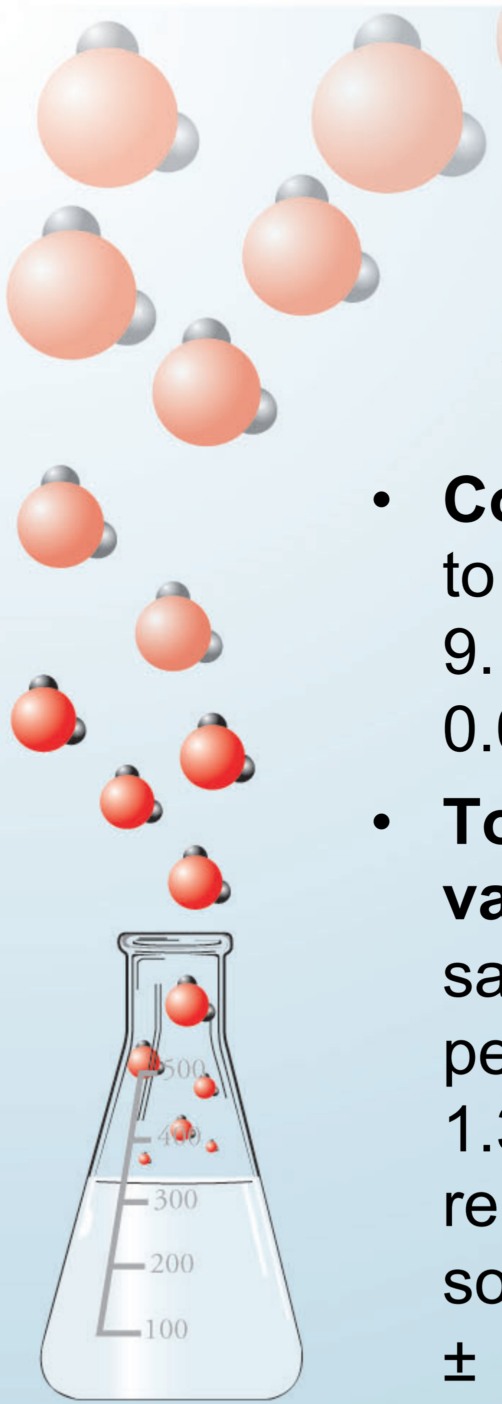
$$0.00056 = 5.6 \times 10^{-4}$$

Scientific Notation to Decimal Number

- Shift the decimal point in the coefficient to the right if the exponent is positive and to the left if it is negative.
- The number in the exponent tells you the number of positions to shift the decimal point.

2.2×10^{4} goes to 22,000

5.6×10^{-4} goes to 0.00056



Reasons for Using Scientific Notation

- **Convenience -** It takes a lot less time and space to report the mass of an electron as 9.1096×10^{-28}, rather than 0.00000000000000000000000000091096 g.
- **To more clearly report the uncertainty of a value -** The value 1.4×10^{3} kJ per peanut butter sandwich suggests that the energy from a typical peanut butter sandwich could range from 1.3×10^{3} kJ to 1.5×10^{3} kJ. If the value is reported as 1400 kJ, its uncertainty would not be so clear. It could be 1400 ± 1, 1400 ± 10, or 1400 ± 100.

Multiplying Exponential Terms

- When multiplying exponential terms, add exponents.

$10^3 \times 10^6 = 10^{3+6} = 10^9$

$10^3 \times 10^{-6} = 10^{3+(-6)} = 10^{-3}$

$3.2 \times 10^{-4} \times 1.5 \times 10^9$

$= 3.2 \times 1.5 \times 10^{-4+9}$

$= 4.8 \times 10^5$

When dividing exponential terms, subtract exponents.

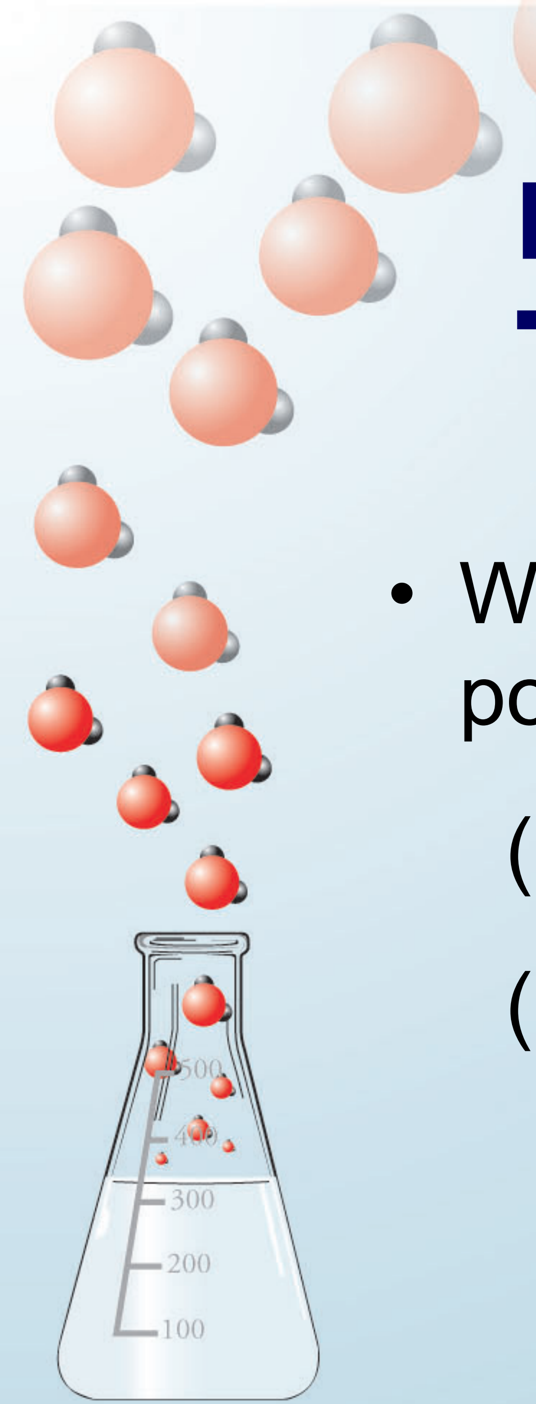
$$\frac{10^{12}}{10^{3}} = 10^{12-3} = 10^{9}$$

$$\frac{10^{6}}{10^{-3}} = 10^{6-(-3)} = 10^{9}$$

$$\frac{9.0 \times 10^{11}}{1.5 \times 10^{-6}} = \frac{9.0}{1.5} \times 10^{11-(-6)} = 6.0 \times 10^{17}$$

$$\frac{10^{2} \cdot 10^{-3}}{10^{6}} = 10^{2+(-3)-6} = 10^{-7}$$

$$\frac{1.5 \times 10^{4} \cdot 4.0 \times 10^{5}}{2.0 \times 10^{12} \cdot 10^{3}} = \frac{1.5 \cdot 4.0}{2.0} \times 10^{4+5-12-3} = 3.0 \times 10^{-6}$$



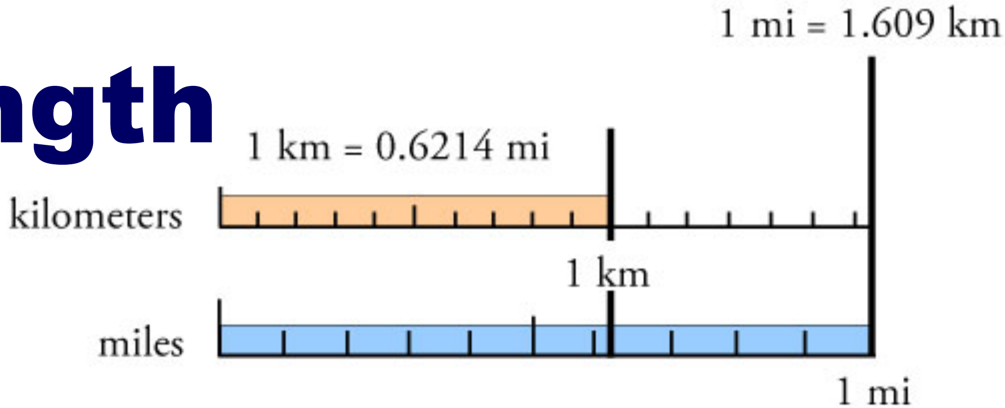
Raising Exponential Terms to a Power

- When raising exponential terms to a power, multiply exponents.

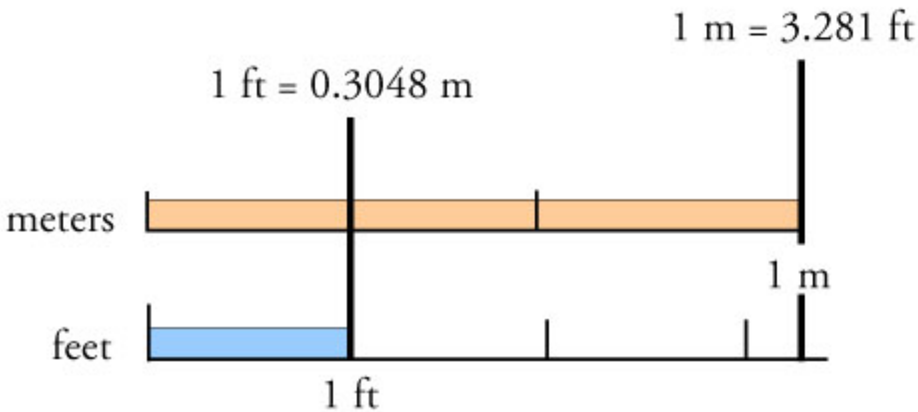
$$(10^4)^3 = 10^{4 \cdot 3} = 10^{12}$$

$$(3 \times 10^5)^2 = (3)^2 \times (10^5)^2 = 9 \times 10^{10}$$

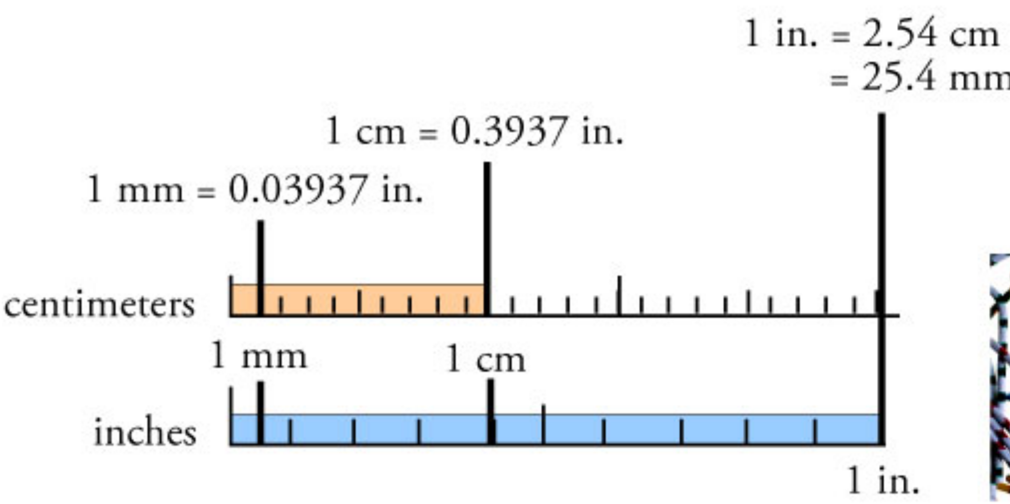
Length



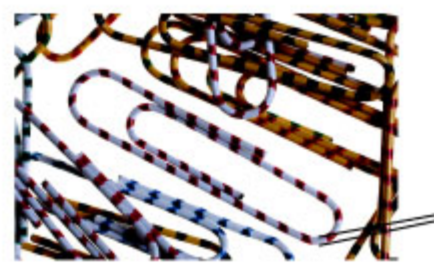
The Stanford linear accelerator is two miles long.



1 meter

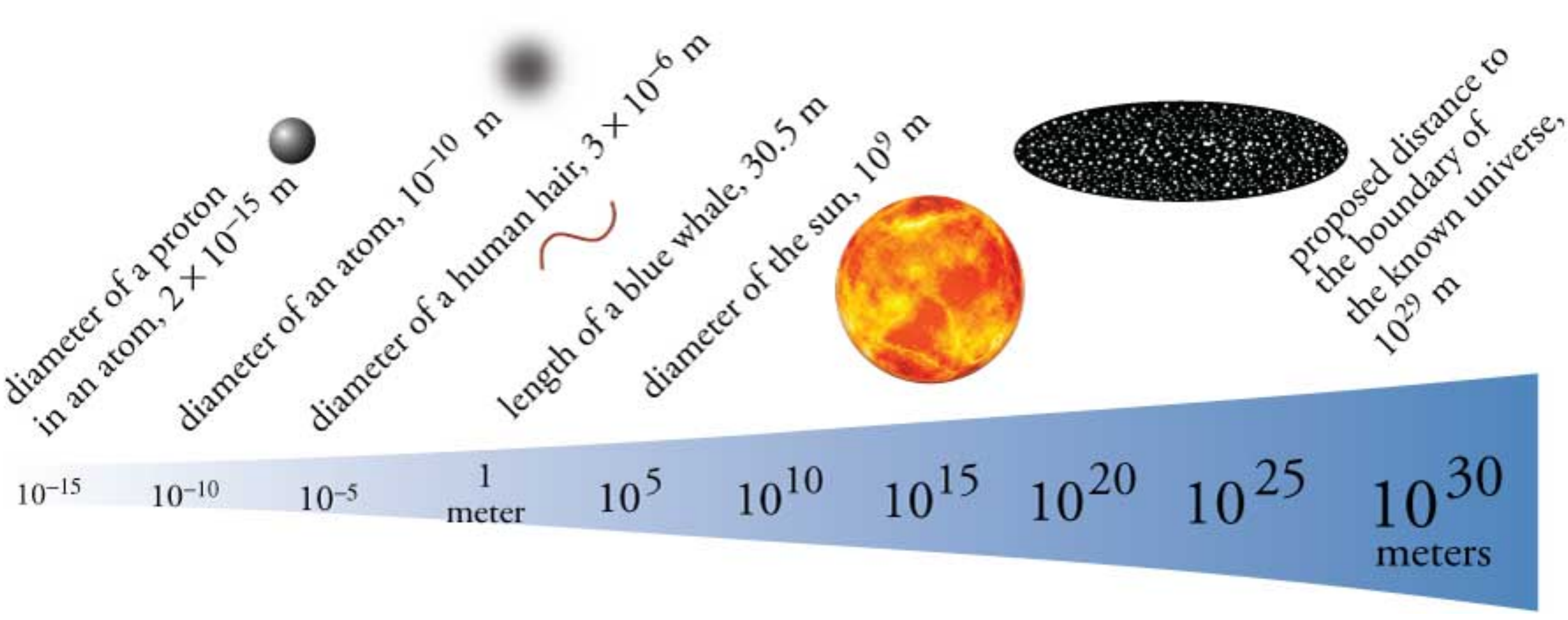


1 centimeter



1 millimeter

Range of Lengths



Volume

1 fluid ounce (fl oz)

1 fl oz = 29.57 mL

1 mL = 0.03381 fl oz

1 milliliter (mL)
= about 20 drops

1 gal = 3.785 L

1 gallon (gal)
or 4 quarts (qt)

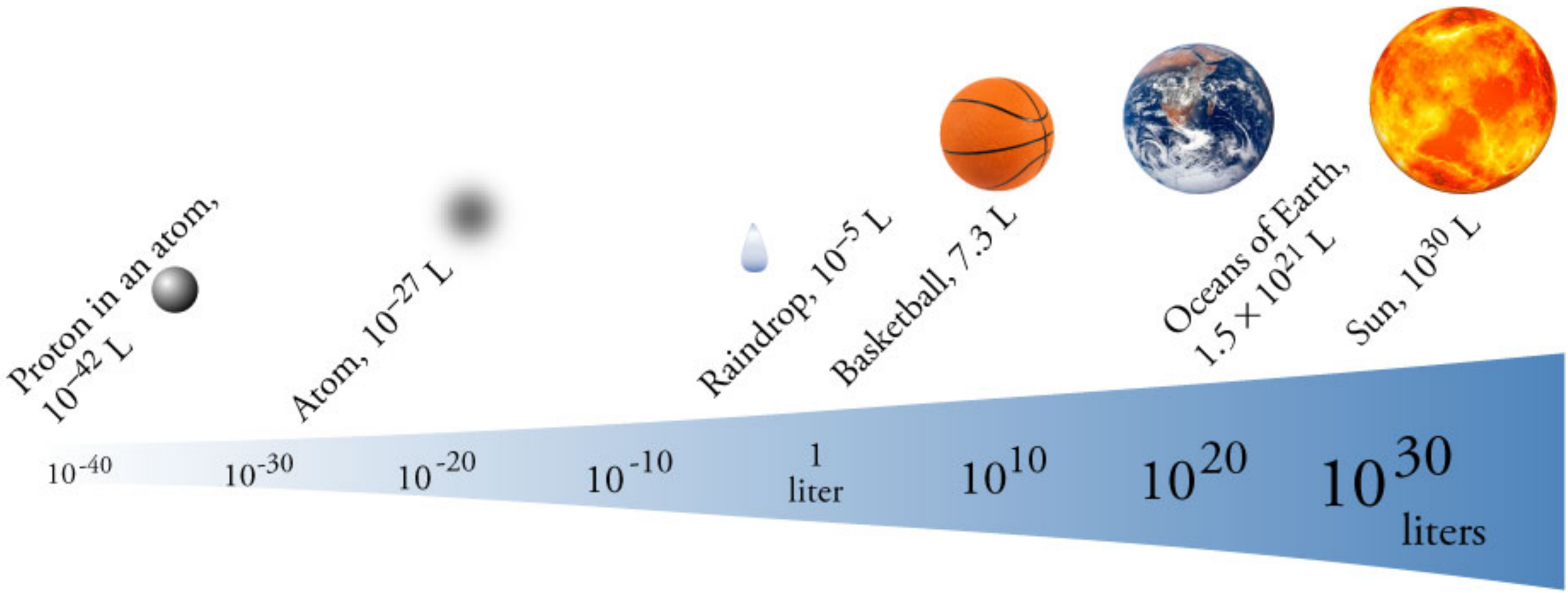
1 qt = 0.9464 L

1 qt or 32 fl oz

1 L = 1.057 qt
= 0.2642 gal

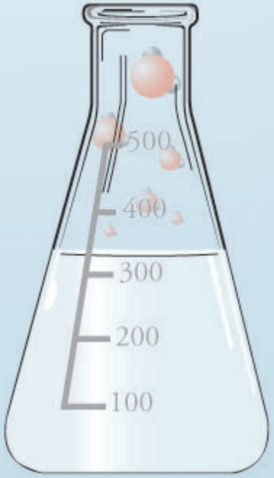
1 liter (L)
or 1000 mL

Range of Volumes



Mass and Weight

- ***Mass*** is usually defined as a measure of the amount of matter in an object. Mass can be defined as the property of matter that leads to gravitational attractions between objects and therefore gives rise to weight.
- ***Matter*** is anything that occupies a volume and has a mass.
- The ***weight*** of an object, on the Earth, is a measure of the force of gravitational attraction between the object and the Earth.



Comparison of the Mass and Weight of a 65 kg Person

	On Earth	Between Earth and Moon	On Moon
Mass	65 kg	65 kg	65 kg
Weight	637 N	≈0 N	1/6(637 N) = 106 N

Mass

1 oz = 28.35 g

About 2.5 grams (g) or
about 0.088 ounce (oz)

1 lb = 453.6 g

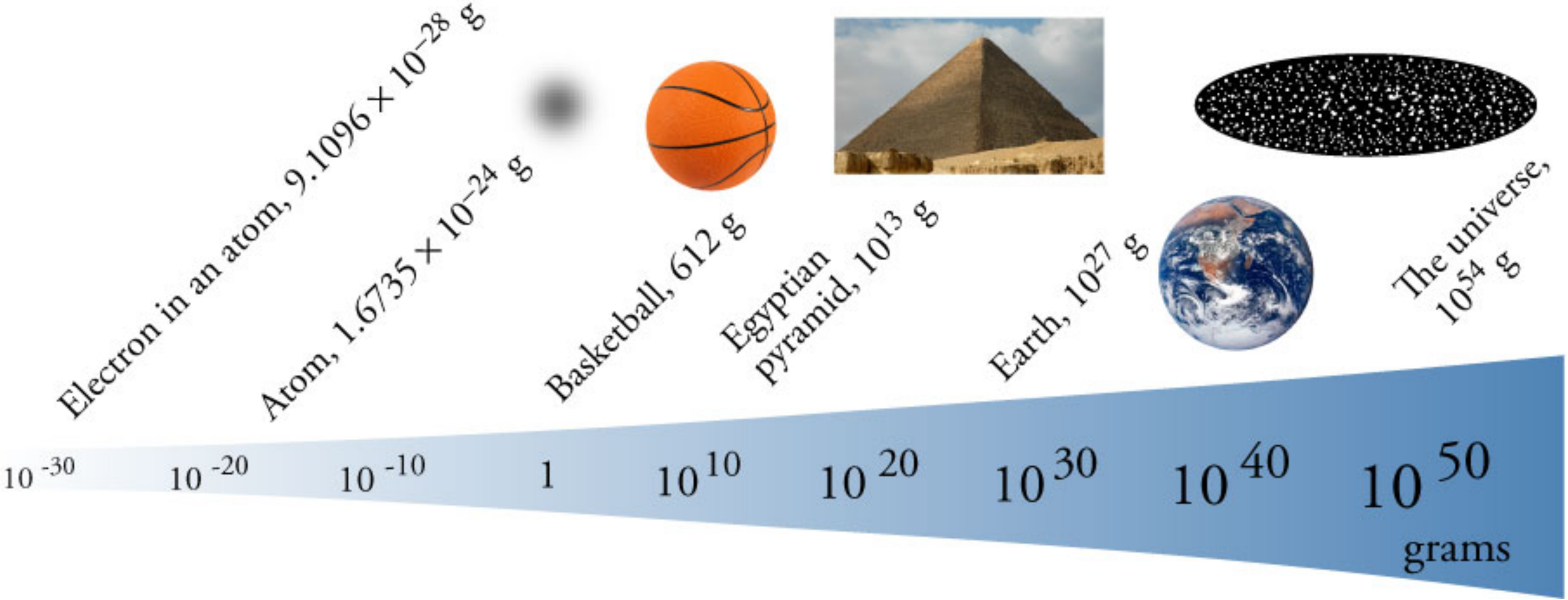
1 kg = 2.205 lb

About 1 kilogram (kg) or
about 2.2 pounds (lb)

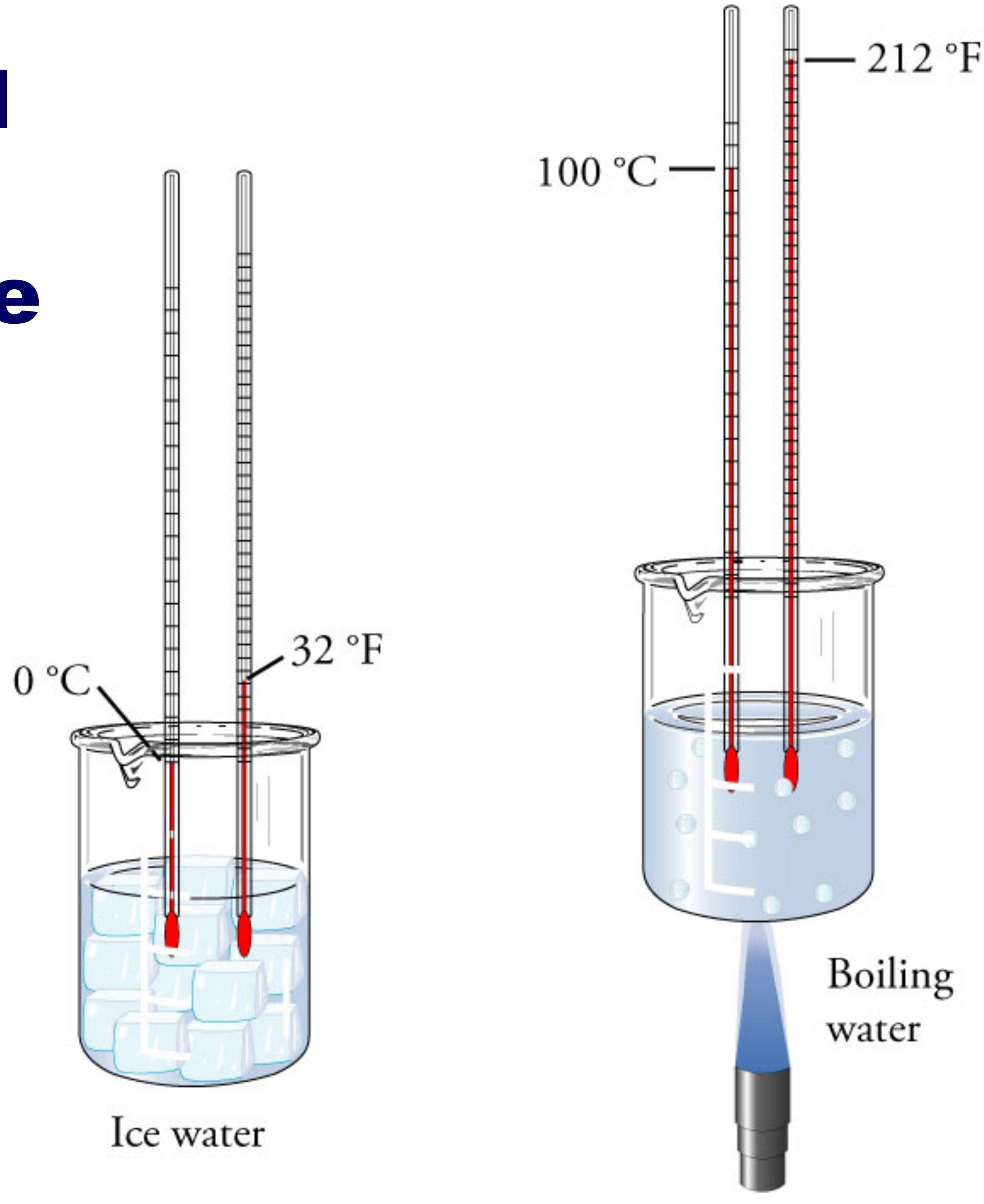
1 Mg = 1000 kg = 1 t

About 1 megagram (Mg) or 1 metric ton (t)

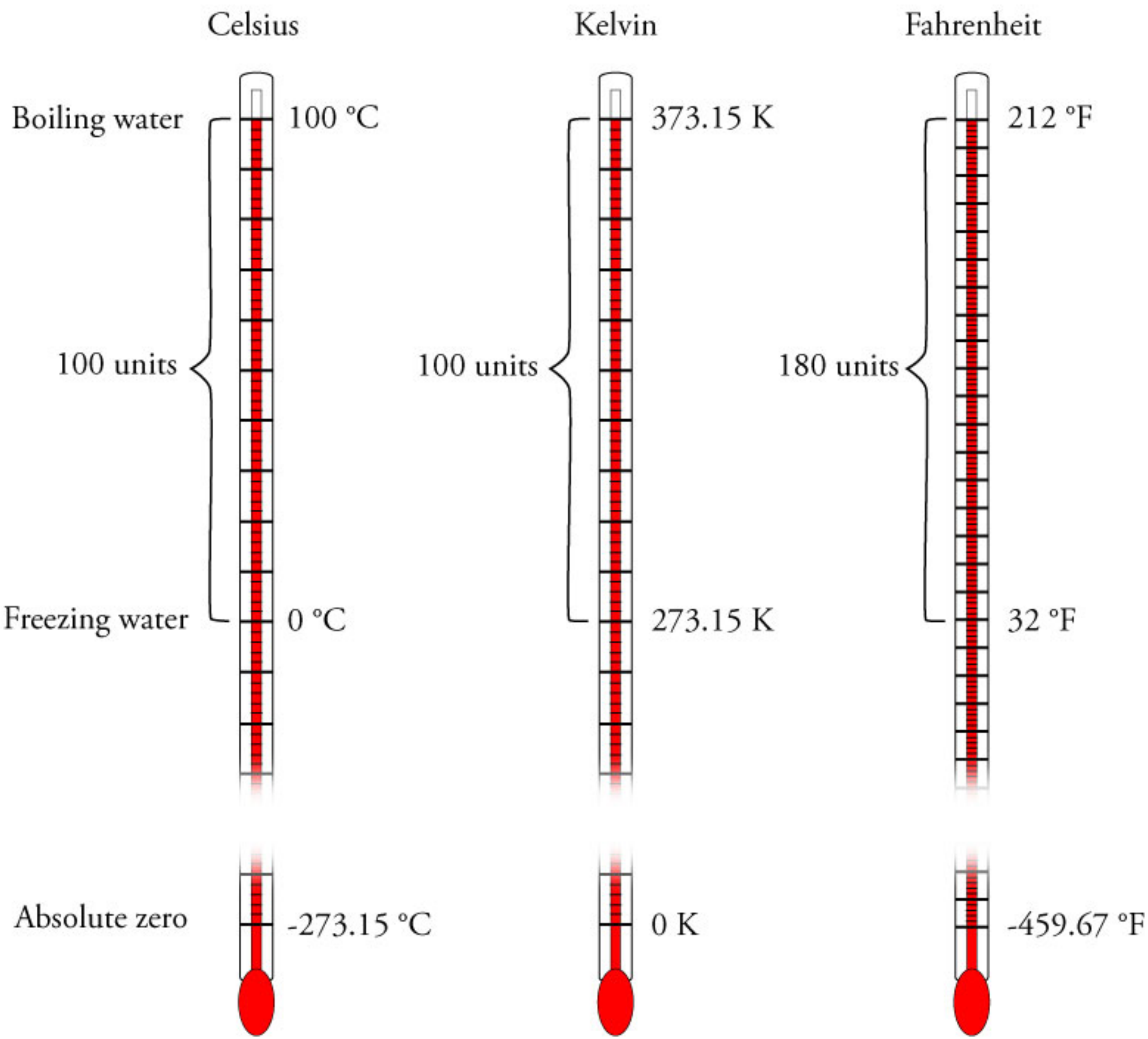
Range of Masses



Celsius and Fahrenheit Temperature



Comparing Temperature Scales



Calculations – Two Types

- **Unit conversions** (using unit analysis)
- **Equation-based calculations** (using algebra)

Calculations are often a blend of the two.

Unit Conversions

All science requires mathematics. The knowledge of mathematical things is almost innate in us. . . [Mathematics] is the easiest of sciences, a fact which is obvious in that no one's brain rejects it…

Roger Bacon (c. 1214-c. 1294)

Problem: Using the following data, calculate the density of seawater in kg/L.

- The total mass of the hydrosphere is about 1.4×10^{15} Gg, which is about 0.023 percent of the Earth's total mass.
- Less than 3 percent is freshwater; the rest is saltwater, mostly in the ocean.
- The area of the world’s oceans is 3.61×10^{8} km^2 and the volume is approximately 1.3×10^{9} km^3.

Unit Analysis Step 1

- **Step 1:** State your question in an expression that sets the unknown unit equal to the value given.
  - Start with the same number of units as you want.
    - If you want a single unit, start with a value that has a single unit.
    - If you want a ratio of two units, start with a value that has a ratio of two units, or start with a ratio of two values, each of which have one unit.
  - Put the correct type of unit in the correct position.

Density

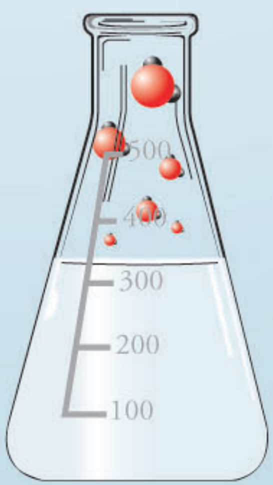
- ***Mass density*** is mass divided by volume. It is usually just called density.

$$\text{Density} = \frac{\text{mass}}{\text{volume}}$$

- It can be used as a unit analysis conversion factor that converts mass to volume or volume to mass.

Unit Analysis Step 2

- **Step 2:** Multiply the expression to the right of the equals sign by one or more conversion factors that cancel the unwanted units and generate the desired unit.
  - If you are not certain which conversion factor to use, ask yourself, "What is the fundamental conversion and what conversion factor do I use for that type of conversion?"



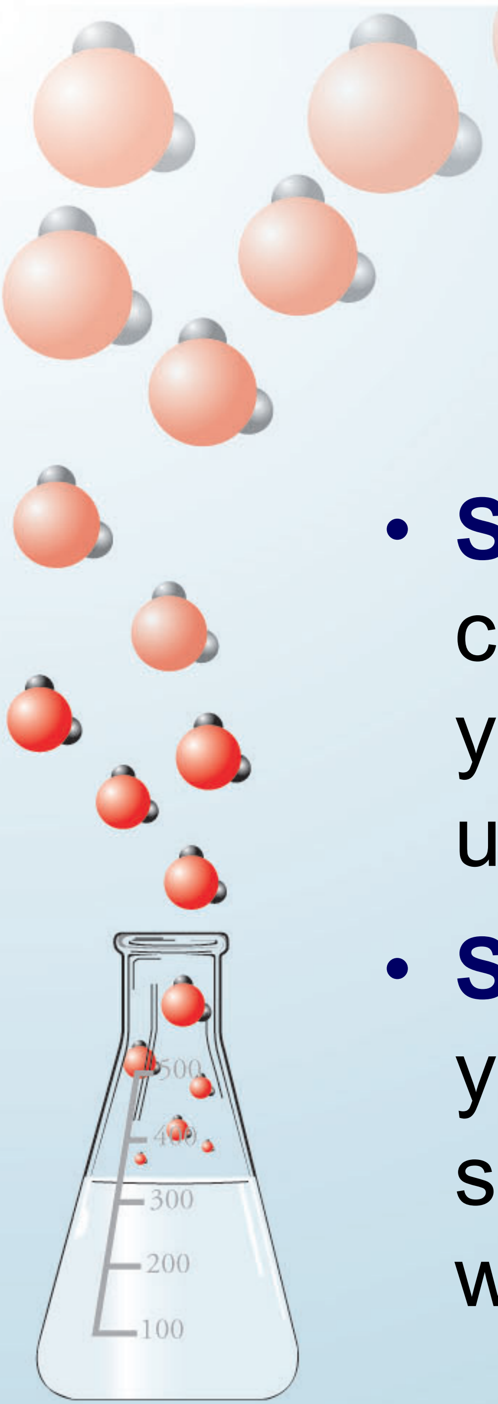
Percentage and Percentage Calculations

- Mass percentages and volume percentage can be used as unit analysis conversion factors to convert between units of the part and units of the whole.

For X% by mass $\dfrac{\text{X (any mass unit) part}}{\text{100 (same mass unit) whole}}$

For X% by volume $\dfrac{\text{X (any volume unit) part}}{\text{100 (same volume unit) whole}}$

Unit Analysis Steps 3 & 4



- **Step 3:** Check to be sure you used correct conversion factors and that your units cancel to yield the desired unit.
- **Step 4:** Do the calculation, rounding your answer to the correct number of significant figures and combining it with the correct unit.

Problem: Using the following data, calculate the density of seawater in kg/L.

- The total mass of the hydrosphere is about 1.4×10^{15} Gg, which is about 0.023 percent of the Earth's total mass.
- Less than 3 percent is freshwater; the rest is saltwater, mostly in the ocean.
- The area of the World Ocean is 3.61×10^{8} km^2 and its volume is approximately 1.3×10^{9} km^3.

$$\frac{?\ \text{kg ocean}}{\text{L ocean}} = \frac{1.4 \times 10^{15}\ \cancel{\text{Gg all water}}}{1.3 \times 10^{9}\ \cancel{\text{km}^3}\ \text{ocean}} \left(\frac{97\ \cancel{\text{Gg}}\ \text{ocean}}{100\ \cancel{\text{Gg all water}}}\right) \left(\frac{10^9\ \cancel{\text{g}}}{1\ \cancel{\text{Gg}}}\right) \left(\frac{1\ \text{kg}}{10^3\ \cancel{\text{g}}}\right) \left(\frac{1\ \cancel{\text{km}}}{10^3\ \cancel{\text{m}}}\right)^3 \left(\frac{1\ \cancel{\text{m}^3}}{10^3\ \text{L}}\right)$$

$$= 1.0446153846153846153846153846154\ \text{kg/L} \approx \mathbf{1.0\ kg/L}$$

English-Metric Conversion Factors

Type of Measurement	Probably Most Useful to Know	Others Useful to Know		
Length	$\frac{2.54\ \text{cm}}{1\ \text{in.}}$	$\frac{1.609\ \text{km}}{1\ \text{mi}}$	$\frac{39.37\ \text{in.}}{1\ \text{m}}$	$\frac{1.094\ \text{yd}}{1\ \text{m}}$
Mass	$\frac{453.6\ \text{g}}{1\ \text{lb}}$	$\frac{2.205\ \text{lb}}{1\ \text{kg}}$		
Volume	$\frac{3.785\ \text{L}}{1\ \text{gal}}$	$\frac{1.057\ \text{qt}}{1\ \text{L}}$		

Rounding Answers from Multiplication and Division Step 1

- **Step 1:** Determine whether each value is exact, and ignore exact values.
  - Exact values
    - Numbers that come from definitions are exact.
    - Numbers derived from counting are exact.
  - Do Step 2 for values that are not exact.
    - Values that come from measurements are never exact.
    - We will assume that values derived from calculations are not exact unless otherwise indicated.

Rounding Answers from Multiplication and Division Step 2

- **Step 2:** Determine the number of significant figures in each value that is not exact.
  - All non-zero digits are significant.
  - Zeros between nonzero digits are significant.
  - Zeros to the left of nonzero digits are not significant.
  - Zeros to the right of nonzero digits in numbers that include decimal points are significant.
  - Zeros to the right of nonzero digits in numbers without decimal points are ambiguous for significant figures.

Rounding Answers from Multiplication and Division Step 3

- **Step 3:** When multiplying and dividing, round your answer off to the same number of significant figures as the value used with the fewest significant figures.
  - If the digit to the right of the final digit you want to retain is less than 5, round down (the last digit remains the same).
  - If the digit to the right of the final digit you want to retain is 5 or greater, round up (the last significant digit increases by 1).

Rounding Answers from Addition and Subtraction

- **Step 1:** Determine whether each value is exact, and ignore exact values.
  - Skip exact values.
  - Do Step 2 for values that are not exact.
- **Step 2:** Determine the number of decimal positions for each value that is not exact.
- **Step 3:** Round your answer to the same number of decimal positions as the inexact value with the fewest decimal places.

Problem: Using the following data, calculate the approximate productivity of Earth's cultivated land in metric tons per hectare (Ha) per year.

- 15×10^6 km^2 cultivated land
- Global population is about 6.6×10^9 people
- Average food intake is 1 kg food per person per day
- 1 Ha = 10^4 m^2

Solution: Calculate the approximate productivity of Earth's cultivated land in metric tons per hectare (Ha) per year.

$$\frac{?\ \text{t}}{\text{Ha}\bullet\text{yr}} = \frac{6.6\times10^{9}\ \cancel{\text{pers}}}{1.5\times10^{7}\ \cancel{\text{km}^2}}\left(\frac{1\ \cancel{\text{kg}}}{\cancel{\text{pers}}\bullet\cancel{\text{day}}}\right)\left(\frac{1\ \text{t}}{10^{3}\ \cancel{\text{kg}}}\right)\left(\frac{1\ \cancel{\text{km}}}{10^{3}\ \cancel{\text{m}}}\right)^{2}\left(\frac{10^{4}\ \cancel{\text{m}^2}}{1\ \text{Ha}}\right)\left(\frac{365\ \cancel{\text{day}}}{1\ \text{yr}}\right)$$

$$= \frac{\mathbf{1.6\ t}}{\mathbf{Ha\bullet yr}}$$

Problem: Using the following data, calculate the approximate volume of the ocean in km^3 and mass in metric tons.

- Surface area of Earth = 5.1×10^8 km^2
- 70% of Earth covered by oceans
- Average depth of ocean about 4 km
- Density of water 1.0 g/cm^3

Solution: Calculate the approximate volume of the ocean in km^3 and mass in metric tons.

$V = A \bullet h$

$$? \text{ km}^3 \text{ ocean} = 5.1 \times 10^8 \cancel{\text{km}^2 \text{ total}} \left(\frac{70 \text{ km}^2 \text{ ocean}}{100 \cancel{\text{km}^2 \text{ total}}} \right) \bullet 4 \text{ km}$$

$$= \mathbf{1 \times 10^9 \text{ km}^3 \text{ ocean}}$$

$$? \text{ t ocean} = 1 \times 10^9 \cancel{\text{km}^3} \text{ ocean} \left(\frac{10^3 \cancel{\text{m}}}{1 \cancel{\text{km}}} \right)^3 \left(\frac{10^2 \cancel{\text{cm}}}{1 \cancel{\text{m}}} \right)^3 \left(\frac{1.0 \cancel{\text{g}}}{1 \cancel{\text{cm}^3}} \right) \left(\frac{1 \text{ t}}{10^6 \cancel{\text{g}}} \right)$$

$$= \mathbf{1 \times 10^{18} \text{ t ocean}}$$

Significance of Volume and Mass of Ocean

With all this volume and mass, why worry about polluting the ocean? - seems you could dilute anything to a very low concentration with all this water

- One reason is bioconcentration of pollutants in the food chain.
- Most pollution goes into the shallow coastal zone where biodiversity and productivity are concentrated.

"Something per Something"

- Anything that can be described as "something per something" can be written as a conversion factor and used to make conversions.

Calculate the number of cobblers in the U.S. using the following estimates.

- $20 per cobbler's job
- Cobbler's income of about $100,000 per year
- There's about one cobbler job per person every four years
- There are about 310 million people in the U.S.

“Something per Something”

Calculate the number of cobblers in the U.S. using the following estimates.

- \$20 per cobbler’s bill
- Cobbler’s income of about \$100,000 per year
- There’s about one cobbler job per person every four years
- There are about 310 million people in the U.S.

$$? \text{ cobblers} = 3.1 \times 10^8 \cancel{\text{persons}} \left(\frac{1 \cancel{\text{job}}}{4 \cancel{\text{yr}} \bullet \cancel{\text{person}}} \right) \left(\frac{20 \cancel{\$}}{1 \cancel{\text{job}}} \right) \left(\frac{1 \cancel{\text{yr}} \bullet \text{cobbler}}{10^5 \cancel{\$}} \right)$$

$$= 15500 \text{ cobblers} \approx \mathbf{2 \times 10^4 \ cobblers}$$

Equations

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

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

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

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

$$V = A \times h$$

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

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

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

Mixed Problems: Equation and Unit Analysis

How many pairs of shoes can be made from a cow?

- Assume that both the cow and the shoe are spherical.
- Find the equation for the surface area of a sphere.

$$A = \pi d^2$$

- Estimate the diameter of a spherical cow and a spherical shoe…about 2 m and 0.15 m (15 cm or about 6 in.)
- Calculate the surface areas of a spherical cow and a spherical shoe, and express these as ratios.
- Use unit analysis to calculate the number of shoes per cow.

Mixed Problems: Equation and Unit Analysis

Solution: How many pairs of shoes can be made from a cow?

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

$$d_{cow} \approx 2\text{ m}$$

$$\text{Surface area of spherical cow} = \pi d^2 = \pi(2\text{ m})^2 \approx \left(\frac{13\text{ m}^2}{1\text{ cow}}\right)$$

$$d_{shoe} \approx 0.15\text{ m} \quad (15\text{ cm or about 6 in.})$$

$$\text{Surface area of spherical shoe} = \pi d^2 = \pi(0.15\text{ m})^2 \approx \left(\frac{0.07\text{ m}^2}{1\text{ shoe}}\right)$$

$$\frac{?\text{ shoe}}{\text{cow}} = \left(\frac{13\ \cancel{\text{m}^2}}{1\text{ cow}}\right)\left(\frac{1\text{ shoe}}{0.07\ \cancel{\text{m}^2}}\right) = 185.71\ldots\text{ shoes/cow} \approx \mathbf{2 \times 10^2\ shoes\ per\ cow}$$

Temperature Conversions

$$? \,°F = \text{---}\, °C \left(\frac{1.8\,°F}{1\,°C}\right) + 32\,°F$$

$$? \,°C = \left(\text{---}\, °F - 32\,°F\right)\left(\frac{1\,°C}{1.8\,°F}\right)$$

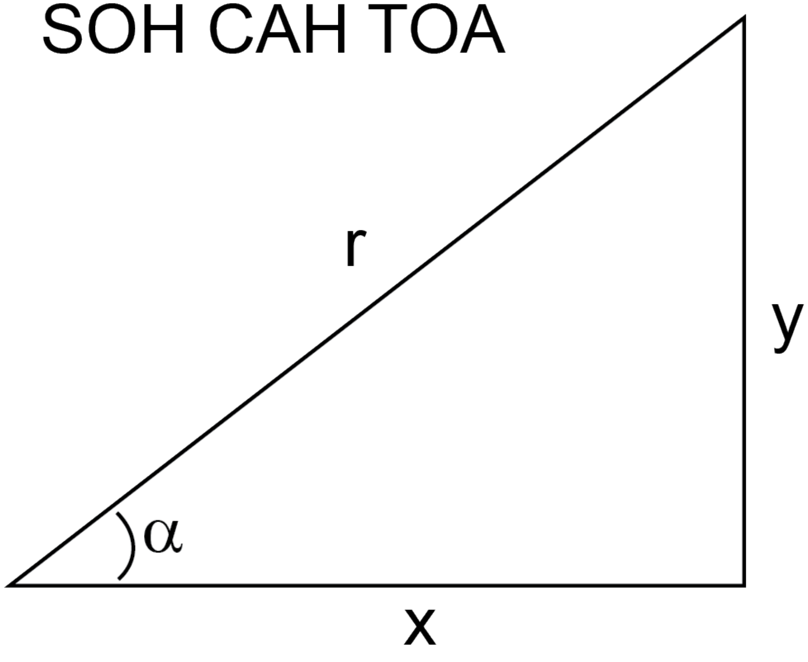
$$? \,K = \text{---}\, °C + 273.15$$

$$? \,°C = \text{---}\, K - 273.15$$

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



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

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

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

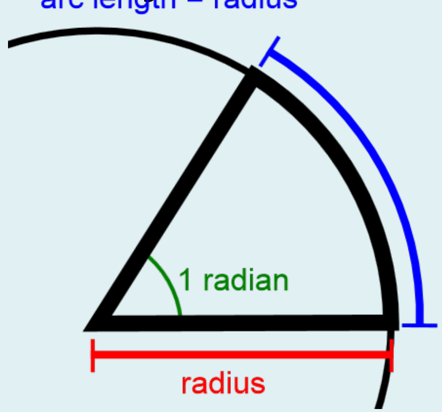
Fractal Units and Lengths of Uneven Surfaces

- 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)

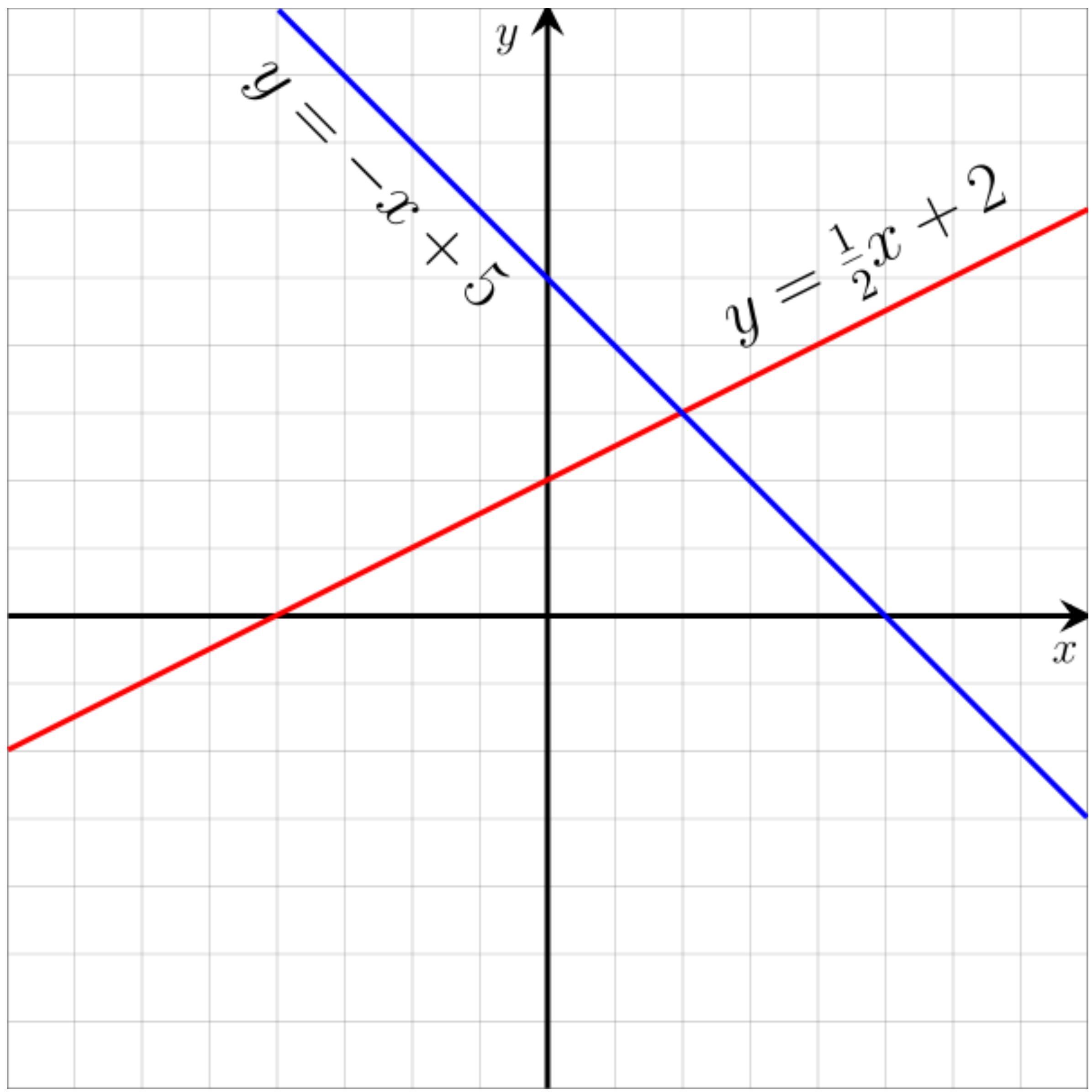
- The origin of the name "linear" comes from the fact that the set of solutions of such an equation forms a straight line in the plane.

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

  b = y-intercept

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

Linear Equation Examples



Reservoirs

- Natural systems can be characterized by the transport or transformation of matter (e.g. water, gases, nutrients, toxics), energy, and organisms between one reservoir and another.
- Reservoirs can be physical (e.g. a human body, the atmosphere, ocean mixed layer), chemical (different chemical species), or biological (e.g. populations, live biomass, dead organic matter)
- Transport/transformation can involve bulk movement of matter, diffusion, convection, conduction, radiation, chemical or nuclear reactions, phase changes, births and deaths, etc.

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

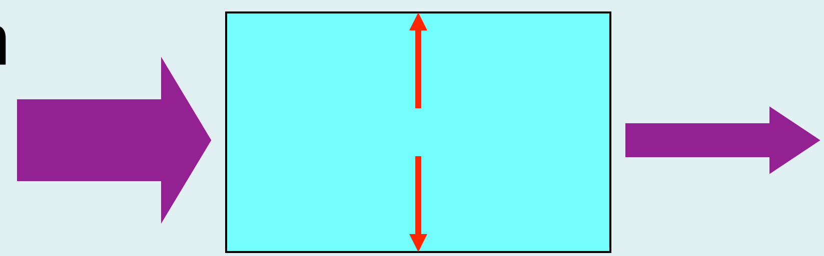
$\Delta S/\Delta t = F_{in} - F_{out}$

Situation 1: Equilibrium

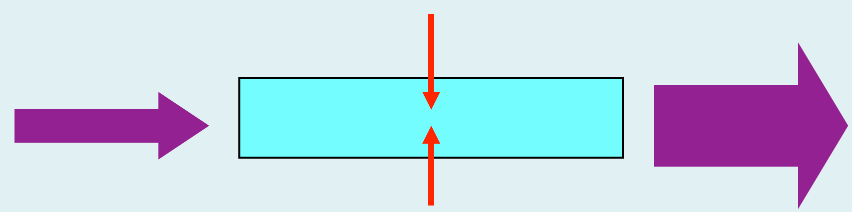
$F_{in} = F_{out}$ $\Delta S/\Delta t = 0$

Situation 2: Non-equilibrium

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



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



Equilibrium: The Balance

- In many problems in environmental science, it is reasonable to start with the assumption that a particular stock is in equilibrium, meaning that *the stock does not change over time*. In this case, we have

$$F_{IN} - F_{OUT} = 0 \rightarrow F_{IN} = F_{OUT} = F$$

- Three types of equilibria
  - static equilibrium: $F_{IN} = 0$, $F_{OUT} = 0$ (nothing is happening)
  - steady state: $F_{IN} = F_{OUT} =$ constant (nothing is changing)
  - dynamic equilibrium: $F_{IN}(t) = F_{OUT}(t)$ (the changes balance)

We can also make a further distinction between stable equilibria (which tend to persist) and unstable equilibria (which are transitory).

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

The precipitation rate on Earth is 5.18×10^{14} m^3/yr. The amount of water in the atmosphere is 1.3×10^{13} m^3. What is the residence time in days of H_2O in Earth's atmosphere?

- Equation-based
- Unit Analysis

Steady-State Calculations

What 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

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

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

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

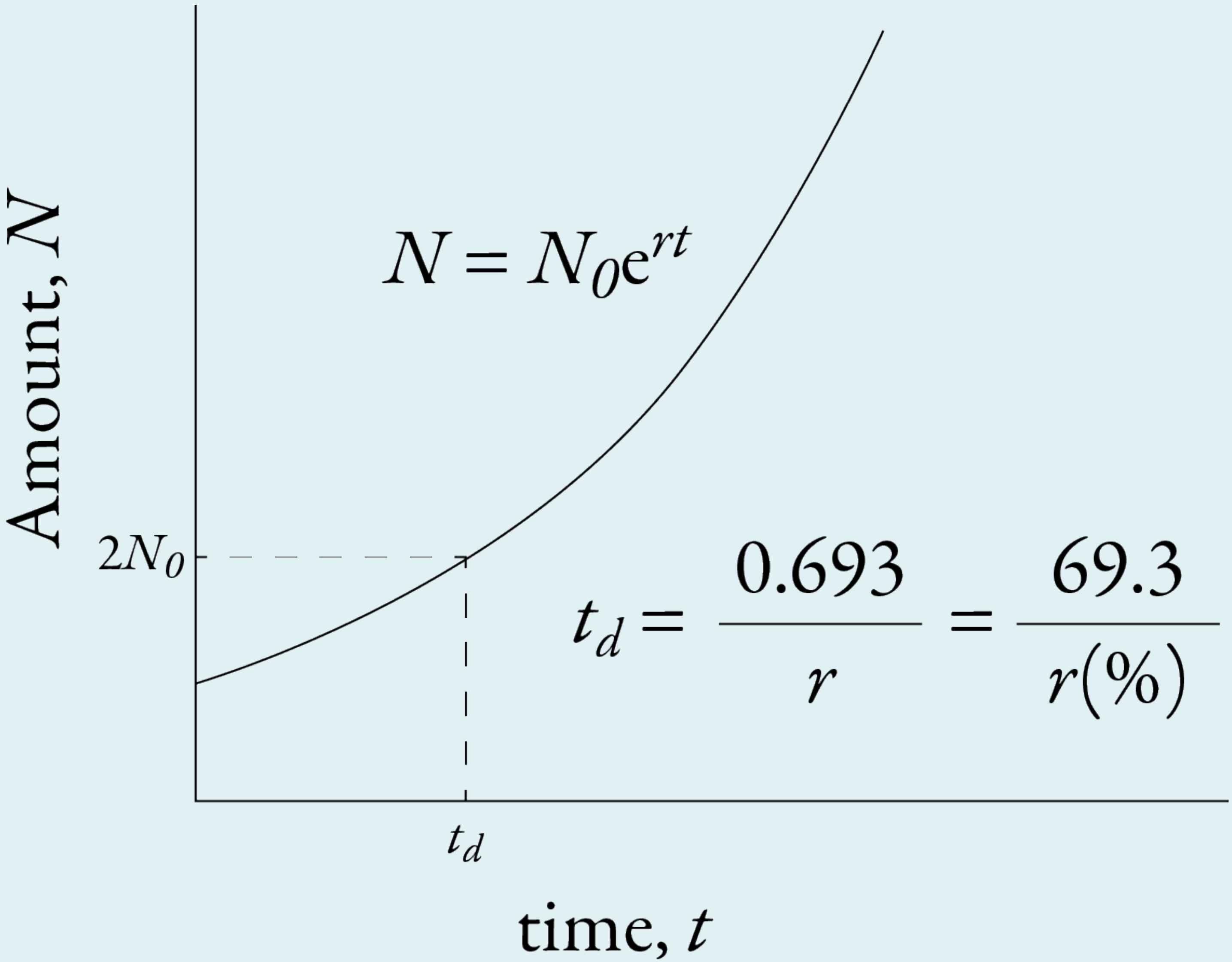
$N(t)$ = amount at time t

N_0 = initial amount

r = rate

t = time

Exponential Growth



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 $\ln e = \ln e^1 = 1$

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

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

$\mathrm{Log}_a b^c = c \log_a b$ 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 $2N_0 = N_0 e^{rt_d}$

$$2 = e^{rt_d}$$

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

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

$$\ln 2 = rt_d$$

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

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

Case C. Exponential Growth of Stocks

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

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

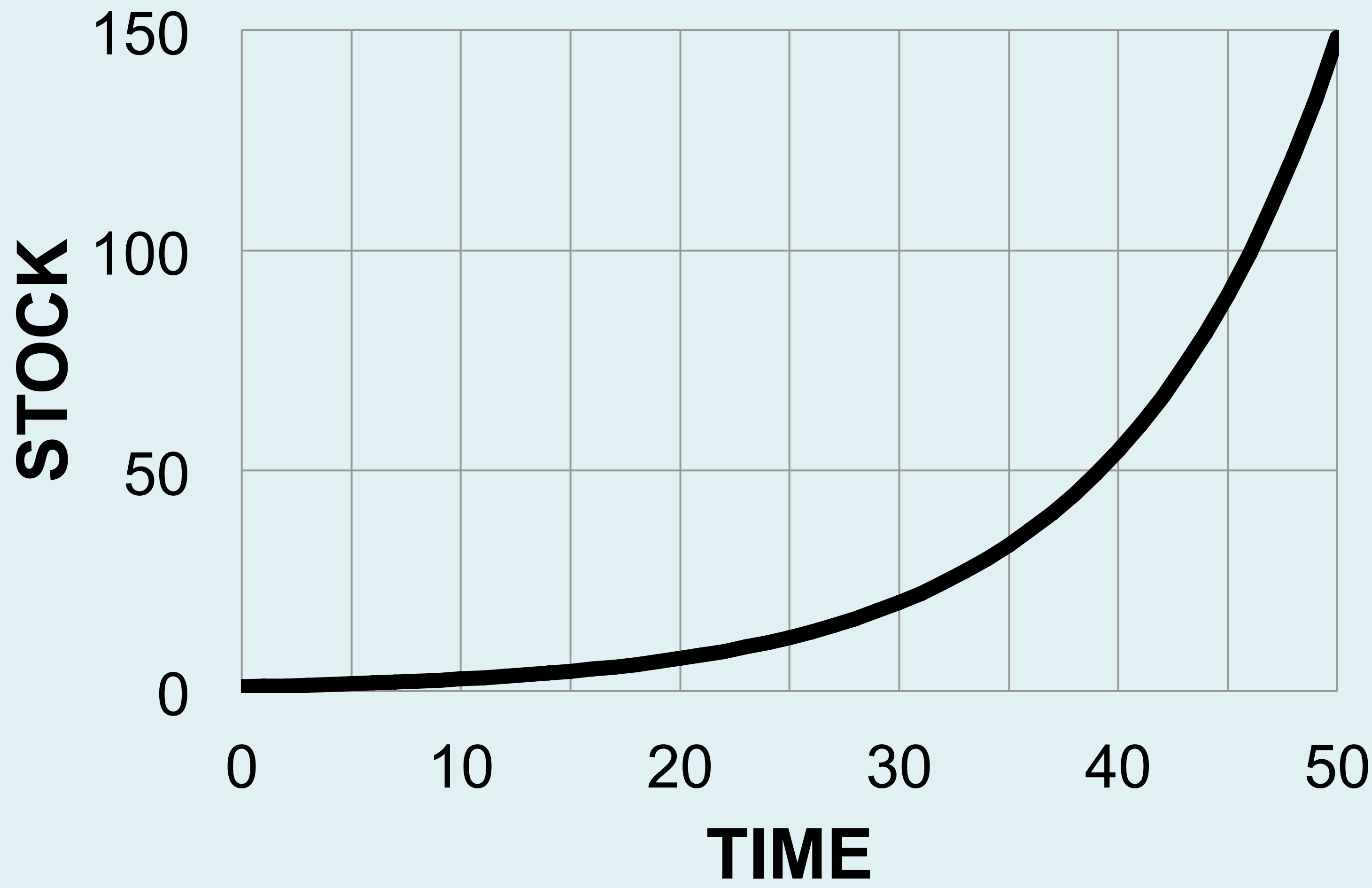
$$\ln(S_t) - \ln(S_0) = \ln\left(\frac{S_t}{S_0}\right) = rt \qquad \boxed{S(t) = S_0\, e^{rt}}$$

- 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: $S(t) = S_0e^{rt}$



Ex. $S_0=1$, $r=0.1/y$

Exponential Decline and Half-Life

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

k = rate $\quad k$ has units of 1/time,

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

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

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

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

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

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

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

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

Exponential Decline of Stocks

- Outflow is proportional to stock.
  $F = -rS$
  $$\boxed{S = S_0 e^{-rt}}$$
- 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?

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

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

Dissociation of Water

- Pure water undergoes a reversible reaction in which both H_3O^+ (H^+) and OH^- are generated.

$$2H_2O(l) \rightleftharpoons H_3O^+(aq) + OH^-(aq)$$

$$H_2O(l) \rightleftharpoons H^+(aq) + OH^-(aq)$$

- The equilibrium constant for this reaction is called the water dissociation constant.

$$K_w = [H^+][OH^-] = 1.01 \times 10^{-14} \quad \text{at } 25\ °C$$

- Because every H^+ (H_3O^+) ion that forms is accompanied by the formation of an OH^- ion, the concentrations of these ions in pure water are the same and can be calculated from K_w.

$$K_w = [H^+][OH^-] = (x)(x) = 1.01 \times 10^{-14}$$

$$x = [H^+] = [OH^-] = 1.01 \times 10^{-7}\ M$$

(1.005×10^{-7} M before

Acidic and Basic Solutions

$$K_w = [H^+][OH^-] = 1.01 \times 10^{-14} \text{ at } 25\ ^\circ C$$

- The equilibrium constant expression shows that the concentrations of H^+ and OH^- in water are linked. As one increases, the other must decrease to keep the product of the concentrations equal to 1.01×10^{-14}.
- If an acid, such as hydrochloric acid, is added to water, the concentration of the H^+ goes up, and the concentration of the OH^- goes down, but the product of those concentrations remains the same. An acidic solution can be defined as a solution in which the $[H^+] > [OH^-]$.
- If a base, such as sodium hydroxide, is added to water, the concentration of the OH^- goes up, and the concentration of the H^+ goes down. A basic solution can be defined as a solution in which the $[H^+] < [OH^-]$.

pH Calculations

- Acidity is measured with pH (from French "pouvoir hydrogene" or "power of hydrogen")

  $pH = -\log [H^+]$

  $[H^+]$ = hydronium ion molarity = 10^{-pH}

  $K_w = [H^+][OH^-] \approx 10^{-14}$

- Example: what is $[H^+]$ and $[OH^-]$ for a solution with a pH = 9?

  $[H^+] = 10^{-pH} = 10^{-9}$ M

  $[OH^-] = K_w/[H^+] = 10^{-14}/10^{-9} = 10^{-5}$ M OH^-