Importance of Heat

Net Primary Resource Consumption ~97 Quads

Source: Production and end-use data from Energy Information Administration, Annual Energy Review 2002.
*Net fossil-fuel electrical imports.
**Biomass/other includes wood, waste, alcohol, geothermal, solar, and wind.

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Vehicle Systems

- In US, transportation uses ~26% of total energy.
Co-Generation in Residential Buildings

In US, residential and commercial buildings consume ~35% energy supply.

Photo by bunchofpants on Flickr.

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Industrial Waste Heat

Photos by arbyreed and toennesen on Flickr.

Fig. ES.1 in Hemrick, James G., et al. "Refractories for Industrial Processing: Opportunities for Improved Energy Efficiency." DOE-EERE Industrial Technologies Program, January 2005.
Renewable Heat Sources

Photos by Jon Sullivan at http://pdphoto.org/ and NASA.
Photos of solar hot water tubes removed due to copyright restrictions. Please see, for example,
http://image.made-in-china.com/2f0j00KeoavBGJycbN/Unpressurized-Solar-Water-Heater-VERIOUS-.jpg
http://ns2.ugurpc.com/productsimages/solarevacuatedtube_202160.jpg

http://www.treehugger.com/Solar-Thermal-Plant-photo.jpg

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Direct Energy Conversion

Thermoelectrics

Photovoltaics

Thermophotovoltaics
Solar Spectrum

- **AM1.5 Solar Spectrum**
- **Energy Usable for Silicon PV Cells**

Bandgap of Silicon (1.1 μm)

Terrestrial Solar Spectrum (W/m² μm)

Wavelength (μm)

0 0.5 1 1.5 2 2.5 3

0 200 400 600 800 1000 1200 1400 1600 1800

Wavelength (μm)

1000 1200 1400 1600 1800

Temperature (°C)

400 600 800 1000 1200 1400 1600 1800

Wavelength (μm)

0 0.5 1 1.5 2 2.5 3

0 200 400 600 800 1000 1200 1400 1600 1800

Wavelength (μm)
Solar Thermophotovoltaics

- Theoretical maximum efficiency: 85.4%; comparable to that of infinite number of multi-junction cells, but with only a single junction PV cell.
- Key Challenges: Selective surfaces absorbing solar radiation but re-emitting only in a narrow spectrum near the bandgap of photovoltaic cells, working at high temperatures.
Solar Thermoelectrics

- Low materials cost and low capital cost, potentially high efficiency.
- Key Challenges: Develop materials with high thermoelectric figure of merit; and selective surfaces that absorb solar radiation but do not re-radiative heat.
1\textsuperscript{st} Law of Thermodynamics

\[ E_2 - E_1 = Q_{12} - W_{12} \]

\[ dE = \delta Q - \delta W \]

\[ \frac{dE}{dt} = \dot{Q} - \dot{W} \]

State Properties:
- Process Dependent Quantities

\[ E = KE + PE + U \text{ (Internal Energy)} + \ldots \]

Specific Heat \( C = \frac{du}{dT} \) [J/K - kg, or J/K - m\(^3\)]
2\textsuperscript{nd} Law of Thermodynamics

\[ S_2 - S_1 = \int \frac{\delta Q}{T_{\text{boundary}}} + S_{\text{gen}} \ (S_{\text{gen}} \geq 0) \]

Entropy Change
State Properties
Entropy Transfer
Entropy Generation

During a cycle:
\[ \int dS = 0 \]

No entropy generation

Maximum Efficiency (Carnot Efficiency)
\[ \eta = \frac{W}{Q_h} = \frac{Q_h - Q_c}{Q_h} = 1 - \frac{T_c}{T_h} \]

\[ T_h = 223 \ ^\circ C, \ T_c = 23 \ ^\circ C, \ \eta = 40\% \]
\[ T_h = 5800 \ K, \ T_c = 300 \ K, \ \eta = 95\% \]

Thermal power plant \( \eta \approx 40\% \), IC engines \( \eta \approx 25\% \)
Microscopic Picture of Entropy

- **For Isolated Systems**
  - Microstate: a quantum mechanically allowed state
  - A total of $\Omega$ microstate
  - Principle of equal probability: each microstate is equally possible to be observed

Boltzmann Principle

$$S = k_B \ln \Omega$$

**Probability**

$$P = \frac{1}{\Omega}$$

$k_B = 1.38 \times 10^{-23}$ J/K --- Boltzmann constant

- **Constant Temperature and Closed Systems**

$$P(E) = Ae^{-E/(k_BT)}$$

- **Constant Temperature But Open Systems**

$$P(E) = Ae^{-(E-\mu)/(k_BT)}$$

$\mu$ --- chemical potential (driving force for mass diffusion); average energy needed to move a particle in/out off a system
Maxwell distribution

A box of gas molecules

\[ E = \frac{1}{2} m \left( v_x^2 + v_y^2 + v_z^2 \right) \]

\[ P(v_x, v_y, v_z) = A \exp \left[ \frac{m(v_x^2 + v_y^2 + v_z^2)}{2k_B T} \right] \]

All Probability must normalize to one

1 = \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z A \exp \left[ \frac{m(v_x^2 + v_y^2 + v_z^2)}{2k_B T} \right] \quad \Rightarrow \quad A = \left( \frac{m}{2\pi k_B T} \right)^{3/2}

Maxwell Distribution

\[ P(v_x, v_y, v_z) = \left( \frac{m}{2\pi k_B T} \right)^{3/2} \exp \left[ \frac{m(v_x^2 + v_y^2 + v_z^2)}{2k_B T} \right] \]
One molecule

\[
\langle E \rangle = \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \frac{1}{2} m (v_x^2 + v_y^2 + v_z^2) A \exp \left[ -\frac{m (v_x^2 + v_y^2 + v_z^2)}{2k_BT} \right]
\]

\[
\langle E \rangle = \frac{3}{2} k_B T
\]

Equipartition Principle: every quadratic term in microscopic energy contributes \( k_B T/2 \).

How much is \( k_B T \) at room temperature

\[
k_B T = 1.38 \times 10^{-23} \text{ J/K} \times 300 \text{K} = 5.14 \times 10^{-21} \text{ J}
\]

\[
= \frac{5.14 \times 10^{-21} \text{ J}}{1.6 \times 10^{-19} \text{ J/ eV}} = 26 \text{ meV}
\]

Oxygen Atom at 300 K

\[
v = \sqrt{\frac{3k_B T}{m}} = \sqrt{\frac{3 \times 1.38 \times 10^{-23} \text{ J/K} \times 300 \text{K}}{16 \times 1.67 \times 10^{-27} \text{ kg}} } = 220 \text{ m/s}
\]
Fermi-Dirac Distribution

- From quantum mechanics
  - Energy levels are quantized
  - Each quantum state can have maximum one electron
  - Planck-Einstein Relation
  - Planck constant $\hbar = 6.6 \times 10^{-34}$ Js

- Consider one quantum state with an energy $E$ at constant temperature $T$. The state can have zero electron ($n=0$) or one electron ($n=1$). What is the average number of electrons if one does many observations?

\[
1 = \sum_{n=0,1} A e^{-(E-\mu)/(k_B T)} = A \exp\left(\frac{\mu}{k_B T}\right)\left[1 + \exp\left(-\frac{E}{k_B T}\right)\right]
\]

- Average number of electrons in the state

Energy: $E = h \nu = \hbar \omega$

Momentum: $p = h/\lambda = \hbar k$

\[
\hbar = \frac{h}{2\pi}
\]
Fermi-Dirac Distribution

- Average number of electrons in the state

\[
f = \sum_{n=0,1} nAe^{-(E-\mu)/(k_BT)} = \frac{1}{\exp\left(\frac{E-\mu}{k_BT}\right) + 1}
\]

At T=0K, \( \mu \) is called Fermi level, \( E_f \)

\( F=1 \) for \( E<\mu \)
\( F=0 \) for \( E>\mu \)
Photons and Phonons

- From quantum mechanics
  - EM waves are quantized, basic energy quanta is called a photon
  - Photon has momentum
  - Planck-Einstein Relation
  - Each quantum state of photon (an EM wave mode) can have only integral number of photons

- Classical Oscillator

One Photon

Energy: \( E = h \nu = \hbar \omega \)

Momentum: \( p = h/\lambda = \hbar k \)

\( h = 6.6 \times 10^{-34} \text{ Js}; \hbar = h/(2\pi) \)

Energy of a quantum state:

\[
E = \left(n + \frac{1}{2}\right) \hbar \omega \quad n = 0, 1, 2, ...
\]

↑ Zero point energy

Natural Frequency

\[
\nu = \frac{1}{2\pi} \sqrt{\frac{K}{M}}
\]

Energy of Mode

\[
E = \left(n + \frac{1}{2}\right) \hbar \omega \quad n = 0, 1, 2, ...
\]

Basic vibrational energy quanta \( h\nu \) is called a phonon
Bose-Einstein Distribution

- Consider one quantum state in thermal equilibrium

\[ P(E_n) = A e^{-\frac{(E_n - \mu)}{k_B T}} \]

- Bose-Einstein Distribution

Average number of photons/phonons in one mode (quantum state)

\[ f = \frac{1}{\exp\left(\frac{E - \mu}{k_B T}\right) - 1} \]

Usually \( \mu = 0 \)
Heat Transfer Modes

**Heat Conduction**

- **Fourier Law**
  \[ \dot{Q} = -kA \frac{dT}{dx} \text{ [W]} \]
- **Heat Flux**
  \[ \dot{q} = -k \frac{dT}{dx} \text{ (= -kV)} \text{ [W/m}^2] \]

**Convection**

- **Newton’s law of cooling**
  \[ \dot{Q} = hA(T_w - T_a) \]

**Thermal Radiation**

- **Stefan-Boltzmann Law for Blackbody**
  \[ \dot{Q} = A\sigma T^4 \]
  Stefan-Boltzmann Constant \( \sigma = 5.67 \times 10^{-8} \text{ W/m}^2\text{K}^4 \)

- **Heat transfer**
  \[ \dot{Q} = AF \varepsilon \sigma \left(T_{hot}^4 - T_{cold}^4\right) \]
  View factor \( F = 1 \) for two parallel plates
  Emissivity of two surfaces
Heat Conduction

1D, no heat generation

$$\dot{Q} = kA \frac{T_{\text{hot}} - T_{\text{cold}}}{L} = \frac{T_{\text{hot}} - T_{\text{cold}}}{R_{\text{th}}}$$

Thermal Resistance

$$R_{\text{th}} = \frac{L}{kA}$$

Heat Current $\dot{Q}$

$$\dot{Q} = \frac{1}{hA}$$

Convection
Heat Conduction: Kinetic Picture

- Energy per particle: $E$ [J]
- Number of particles per unit volume: $n$ [1/m$^3$]
- Average random velocity of particles $v$
- Average time between collision of two particles $\tau$---relaxation time
- Average distance travelled between collision $\Lambda = v \tau$---Mean free path

Volumetric specific heat

$$C = \frac{dU}{dT} \left[ \frac{J}{m^3 K} \right]$$

Density

Specific heat per unit mass

$$k = \frac{1}{3} C v \Lambda$$

Energy balance equation:

$$q_x = \frac{1}{2} \left( n E v_x \right) \bigg| _{x-v_x \tau} - \frac{1}{2} \left( n E v_x \right) \bigg| _{x+v_x \tau}$$

$$q_x = -v_x \tau \frac{d(Env_x)}{dx} = -\frac{v^2 \tau}{3} \frac{dU}{dT} \frac{dT}{dx}$$

$$-\frac{v^2 \tau}{3} C \frac{dT}{dx} = -k \frac{dT}{dx}$$

Thermal Conductivity

$$k = \frac{1}{3} C v \Lambda$$
Thermal Radiation: Planck’s Law

Basic Relations

- Frequency $\nu$
- Angular Frequency $\omega = 2\pi \nu$
- Wavelength $\lambda$
- Wavevector magnitude $k = 2\pi / \lambda$
- Wavevector $\mathbf{k} = (k_x, k_y, k_z)$

$$c = \nu \lambda \quad \Rightarrow \quad \omega = ck = c \sqrt{k_x^2 + k_y^2 + k_z^2}$$

$\omega(k)$: Dispersion relation (linear)

How much energy in the cavity?

$$U = 2 \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} \sum_{n_z=1}^{\infty} \hbar \omega f(\omega, T) =$$

$$= 2 \int_0^{\infty} \frac{dk_x}{(2\pi / L_x)} \int_0^{\infty} \frac{dk_y}{(2\pi / L_y)} \int_0^{\infty} \frac{dk_z}{(2\pi / L_z)} \hbar \omega f(\omega, T)$$

Two polarization
Thermal Radiation: Planck’s Law

\[ U = \frac{2V}{8\pi^3} \int \int \int_{-\infty}^{\infty} \hbar \omega f(\omega, T) dk_x dk_y dk_z \]
\[ = \frac{2V}{8\pi^3} \int_0^{\infty} \hbar \omega f(\omega, T) 4\pi k^2 dk \]
\[ = \frac{2V}{8\pi^3} \int_0^{\infty} \hbar \omega f(\omega, T) 4\pi \left( \frac{\omega}{c} \right)^2 d\left( \frac{\omega}{c} \right) \]
\[ \frac{U}{V} = \int_0^{\infty} \hbar \omega f(\omega, T) \frac{\omega^2}{\pi^2 c^3} d\omega \]
\[ = \int_0^{\infty} \hbar \omega f(\omega, T) D(\omega) d\omega \]
\[ = \int_0^{\infty} u(\omega) d\omega \]

\( D(\omega) \)-density of states per unit volume per unit angular frequency interval

- Energy density per \( \omega \) interval
  \[ u(\omega) = \hbar \omega f(\omega, T) D(\omega) \]
  \[ = \frac{\hbar \omega^3}{\pi^2 c^3} \frac{1}{\exp\left( \frac{\hbar \omega}{k_B T} \right) - 1} \]
  Planck’s law

- Intensity: energy flux per unit solid angle
  \[ I(\omega) = \frac{c u(\omega)}{4\pi} = \frac{\hbar \omega^3}{4\pi^2 c^2} \frac{1}{\exp\left( \frac{\hbar \omega}{k_B T} \right) - 1} \]

\[ d\Omega = \frac{dA_p}{R^2} \]

\[ I(\lambda) = \frac{I(\omega)d\omega}{d\lambda} = \frac{4\pi \hbar}{\lambda^5} \frac{1}{\exp\left( \frac{2\pi \hbar c}{k_B T \lambda} \right) - 1} \]

Planck’s law
Thermal Radiation: Planck’s Law

Wien’s displacement law

\[ \lambda_{\text{max}} T = 2898 \ \text{K}\mu\text{m} \]

Emissive Power

\[
\dot{Q}(\lambda) = A \pi l(\lambda)
= A \frac{\hbar \omega^3}{4\pi^2 c^2} \frac{1}{\exp\left(\frac{\hbar \omega}{k_B T}\right) - 1}
\]

Total

\[
\dot{Q} = \int_0^{\infty} \dot{Q}(\lambda) d\lambda = A \sigma T^4
\]
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