Nano-materials for Energy conversion and storage

NAC 2401

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Chemistry New Building - 1st Floor

Ahmad Alakraa

Reference

- Energy Production, Conversion, Storage, Conservation, and Coupling, Yasar Demirel, **2012**, Springer.

- Nanostructured Materials for Electrochemical Energy Production and Storage, Edson Roberto Leite, **2009**, Springer.

- Thermodynamics: an engineering approach, 8th edition, Yunus A. Çengel and Michael A. Boles, **2015**, McGraw-Hill Education.

Outline

- Introduction & Basic Definitions
- Energy Types
- Energy Production
- Energy Conversion
- Energy Storage
- Electrocatalytic Applications of Nanomaterials

Lecture 1

Introduction and Basic Definitions

Energy: Applications

- All activities in nature involve some interaction between energy and matter

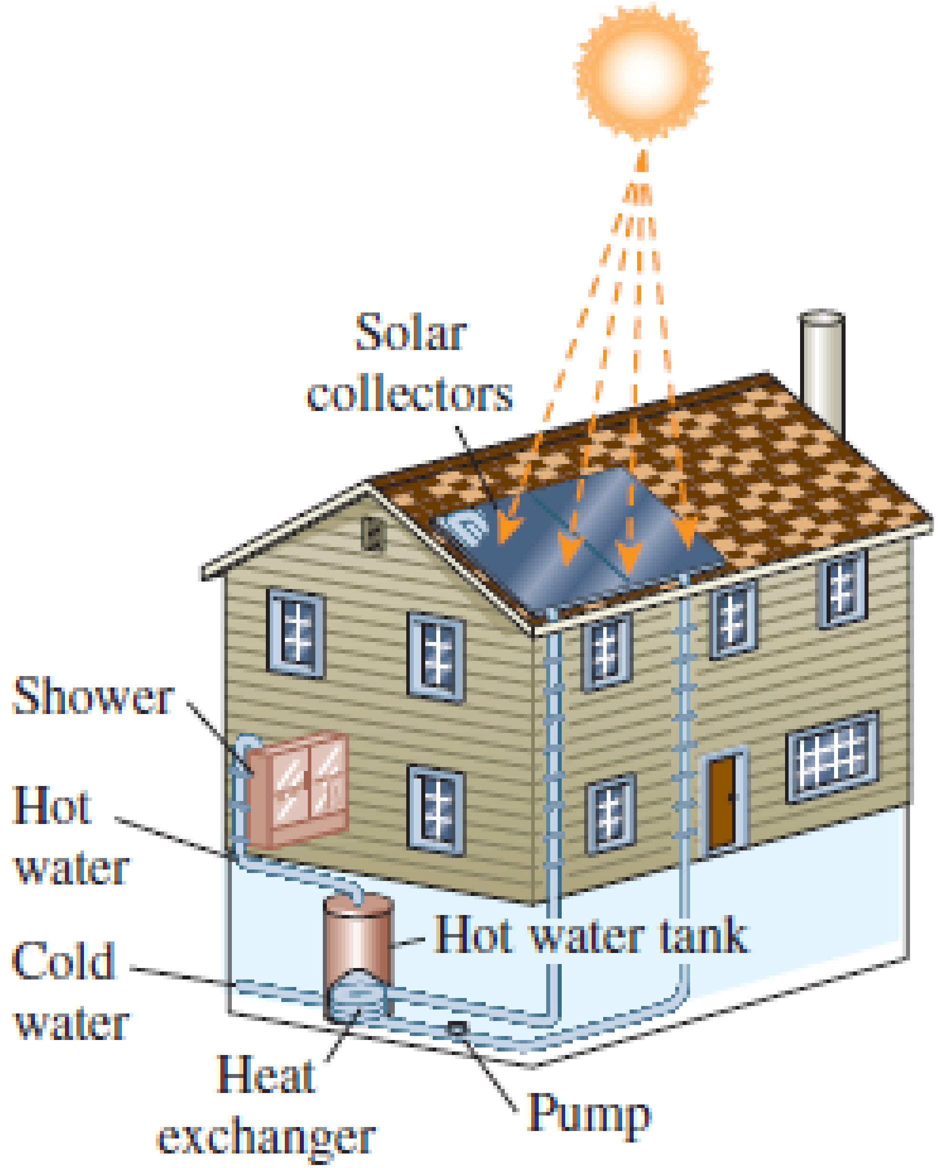
- The body **heat** generated is constantly rejected to the environment.
- The human **comfort** is closely tied to the **rate** of this metabolic heat rejection.
- We try to control this heat transfer rate by adjusting our clothing to the environmental conditions.

- The **heart** is constantly pumping blood to all parts of the human body.
- Various energy conversions occur in trillions of body cells.

Energy: Applications

- The energy-efficient home is designed on the basis of minimizing heat loss in winter and heat gain in summer.

Solar hot water system



Computer and TV

Iron

Refrigerator

Electric/gas range

Humidifier

Water heater

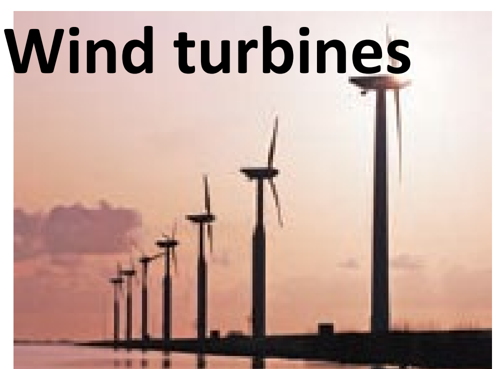
Shower

air-conditioning

Pressure cooker

household utensils أواني and appliances الأجهزة

Energy: applications



0^{th} law of thermodynamics

R H Fowler / 1931

If two bodies are in thermal equilibrium with a third body, they are also in thermal equilibrium with each other

If the third body with a thermometer

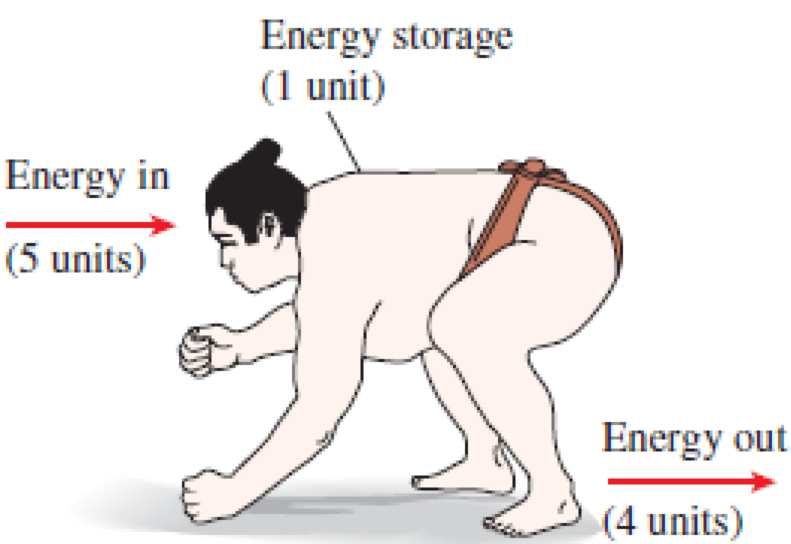
Two bodies are in thermal equilibrium if both have the same temperature reading even if they are not in contact

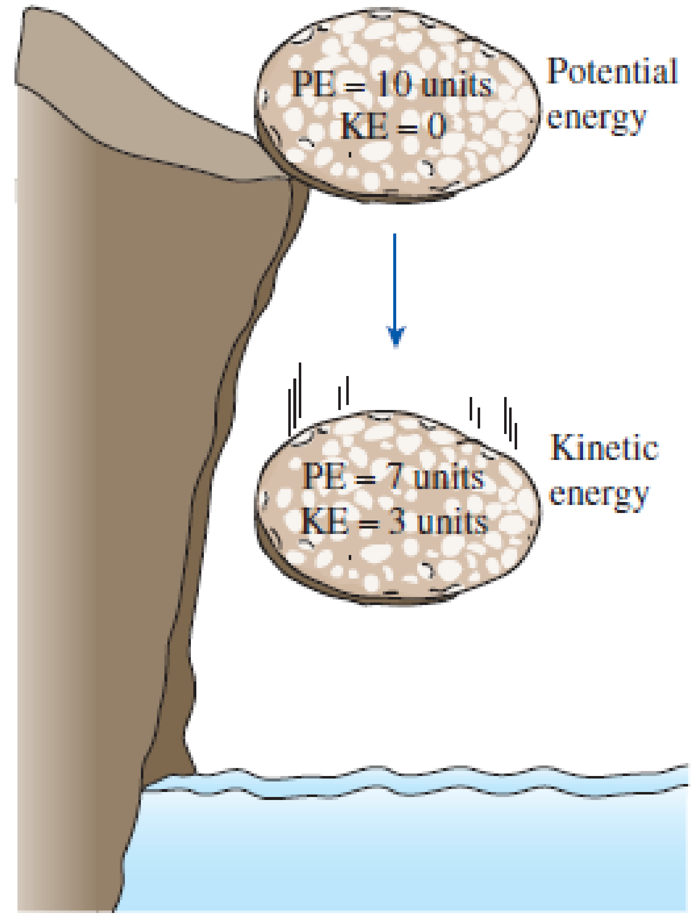
- The 0^{th} law was recognized more than half a century after the formulation of the 1^{st} & 2^{nd} laws of thermodynamics.
- "Zeroth" since it should have preceded the first and the second laws of thermodynamics.

First Law of Thermodynamics

Principle of Energy Conservation

- During an interaction, energy can change from one form to another but the total amount of energy remains constant.
- Energy cannot be created or destroyed.





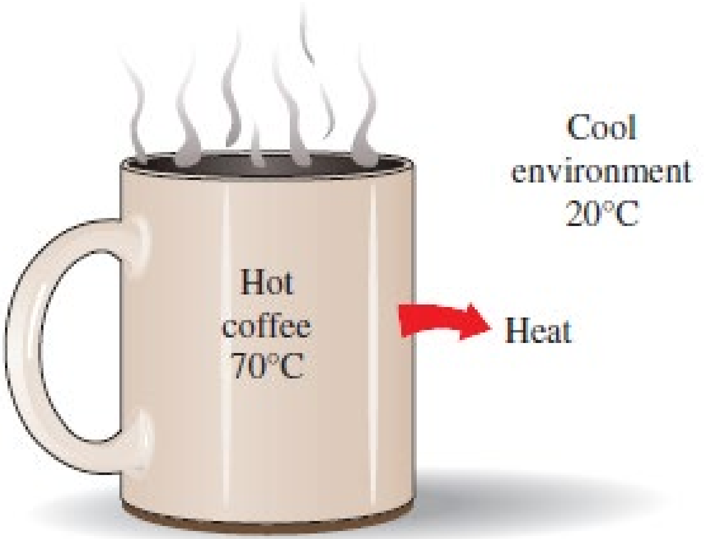
Energy is conserved

You don't get something for nothing

Second Law of Thermodynamics

Energy has quality as well as quantity, and actual processes occur in the direction of decreasing quality of energy.

- Even within the framework of energy conservation, you can not have it just any way you might like it.
- If you think things are going to be perfect, forget it.



Heat flows in the direction of decreasing T

The high-T energy of the coffee is degraded (transformed into a less useful form at a lower T) once it is transferred to the surrounding air.

A cup of hot coffee left on a table eventually cools, but a cup of cool coffee in the same room never gets hot by itself

Absolute Entropy
Third Law of Thermodynamics

The entropy of any pure perfectly crystalline solid is ZERO at the absolute zero (0 K).

Criteria

- Pure: because impure substances would have a finite entropy at 0K (ΔS of mixing the substance with impurities)
- Perfectly: because imperfections would add crystal defects that increase the disordering and S
- Solid: because liquids have a finite entropy even at 0K which equals ΔS of fusion

Energy

- The capacity to do work or to produce heat.
- The ability to cause **changes.**

Basic forms of Energy

Potential Energy

energy due to position or composition.

e.g., attractive and repulsive forces

Kinetic Energy

energy due motion of an object of a mass m and a velocity υ.

$$K.E. = \frac{1}{2} m \upsilon^2$$

Potential Energy

- Any type of stored energy: Chemical, nuclear, gravitational, mechanical.

Kinetic Energy

- is found in movement, e.g., a flying airplane; or vibrating atoms (if they are hot or transmitting sound waves).
- Electricity is the kinetic energy of flowing electrons between atoms.

Energy Conversion/Transformation

- Energy may transfer between systems in three basic forms:
  - → Mass
  - → Heat, q
  - → Work, w

Mechanical work

- When a force acts upon an object to cause a displacement of the object, it is said that work was done upon the object

$$W = F \cdot d = m \cdot g \cdot h \quad (J)$$

(force) . (distance) = (mass). (acceleration) .(height)

$$= P \cdot A \cdot h = P \cdot V$$

(pressure) . (area).(height) (pressure) . (volume)

Work, J

a form of **energy** (force times distance)

$$W = N \times m = J$$

Calorie, Cal

The amount of energy needed to raise the temperature of 1 g of water at 14.5°C by 1°C.

$$1\ \text{cal} = 4.1868\ \text{J}$$

Feel the Unit

If you light a typical match and let it burn itself out, it yields approximately one **kJ** of energy

Units of measurements

SI system

French Système International d'Unités.

7 SI Base UNITS from which all other units are derived

Dimension	Unit	Unit Symbol
Length	meter	m
Mass	kilogram	kg
Time	second	s
Temperature	kelvin	K
Electrical Current	ampere	A
Amount of light	candela	cd
Amount of matter	mole	mol

Recognize the capital and small letters

Standard prefixes in SI Base units

Multiple	Prefix
10^{24}	yotta, Y
10^{21}	zetta, Z
10^{18}	exa, E
10^{15}	peta, P
10^{12}	tera, T
10^{9}	giga, G
10^{6}	mega, M
10^{3}	kilo, k
10^{2}	hecto, h
10^{1}	deka, da
10^{-1}	deci, d
10^{-2}	centi, c
10^{-3}	milli, m
10^{-6}	micro, μ
10^{-9}	nano, n
10^{-12}	pico, p
10^{-15}	femto, f
10^{-18}	atto, a
10^{-21}	zepto, z
10^{-24}	yocto, y

Other Derived SI Units

Physical quantity	Symbol (s)	Name of SI unit	Derived Unit	Definition
Frequency	v, f	Hertz	Hz	s^{-1}
Force	F	Newton	N	$kg\ m\ s^{-2} = J\ m^{-1}$
Energy	E, H,V, etc	Joule	J	$N\ m = kg\ m^2\ s^{-2}$
Pressure	P	Pascal	Pa	$N\ m^{-2} = kg\ m^{-1} s^{-2}$
Power	p	Watt	W	$J\ s^{-1} = kg\ m^2\ s^{-3}$
Charge	Q	Coulomb	C	A s
Potential	E,…etc	Volt	V	$J\ A\ s^{-1}$
Resistance	R	Ohm	Ω	$V\ A^{-1}$
Conductance	G	Siemens	S	Ω^{-1}
Capacitance	C	Farad	F	$C\ V^{-1}$

Other Units

Physical quantity	Symbol	SI unit
Area	A	m^2
Volume	V	m^3
Velocity	U, V, c	$m\ s^{-1}$
Acceleration	a, g	$m\ s^{-2}$
Weight	G,W	N
Density	p	$kg\ m^{-3}$
Volume	liter (l)	dm^3
Force	dyne (dyn)	10^{-5} N
Concentration	Molar (M)	$mol\ dm^{-3}$
Energy	Calorie (Cal)	4.18 J
Energy	Erg (erg)	10^{-7} J
Pressure	Atmosphere (atm)	1.013×10^5 Pa
Pressure	(mm Hg)	133.322 Pa
Pressure	Torr (torr)	133.322 Pa
Pressure	Bar	10^5 Pa
Pressure	Atmosphere	760 mm Hg = 76 cm Hg

Mass and length units

Measure	Symbol	Unit name and Abbreviation
Kilogram	kg	1000 g = 2.204 lb = 32.17 oz
Ounce	oz	28.35 g = 6.25×10^{-2} lb
Pound	lb	0.453 kg = 453 g = 16 oz
Ton, long	ton	2240 lb = 1016.046 kg
Ton, short	sh ton	2000 lb = 907.184 kg
Tonne	t	1000 kg
Ångstrőm	Å	1×10^{-10} m = 0.1 nm
Foot	ft	1/3 yd = 0.3048 m = 12 inches
Inch	in	1/36 yd = 1/12 ft = 0.0254 m
Micron	μ	1×10^{-6} m
Mile	mi	5280 ft = 1760 yd = 1609.344 m
Yard	yd	0.9144 m = 3 ft = 36 in

Pressure

is the force per unit cross-sectional area applied in a direction perpendicular to the surface of an object.

‘psi’: pounds force per square inch.

1 atm = 14.659 psi.

Table 1.6 Pressure conversion factors [2]

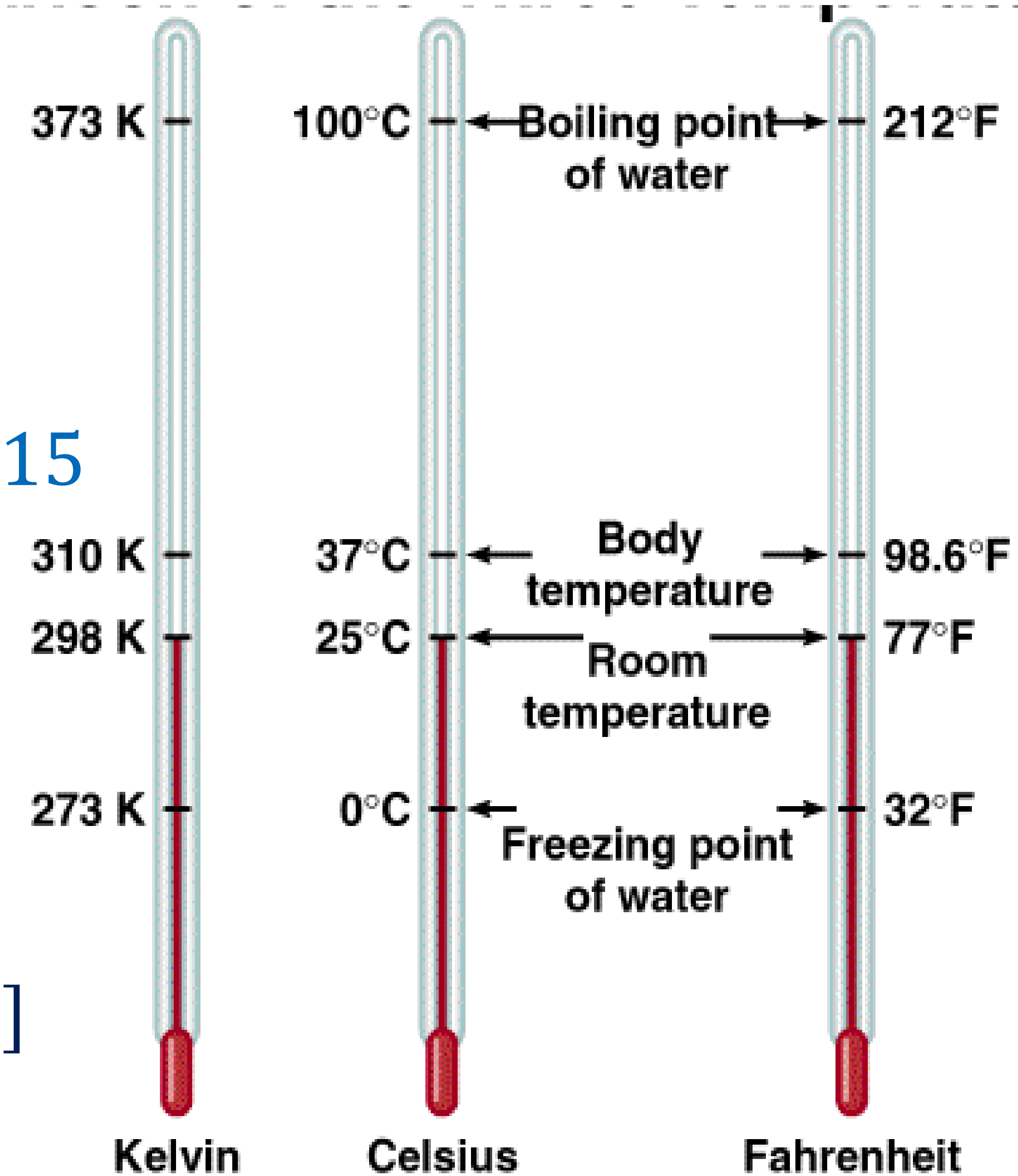
	kPa	Bar	Atm	mm Hg	Psi
kPa	1	10^{-2}	9.869×10^{-3}	7.50	145.04×10^{-3}
Bar	100	1	0.987	750.06	14.503
Atm	101.32	1.013	1	760	14.696
mm Hg	0.133	1.333×10^{-3}	1.316×10^{-3}	1	19.337×10^{-3}
Psi	6.894×10^{3}	68.948×10^{-3}	68.046×10^{-3}	51.715	1

Temperature

$$T(°F) = \frac{9}{5}(°C) + 32$$

$$T(K) = T(°C) + 273.15$$

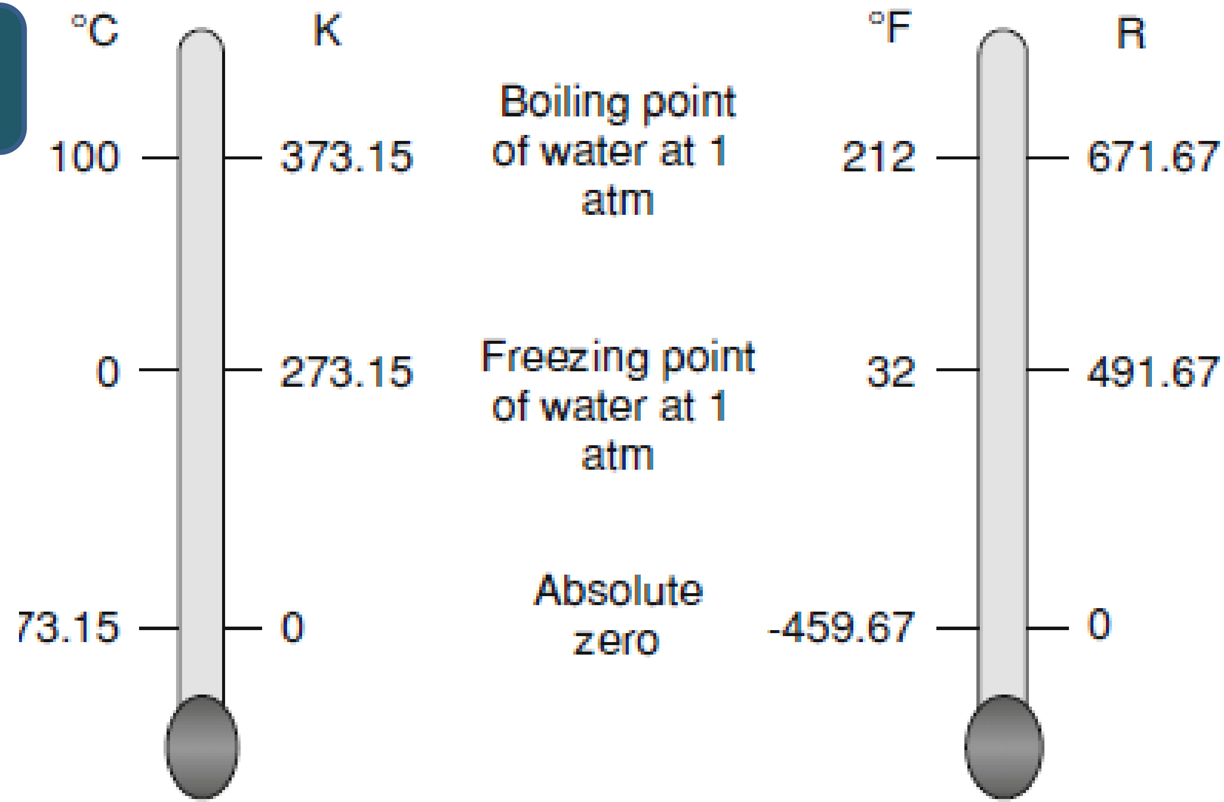
$$T(°C) = \frac{5}{9}[T(°F) - 32]$$



Scales

Rankine scale

Thermodynamic temperature scale in the English engineering system units



Rankine and Fahrenheit temperature scales have the same degree **intervals,** 1R= 1F (difference)

Table 1.5 Temperature units and their definitions

Unit	Symbol	Definition	Conversion	Equation
degree Celsius	°C	°C = K − 273.15	°C = (°F − 32)/1.8	(1.8)
degree Fahrenheit	°F	°F = R − 459.67	°F = °C × 1.8 + 32	(1.9)
degree Rankine	R	R = °F + 459.67	R = K × 1.8	(1.10)
degree Kelvin	K	K = °C + 273.15	K = R/1.8	(1.11)

Exercise

(*a*) Convert 27°C to °F, K, and R.

(*b*) Express a change of 25°C in K and a change of 70 °F in R.

Answer

(*a*)

$$T(°F) = \frac{9}{5}(°C) + 32 = \frac{9}{5}(27) + 32 = \ 80.6°F$$

$$T(K) \ = T(°C) + \ 273.15$$
$$= 27 + 273.15 = 300.1\ K$$

$$T(R) = T(°F) + 460 = 80.6 + 460 = 540.6\ R$$

(*b*) $25\ K$ $\qquad$ $70\ R$

Volume

- is how much a three-dimensional space occupies or contains a substance.

- **Total volume,** V_t of a system may be divided by the mass to calculate specific volume v which is the inverse of density.

Volume Conversions

Name of unit	Symbol	Definitions
Barrel (Imperial)	bl (Imp)	36 gal (Imp) = 0.163 m^3
Barrel	bl; bbl	42 gal (US) = 0.158 m^3
Cubic foot	cu ft	0.028 m^3
Cubic inch	cu in	16.387×10^{-6} m^3
Cubic meter	m^3	1 m^3 = 1000 l
Cubic yard	cu yd	27 cu ft = 0.764 m^3
Gallon (U.S.)	gal (US)	3.785×10^{-3} m^3 = 3.785 l
Ounce	US fl oz	1/128 gal (US) = 29.573×10^{-6} m^3
Pint	pt (US dry)	1/8 gal(US dry) = $550.610 \times 10^{-6} m^3$
Quart	qt (US)	¼ gal (US dry) = 1.101×10^{-3} m^3
Liter	l	1000 cm^3 = 10^{-3} m^3

	in^3	ft^3	U.S. gal	Liters	m^3
in^3	1	5.787×10^{-4}	4.329×10^{-3}	1.639×10^{-2}	1.639×10^{-5}
ft^3	1.728×10^3	1	7.481	28.32	2.832×10^{-2}
U.S. gal	231	0.133	1	3.785	3.785×10^{-3}
Liters	61.03	3.531×10^{-2}	0.264	1	1.000×10^{-3}
m^3	6.102×10^4	35.31	264.2	1000	1

Power

- It is the time **rate** of energy or the rate of doing work.

- Its unit is (**J/s**) $\Rightarrow$ that is called watt (W).

- **Electrical energy** is expressed in kilowatt-hour (kWh), which is equivalent to 3600 kJ.
  - An electric appliance with a rated power of 1 kW consumes 1 kWh of electricity when running continuously for one hour.
  - Do not get confused between kW (power or rate) and kWh (energy) are often confused.

"the new wind turbine will generate **50 kW** of electricity per year"

Incorrect statement

"the new wind turbine with a power of **50 kW** will generate 438000 kWh of electricity per year"

correct statement

Energy of 50 kW for a year

$$= \frac{50\ kJ}{s} \times 1y = \frac{50\ kJ}{s} \times 365 \times 24 \times 60 \times 60\ s = 1576800000\ \mathrm{kJ}$$

$$= 1576800000\ \mathrm{kJ} \times \frac{1\ kWh}{3600\ kJ} = 438000\ kWh$$

Exercise

Energy production from wastewater

What is potential energy benefit of maximum energy recovery using domestic wastewater to a town of 100,000 people?

- Calculate the maximum energy production for assuming 500 L/d per capita, 300 mg/L of COD (chemical oxygen demand), and 14.7 kJ/g COD (based on wastewater solids)?
- How much is this electricity worth at $0.44/kWh?
- How many homes would this power, assuming 1.5 kW/home?

Solution

Environ. Sci. Technol. 2016, 50, 4439−4447

Calculate power in megawatts (MW)

$$P = (10^5 \text{cap})\left(\frac{500\ \text{L}}{\text{d cap}}\right)\left(\frac{1\ \text{d}}{24\ \text{h}}\right)\left(300\,\frac{\text{mg COD}}{\text{L}}\right)\left(\frac{\text{g COD}}{10^3 \text{mg}}\right)\left(\frac{14.7\ \text{kJ}}{\text{g COD}}\right)\left(\frac{1\ \text{kWh}}{3600\ \text{kJ}}\right)\left(\frac{\text{MW}}{10^3\ \text{kW}}\right) = 2.6\ \text{MW}$$

Cost per year

$$\text{Value} = (2.6\ \text{MW})\left(\frac{10^3 \text{kW}}{\text{MW}}\right)\left(\frac{24 \times 365\ \text{h}}{1\ \text{yr}}\right)\left(\frac{\$\,0.44}{\text{kWh}}\right) = \$10 \times 10^6 \text{yr}^{-1}$$

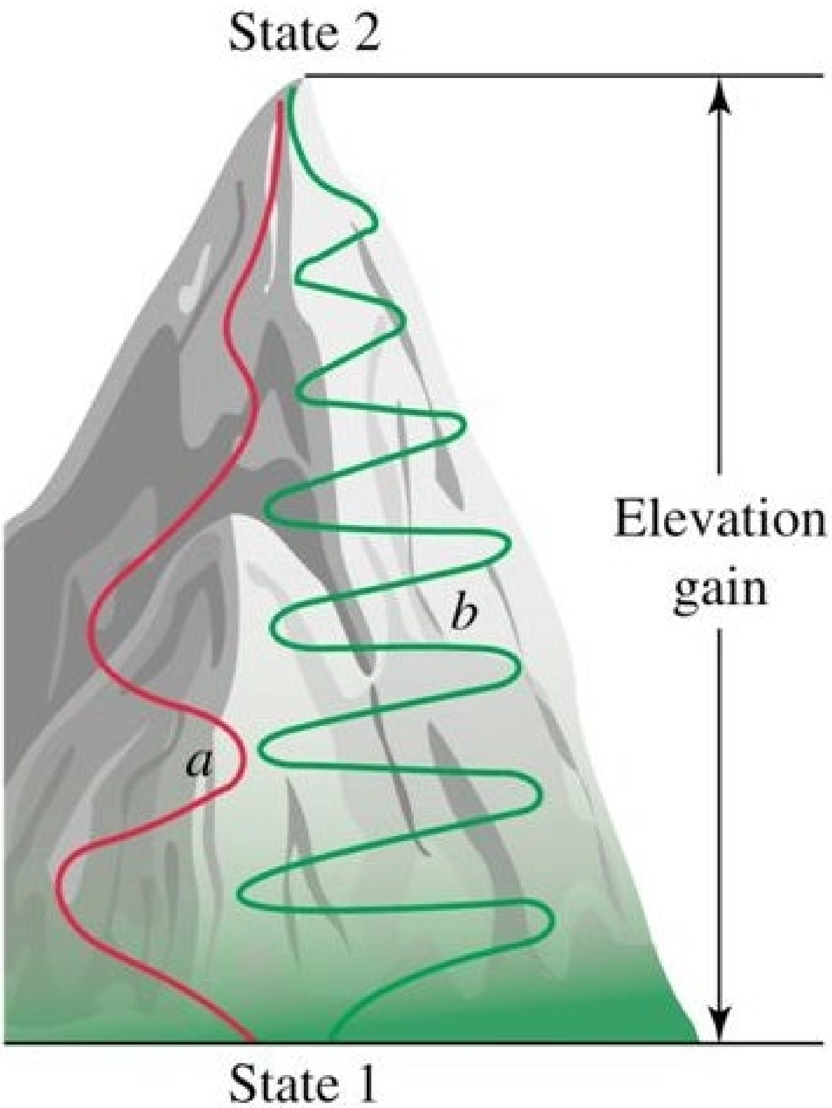
no. of homes

$$\text{homes} = (2.6\ \text{MW})\left(\frac{10^3\text{kW}}{\text{MW}}\right)\left(\frac{\text{home}}{1.5\ \text{kW}}\right)$$

$$= 1700\ \text{home}$$

- This assumed **100 %** energy recovery, which is hopeful but not reasonable. A recovery of 25-50 % of the energy is more logic.

State (path-independent) functions



- ✓ A change in state functions is independent of the particular pathway taken between the two states.

- ✓ ΔE is a state function; however, work and heat are both non-state functions (depend on the pathway) .

State/Non-state functions

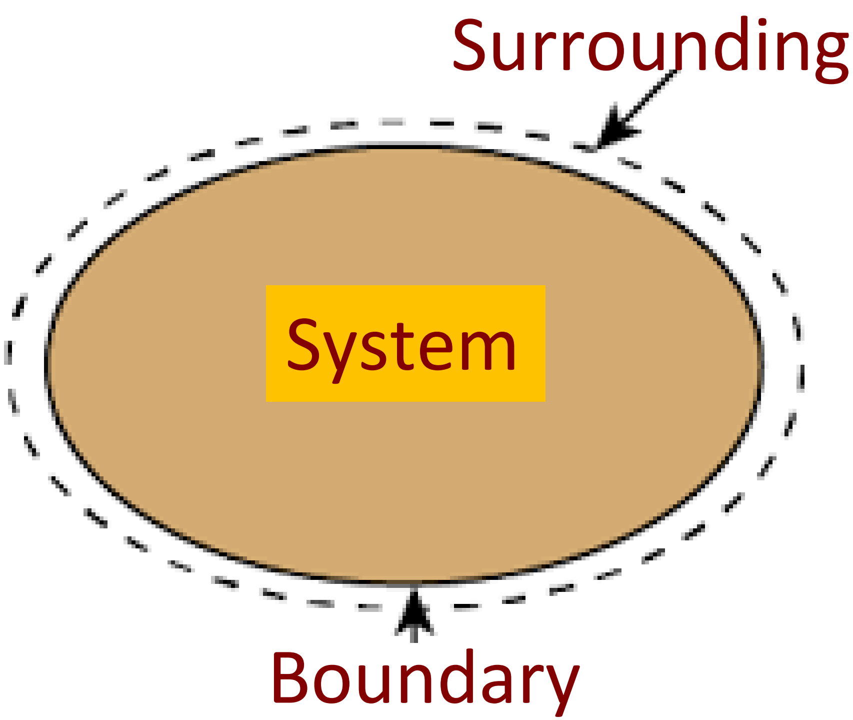
- **State property (Functions):** Functions which depend on the initial and final states of the system, not on the path it takes. (e.g., Internal energy, Temperature, Volume, Pressure).

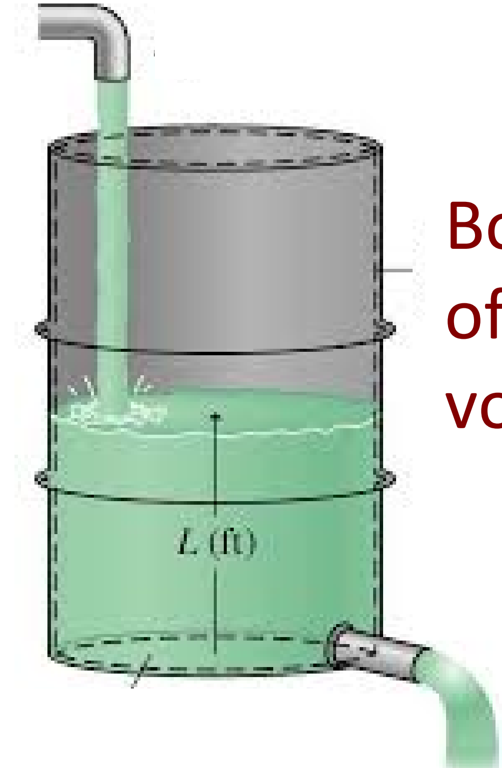
- **Path or non-State property (Functions):** Functions which depend not only on the initial and final states of the system, but also on the path it takes. (e.g., **Heat** and **Work**; written dq or dw. Never written **Δq** or **Δw**).

Thermodynamics is largely concerned with relations between state functions which characterize systems.

System/Surroundings

- **System**: volume of interest (reaction vessel, test tube, biological cell, atmosphere, etc.)
- **Surroundings**: volume outside a system



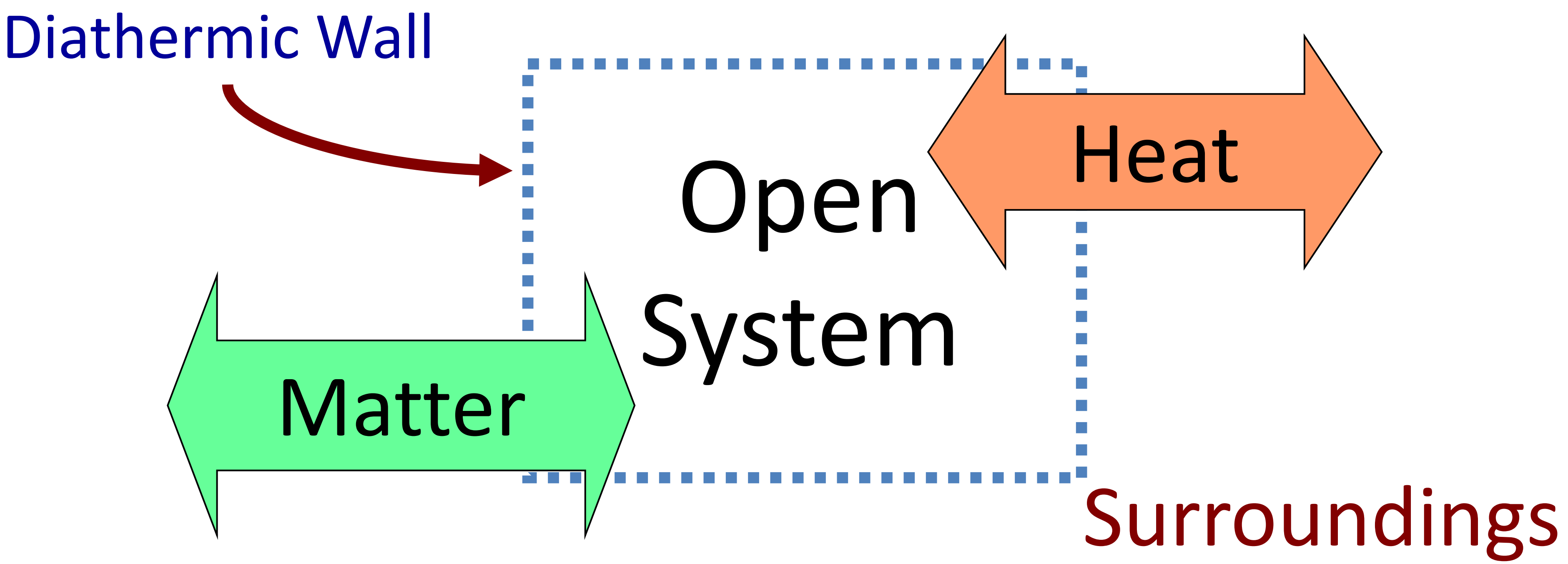


- Mathematically speaking, the **boundary** (fixed or movable) has zero thickness, and thus it can neither contain any mass nor occupy any volume in space.

Open (control volume) systems

A system permitting the heat (Energy) and mass transfer between system & surroundings

- **Diathermic Walls:** Walls permitting energy transfer as heat (such as steel and glass) ('dia' is the Greek word for "through").



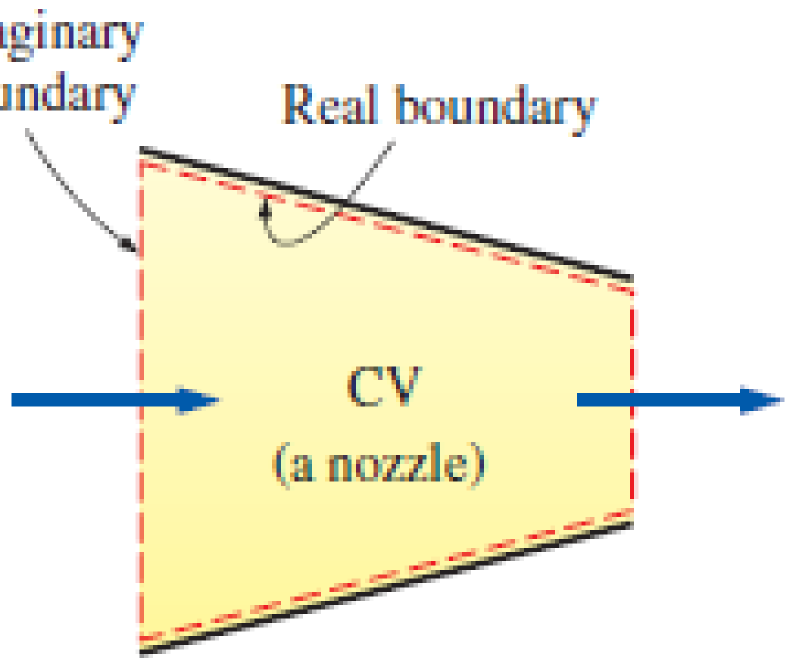
Open (control volume) systems

- usually encloses a device that involves mass flow such as a water heater, a car radiator, compressor, turbine, or nozzle.

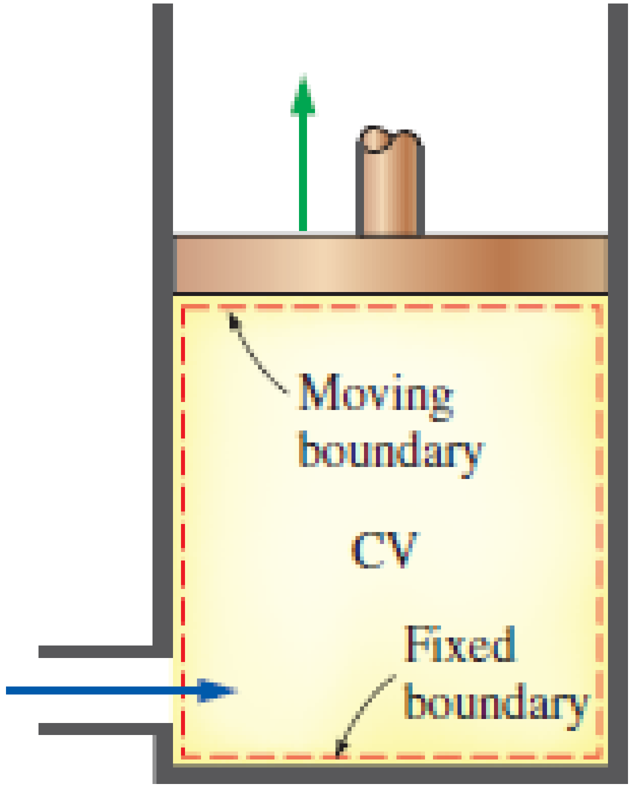
- Flow of air through a nozzle is a good example for the **control volume** would be the region within the nozzle.

- The boundaries of a control volume are called a **control surface**, and they can be real or imaginary.
  - In the case of a nozzle, the inner surface of the nozzle forms the real part of the boundary, and the entrance and exit areas form the imaginary part, since there are no physical surfaces there.

Open Systems



A control volume with real and imaginary boundaries

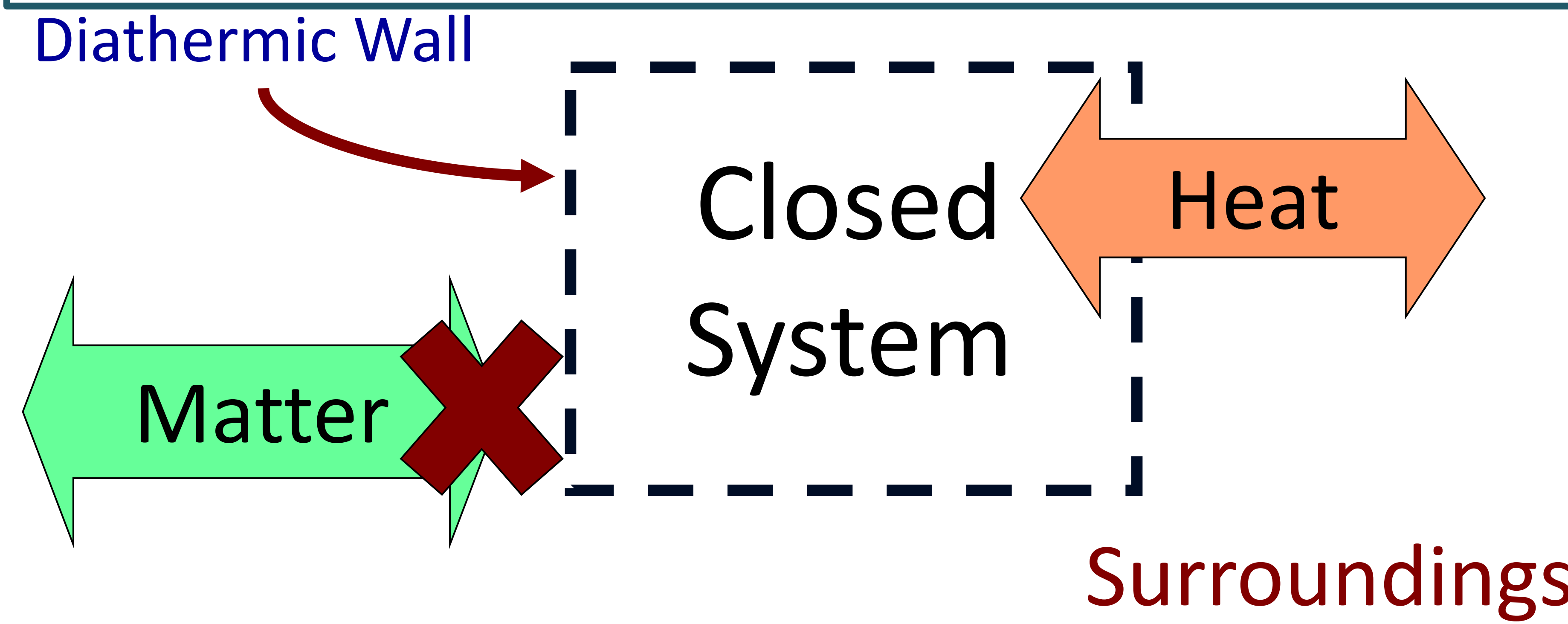


A control volume with fixed and moving boundaries as well as real and imaginary boundaries

Control volume systems can involve heat, work, and mass interaction.

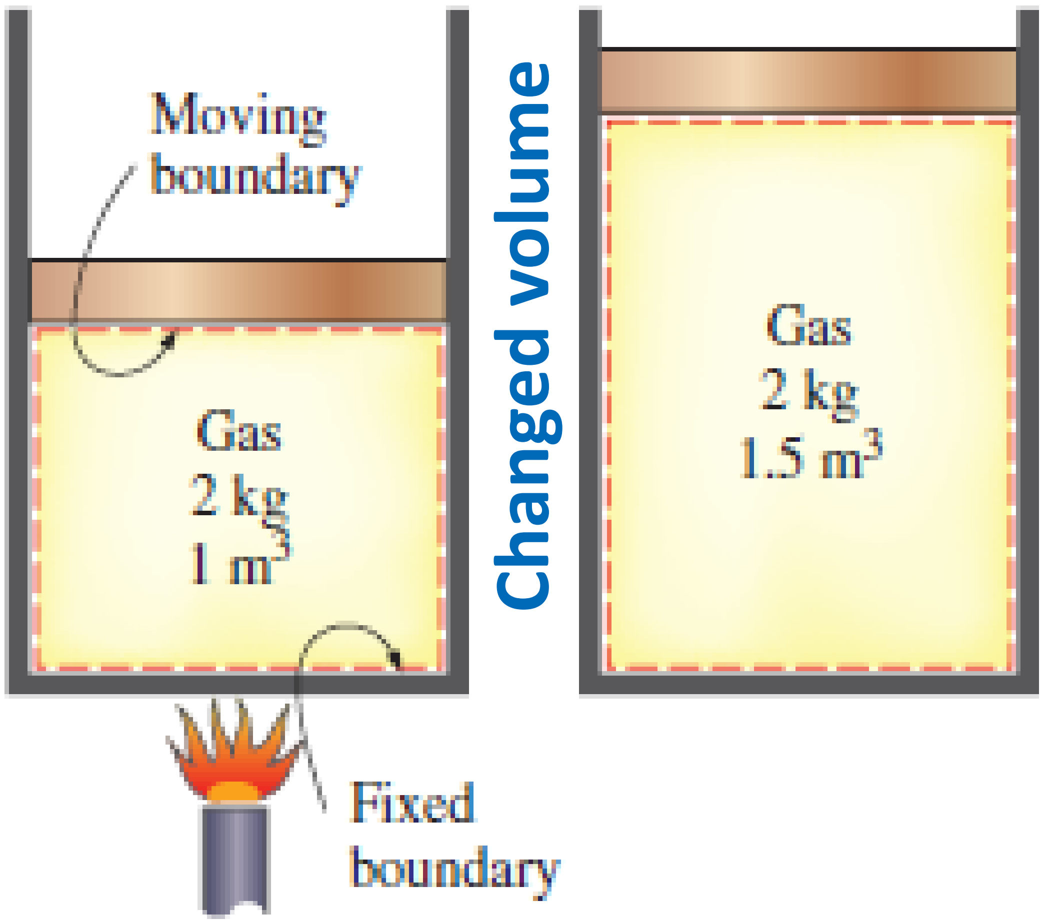
Closed (or control mass) systems

- consists of a fixed amount of mass, and no mass can cross its boundary.
- permits the exchange of heat and work but not mass between system & surroundings



A closed system with a moving boundary

- The volume of a closed system does not have to be fixed.
- If, as a special case, energy is not allowed to cross the boundary, that system is called an isolated system.

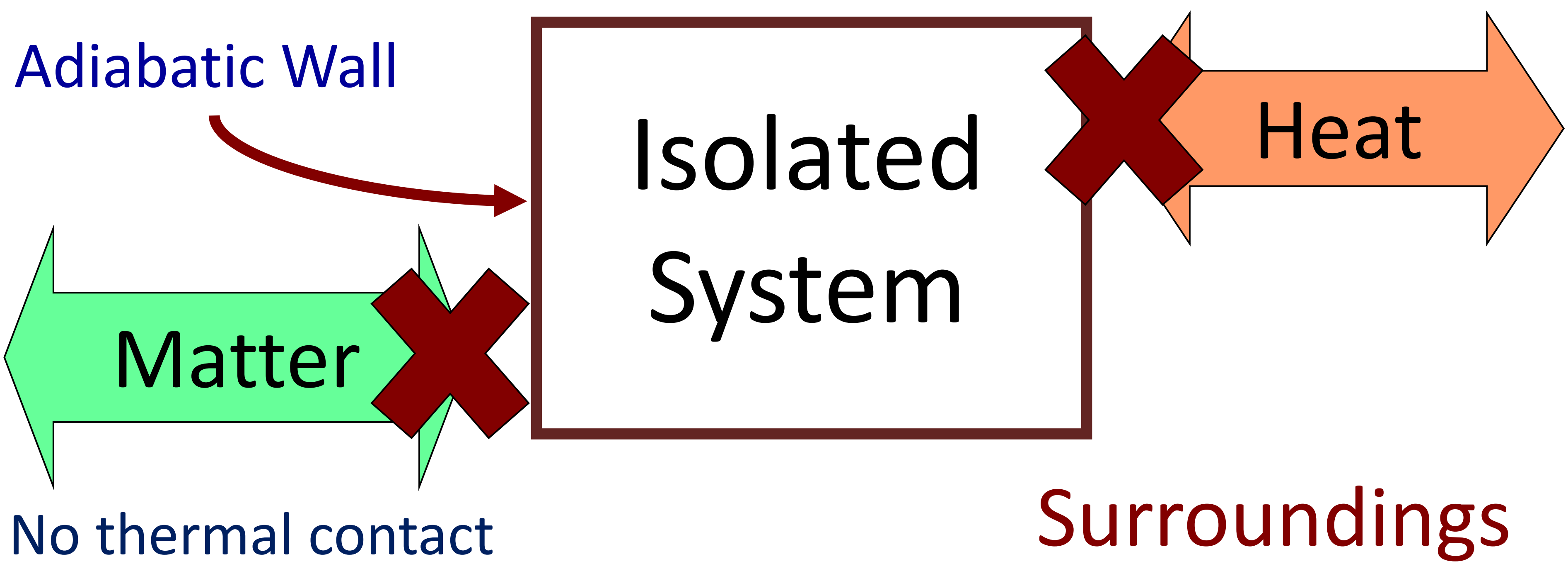


Isolated Systems

A system permitting neither the heat (Energy) nor mass transfer between system & surroundings

- **Adiabatic Walls**: Walls that DO NOT permit energy transfer as heat.

No change in internal energy ($\Delta E=0$)



Systems

homogeneous

- The system has the same properties throughout its extension (a **single** phase)

heterogeneous

- The system is composed of a **number** of homogeneous parts (called **phases**)

Phase

- is a homogeneous, physically distinct, and mechanically separable portion of any heterogeneous system.

Chemical-Heat Energy Transformations

- The combustion of methane: heating homes

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O\,(g) + \text{energy (heat)}$$

- Exothermic Reactions: reactions result in the evolution of heat.

- Endothermic Reactions: reactions that absorb energy from the surroundings.