Nano-materials for Energy conversion and storage

NAC 2401: Lecture 3

Energy: types

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Energy Types

Energy

Primary

- extracted or captured directly from environment, e.g.,
  - **Nonrenewable** (fossil fuels): coal, crude oil, natural gas, nuclear fuel.
  - **Renewable**: hydropower, biomass, solar energy, wind, geothermal, and ocean energy.
  - **Waste**.

Secondary

- is converted from the primary energy in the form of electricity or fuel (gasoline, fuel oil, methanol, ethanol, and hydrogen).

Final Energy:

Electricity + Fuel

Fossil Fuels: Coal, Crude Oil, Natural Gas

- are formed from the **remains** of dead plants and animals by exposure to heat and pressure in the earth's crust over the millions of years.

- contain high percentages of **carbon**.

Coal

Black Anthracites Hard Coal

Black bituminous coal

Brown coal (lignite)

https://energyeducation.ca/encyclopedia/Types_of_hydrogen_fuel

Coal

- are sedimentary rocks containing combustible and incombustible matters as well as water.
- comes in various composition and energy content depending on the source and type.
- cheaper than petroleum oil.
- has impurities like sulfur and nitrogen and when it burns the released impurities can combine with water vapor in air to form droplets that fall to earth as weak forms of sulfuric and nitric acid (**acid rain**).
- contains **minerals**, which do not burn and make up the **ash** left behind in a coal combustor.

- **Anthracites:** ~ 90% C, is very hard and shiny and the ultimate maturation, creates a steady and clean flame and is preferred for domestic heating, burns longer with more heat than the other types.

- **Bituminous:** ~70-75% C, ignites easily and burns with a relatively long flame. If improperly fired, excess smoke and soot (amorphous carbon) result.

- **Lignite:** poorest coal with < 50% C and an energy density lower than wood

Table 2.2 Typical properties of various coals

	Anthracite coal	Bituminous coal	Lignite coal
Fixed carbon, weight%	80.5–85.7	44.9–78.2	31.4
Moisture, weight%	2.8–16.3	2.2–15.9	39
Bulk density, lb/ft^3	50–58	42–57	40–54
Ash, weight%	9.7–20.2	3.3–11.7	3.3–11.7
Sulfur, weight%	0.6–0.77	0.7–4.0	0.4

- Because of high carbon content, coals generate more CO_2 per unit of released energy than any other fossil fuel such as crude oil.

- Sulfur content of coal is also a drawback.

- Advanced coal technology can filter out 99% of the tiny particles, remove more than 95% of the acid rain pollutants and reduce the release of CO_2 by burning coal **more efficiently.**

- Many new plants are required to have flue gas desulfurization (FGD) units called **scrubbers**.

Petroleum Oil

Petroleum (Crude Oil)

- is a naturally occurring flammable liquid consisting of a complex **mixture** of **hydrocarbons** of various molecular masses, which define its physical and chemical **properties:** (heating value, color, viscosity).
- The composition of **hydrocarbons** (mostly *alkanes, cycloalkanes* and *various aromatic hydrocarbons*) ranges from as much as 97% by mass in the lighter oils to as little as 50% in the heavier oils.
- Other organic compounds containing nitrogen, oxygen, sulfur, and trace amounts of metals exist.

Typical elemental composition by weight of crude oil

Element	Percent range (%)
Carbon	83–87
Hydrogen	10–14
Nitrogen	0.1–2
Oxygen	0.1–1.5
Sulfur	0.5–6
Metals	<0.1

Composition by weight of hydrocarbons in petroleum

Hydrocarbon	Average (%)	Range (%)
Paraffins (alkanes)	30	15–60
Naphtanes (cycloalkanes)	49	30–60
Aromatics	15	3–30
Asphaltics	6	Remainder

Alkanes (paraffin)

- are saturated **hydrocarbons** with straight or branched chains with formula C_nH_{2n+2}.
- generally, have from 5 to 40 carbon atoms per molecule.
- Paraffin wax is an alkane with approximately 25 carbon atoms, while asphalt has 35 and up.
- These long chain alkanes are usually cracked by modern refineries into lighter and more valuable products.

Cycloalkanes (naphthenes)

- are saturated **hydrocarbons** with one or more carbon rings to which hydrogen atoms are attached according to the formula C_nH_{2n}.
- have similar properties to alkanes with **higher** boiling points.

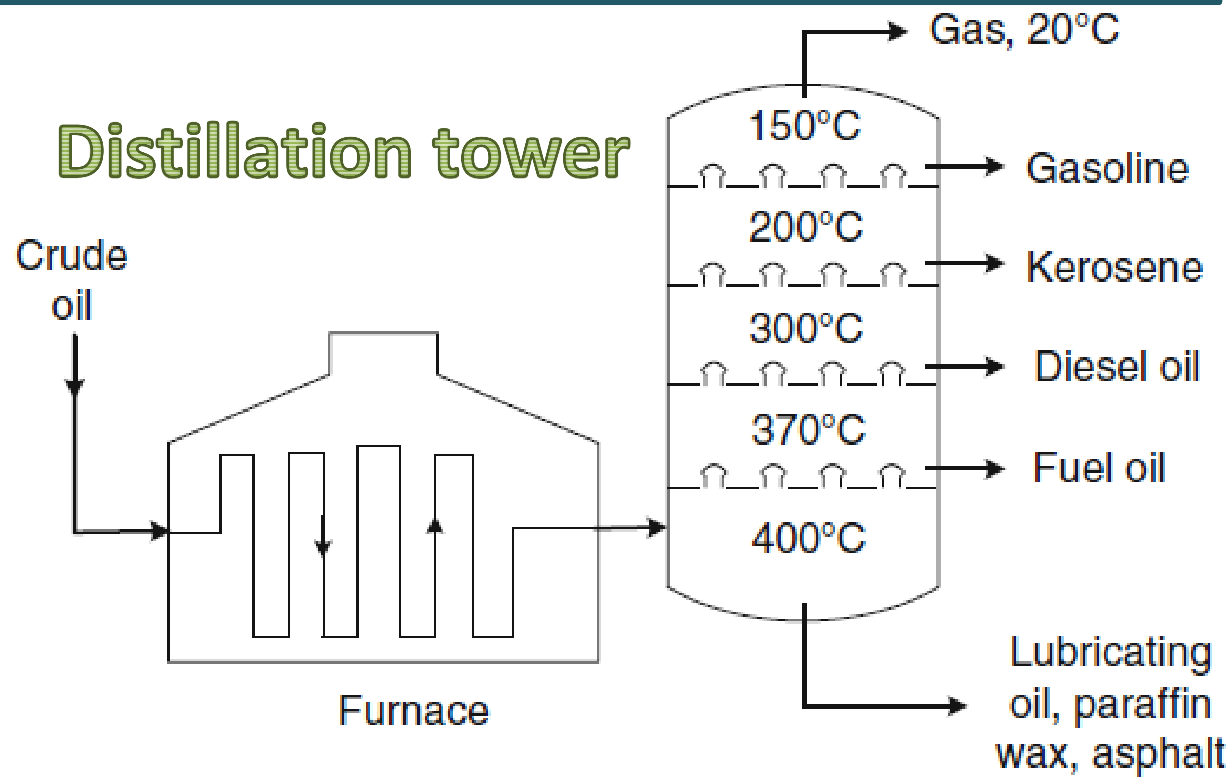
Aromatics (unsaturated hydrocarbons)

- have one or more **six-carbon rings** called **benzene** rings with double and single bonds and hydrogen atoms attached according to the formula C_nH_n.

Petroleum Fractions

- Oil is refined and separated into many products, from gasoline and kerosene to asphalt and chemical reagents used to make plastics and pharmaceuticals.

84% by volume of the hydrocarbons in petroleum is converted into energy-rich fuels



Liquefied petroleum gas (LPG)

- is a flammable mixture of propane (C_3H_8) (~ 38% by volume and more in winter) and butane (C_4H_{10}) (about 60% by volume and more in summer).
- is used as a fuel in **heating** appliances and **vehicles**.
- has energy content per kilogram higher than that of gasoline because of higher **H/C ratio**.
- emits 81% of the CO_2 per kWh produced by oil and 70% of that of coal.
- has a typical specific heat of **46.1 MJ/kg** compared with **43.5 MJ/kg** for gasoline. However, its volumetric energy density of **26 MJ/L** is lower than that of gasoline (~ 34.9 MJ/L).
- Pure n-butane is liquefied at ~ 220 kPa (2.2 bar), while pure propane at 2200 kPa (22 bar). At liquid state, the vapor pressure of liquefied petroleum gas is ~ 550 kPa (5.5 bar).

Gasoline

- is primarily used as a fuel in internal combustion engines.
- A typical gasoline consists of hydrocarbons with between 4 and 12 carbon atoms per molecule.
- It consists **mostly** of aliphatic hydrocarbons enhanced with iso-octane or the aromatic toluene and benzene to increase its octane rating (measure of burning efficiency).
- has a specific density of ~ 0.71 to 0.77 (6.175 lb/US gal). Higher densities having a greater volume of aromatics.
- has ~132 MJ/US gal (~34.9 MJ/L, higher heating value than LPG, **26 MJ/L**), while its blends differ by up to 4% more or less than the average.
- CO_2 emission from gasoline is ~ 73.38 g/MJ.

Kerosene

- is a thin, clear liquid formed containing between 6 and 16 carbon atoms per molecule, with density of 0.78–0.81 g/cm^3.

- its **flash point** (*lowest temperature at which the vapor of a combustible liquid can be ignited in air*) is between 37 and 65°C and its autoignition temperature (*temperature required to supply the activation energy needed for combustion*) is 220°C.

- its heat of combustion is like that of diesel: its lower heating value is ~ 43.1 MJ/kg (18,500 Btu/lb), and its higher heating value is 46.2 MJ/kg (19,861 Btu/lb).

Petroleum Diesel/Diesel Oil

- contains 8–21 carbon atoms per molecule with a boiling point in the range of 180–360°C and density of ~ 6.943 lb/gal.
- ~86.1% of the fuel mass is carbon and it offers a net heating value of around 43.1 MJ/kg (lower than LPG, 46.1 MJ/kg).
- With its higher density, it offers a higher volumetric energy density at 128,700 Btu/gal versus 115,500 Btu/gal for gasoline.
- CO_2 emissions are 73.25 g/MJ, (like gasoline).
- additional refining is required to remove sulfur which lead to a higher cost.

Jet Fuel

- is a **mixture** of many different hydrocarbons with density of 0.775-0.840 kg/L at 15°C.
- is a type of ***aviation fuel*** designed for use in aircraft powered by gas turbine engines.
- The commonly used fuels are Jet A and Jet A-1. Both have carbon number between about 8 and 16
- Jet B (containing C number between ~ 5 and 15) is used for its enhanced cold-weather performance.

Fuel Oil

- is made of long hydrocarbon chains, particularly alkanes, cycloalkanes, and aromatics and is heavier than gasoline and naphtha.
- is classified into six classes, numbered 1 through 6, according to its boiling point (175 to 600°C), composition (9-70 C atoms), and purpose.
- With number ↑, price ↓, but heating value ↑ and viscosity ↑, and the heaviest oil must be heated to get it to flow.
- **Number 1** is like kerosene, **number 2** is the diesel fuel that trucks and some cars run on, leading to the name "road diesel". **Number 4** fuel oil is usually a blend of heavy distillate and residual fuel oils. **Number 5 and 6** fuel oils are called residual fuel oils or heavy fuel oils.

Natural Gas

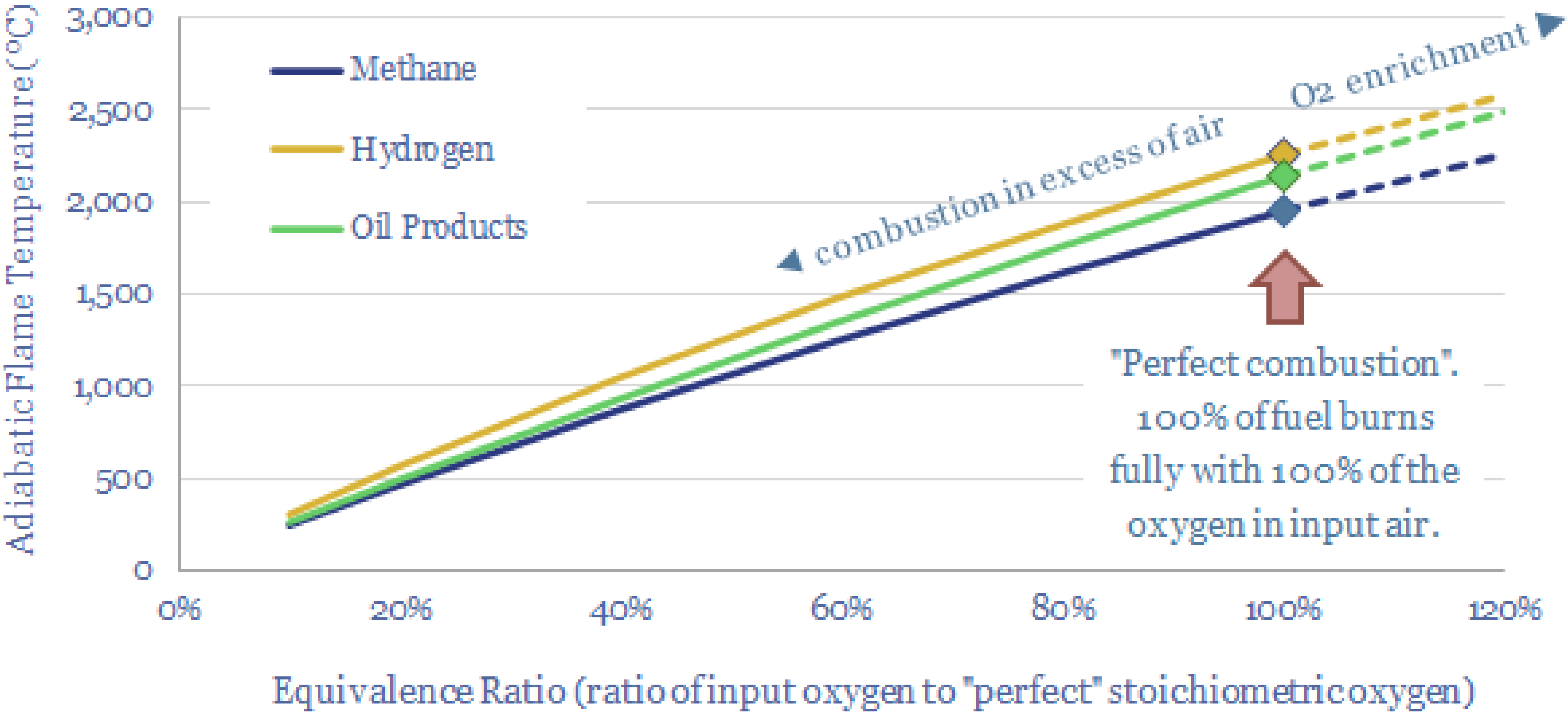
Natural Gas

- is naturally occurring mixture, consisting mainly of methane.

- provides 23% of all energy consumed in the world.

- Typical theoretical flame temperature [**adiabatic flame temperature** *is the temperature reached by a flame under ideal conditions*] of natural gas is 1960°C, [H_2 burns 300°C hotter at 2250°C and oil products burn somewhere in between, at around 2150°C].

https://www.stovepedia.com/



https://thundersaidenergy.com/

Natural Gas

- ignition point [or **fire point:** *is lowest T at which rapid combustion of a fuel will take place in air*] is 593°C.
- is a major source of **electricity** production using gas turbines and steam turbines.
- burns more cleanly and produces about 30% less CO_2 than petroleum and about 45% less than coal for an equivalent amount of heat produced.
- Combined cycle power generation using natural gas is the **cleanest** source of power available using fossil fuels.
- The gross heat of combustion of natural gas is around 39 MJ/m^3 and the typical caloric value is roughly **1,000 Btu/ft^3**, depending on gas composition.

- Liquefied natural gas exists at –161°C.
- ***Impurities*** and ***heavy hydrocarbons*** from the gaseous fossil fuel are removed before cooling.
- Density of liquefied natural gas: 410–500 kg/m^3.
- The volume of the liquid is approximately 1/600 of the gaseous volume at atmospheric conditions.

Typical composition (mole %) of natural gas

Component	Composition	Range
Methane	95.2	87.0–96.0
Ethane	2.5	1.5–5.1
Propane	0.2	0.1–1.5
Butane, *n*-butane	0.03	0.01–0.3
Iso-pentane, *n*-pentane, hexane plus	0.01	Trace–0.14
Nitrogen	1.3	0.7–5.6
Carbon dioxide	0.7	0.1–1.0
Oxygen	0.02	0.01–0.1
Hydrogen	Trace	Trace–0.02
Specific gravity	0.58	0.57–0.62
Gross heating value (MJ/m^3), dry basis	37.8	36.0–40.2

Nuclear Energy

Nuclear Energy, NE

- **NE plants** produce electricity through the **fission** of nuclear fuel (e.g., uranium) with no harmful emissions.
- Nucleus of an atom splits into smaller parts often with the emission of free neutrons and photons in the form of gamma rays and release of large amounts of energy.
- This heat is used to produce steam for turbines producing electricity.
- Typical fission releases about **two hundred million eV** (**200 MeV**) of energy, which is much higher than most chemical oxidation reactions.
- The energy of nuclear fission is released as KE of the fission products and fragments, and as electromagnetic radiation in the form of gamma rays in a nuclear reactor.

Nuclear Energy, NE

- KE is converted to **heat** due to collision of particles and gamma rays with the atoms and working fluid (usually water or occasionally heavy water).
- Products of nuclear fission, however, are far more **radioactive** than the heavy elements which are normally fissioned as fuel, and remain so for a significant amount of time, giving rise to a ***nuclear waste problem***.
- Although **NE** is essentially carbon-free, the electricity from new NE is relatively expensive.
- NE is challenged with waste disposal, threat of nuclear proliferation انتشار, and long licensing times.

Energy Terms

Heating Value, HV

- quantity of heat produced by combustion of a fuel at **constant P** and under "normal" conditions (25°C and 1 atm).
- The combustion process generates water.
- **Higher heating value** (HHV) involves, moreover, recovery of the heat of vaporization contained in the water vapor, i.e., the combustion product of water is condensed.
- **Lower heating value** (LHV) or **Net heating value**: water product of combustion is in vapor state.

- **Gross heating value** (GHV): is like HHV but accounts for liquid water in the fuel prior to combustion, as those in wood and coal.
- If a fuel has no water prior to combustion, then the GHV is equal to HHV.

$$\text{LHV} = \text{HHV} - \Delta H_{\text{vap}} \left[\frac{n_{H_2O,out} \times MW_{H_2O}}{n_{fuel,in} \times MW_{fuel}} \right]$$

HV at 1 atm and 20°C; at 25°C for liquid fuels, and 1 atm and normal boiling temperature for gaseous fuels

Fuel (phase)	Formula	MW (kg/kmol)	ρ (kg/l)	ΔH_v (kJ/kg)	T_b (°F)	C_p (kJ/kg °C)	HHV[a] (kJ/kg)	LHV[a] (kJ/kg)
Carbon (s)	C	12.01	2.000	–		0.71	32,800	32,800
Hydrogen (g)	H_2	2.01	–	–		14.40	141,800	120,000
Methane (g)	CH_4	16.04	–	509	−258.7	2.20	55,530	50,050
Methanol (l)	CH_3OH	32.04	0.790	1168	149.0	2.53	22,660	19,920
Ethane (g)	C_2H_6	30.07	–	172	−127.5	1.75	51,900	47,520
Ethanol (l)	C_2H_5OH	46.07	0.790	919	172.0	2.44	29,670	26,810
Propane(g)	C_3H_8	44.09	0.500	420	−43.8	2.77	50,330	46,340
Butane (l)	C_4H_{10}	58.12	0.579	362	31.1	2.42	49,150	45,370
Isopentane (l)	C_5H_{12}	72.15	0.626	–	82.2	2.32	48,570	44,910
Benzene (l)	C_6H_6	78.11	0.877	433	176.2	1.72	41,800	40,100
Hexane (l)	C_6H_{14}	86.18	0.660	366	155.7	2.27	48,310	44,740
Toluene (l)	C_7H_8	92.14	0.867	412	231.1	1.71	42,400	40,500
Heptane (l)	C_7H_{16}	100.204	0.684	365	209.1	2.24	48,100	44,600
Octane (l)	C_8H_{18}	114.23	0.703	363	258.3	2.23	47,890	44,430
Decane (l)	$C_{10}H_{22}$	142.28	0.730	361		2.21	47,640	44,240
Gasoline (l)	$C_nH_{1.87n}$	100–110	0.72–0.78	350		2.40	47,300	44,000
Light diesel (l)	$C_nH_{1.8n}$	170.00	0.78–0.84	270		2.20	46,100	43,200
Heavy diesel (l)	$C_nH_{1.7n}$	200.00	0.82-0.88	230		1.90	45,500	42,800
Natural gas (g)		~ 18.00	–	–		2.00	50,000	45,000

HHV (gross calorific value) of some common fuels

Fuel	Higher heating value	
	kJ/kg	Btu/lb
Anthracite	32,500–34,000	14,000–14,500
Bituminous coal	17,000–23,250	7,300–10,000
Butane	49,510	20,900
Charcoal	29,600	12,800
Coal(anthracite)	30,200	13,000
Coal(bituminous)	27,900	12,000
Coke	28,000–31,000	12,000–13,500
Diesel	44,800	19,300
Ether	43,000	
Gasoline	47,300	20,400
Glycerin	19,000	
Hydrogen	141,790	61,000
Lignite	16,300	7,000
Methane	55,530	
Oils, vegetable	39,000–48,000	
Peat	13,800–20,500	5,500–8,800
Petroleum	43,000	
Propane	50,350	
Semi anthracite	26,700–32,500	11,500–14,000
Wood (dry)	14,400–17,400	6,200–7,500

HHV (gross calorific value) of some common fuels

	kJ/m^3	Btu/ft^3
Acetylene	56,000	
Butane C_4H_{10}	133,000	3200
Hydrogen	13,000	
Natural gas	43,000	950–1,150
Methane CH_4	39,820	
Propane C_3H_8	101,000	2550
Butane C_4H_{10}		3200
	kJ/l	Btu/gal
Gasoline	32,000	115,000
Heavy fuel oil #6	42,600	153,000
Kerosene	37,600	135,000
Diesel	36,300	130,500
Biodiesel	33,500	120,000
Butane C_4H_{10}	36,200	130,000
Methanol	15,900	57,000
Ethanol	21,100	76,000

Energy Density, ED

- **ED** is the amount of energy per unit volume. it has the same physical unit as pressure.
- **Specific energy**, **SE**, is the amount of energy per unit amount.
- H_2 has a higher **SE** than gasoline but a much lower **ED** even in liquid form.

ED of some fuels

Fuel type	Gross (HHV)			Net (LHV)
	MJ/l	MJ/kg	Btu/gal	Btu/gal
Conventional gasoline	34.8	44.4	125,000	115,400
High octane gasoline	33.5	46.8	120,200	112,000
LPG (60%Pr. + 40%Bu.)	26.8	46.0		
Ethanol	24.0	30.0	84,600	75,700
Methanol	17.9	19.9	64,600	56,600
Butanol	29.2	36.6		
Gasohol E10 (ethanol 10% vol.)	33.2	43.5	120,900	112,400
Gasohol E85 (ethanol 85% vol.)	25.6	33.1		
Gasoline (petrol)	34.2	46.4		115,500
Diesel	38.6	45.4	138,700	128,700
Biodiesel	33.5	42.2	126,200	117,100
Jet fuel (kerosene based)	35.1	43.8	125,935	
Jet fuel (naphtha)	42.8	33.0	127,500	118,700
Liquefied natural gas (160°C)	22.2	53.6	90,800	
Liquefied petroleum gas	26.8	46.0	91,300	83,500
Hydrogen (liquid at 20 K)	10.1	142.0		130
Hydrogen gas	0.0108	143.0		
Methane (1 atm, 15°C)	0.0378	55.6		
Natural gas	0.0364	53.6		
LPG propane	25.3	49.6		
LPG butane	27.7	49.1		
Crude oil	37.0	46.3		
Coal, anthracite	72.4	32.5		
Coal, lignite		14.0		
Coal, bituminous	20.0	24.0		
Wood		18.0		

Exercise

An average daily traveling distance is about 40 miles/day. A car has a city-mileage of 20 miles/gal. If the car is replaced with a new car with a city-mileage of 30 miles/gal and the average cost of gasoline is \$3.50/gal, estimate the amount of fuel, energy, and money conserved with the new car per year. Assume gasoline is incompressible with ρ_{av} = 0.75 kg/L and LHV = 44,000 kJ/kg.

Solution

Fuel needed for old car

$$= (40\, miles/day)/(20\, miles/gal) = 2\, gal/day$$

Fuel needed for new car

$$= (40\, miles/day)/(30\, miles/gal) = 1.34\, gal/day$$

Mass of gasoline used per day for old car

$$m_{gasoline} = (\rho V)_{gasoline} = \left(\frac{0.75\ kg}{L}\right)\left(\frac{2\ gal}{day}\right)\left(\frac{3.785\ L}{gal}\right)$$
$$= 5.7\ kg/day$$

E supplied to the car per year

$$E = (m_{gasoline})\ (LHV)$$

$$= \left(\frac{5.7\ kg}{day}\right)\left(\frac{44{,}000\ kJ}{kg}\right) = \left(\frac{250{,}800\ kJ}{day}\right) = \left(\frac{91{,}542\ MJ}{year}\right)$$

Cost

$$= \left(\frac{\$3.5}{gal}\right)\left(\frac{2\ gal}{day}\right)\left(\frac{365\ day}{year}\right) = \$2555/year$$

Mass of gasoline used per day for new car

$$m_{gasoline} = (\rho V)_{gasoline} = \left(\frac{0.75\ kg}{L}\right)\left(\frac{1.34\ gal}{day}\right)\left(\frac{3.785\ L}{gal}\right)$$

$$= 3.8\ kg/day$$

E supplied to the car per year

$$E = (m_{gasoline})\,(LHV)$$

$$= \left(\frac{3.8\ kg}{day}\right)\left(\frac{44{,}000\ kJ}{kg}\right) = \left(\frac{167{,}200\ kJ}{day}\right) = \left(\frac{61{,}028\ MJ}{year}\right)$$

Cost

$$= \left(\frac{\$3.5}{gal}\right)\left(\frac{1.34\ gal}{day}\right)\left(\frac{365\ day}{year}\right) = \$1712/year$$

New car reduces fuel consumption by ~ 33%, which is significant.