Introduction to Combustion and Economic Analysis

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Alternative Energy

February 3, 2009

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Reading

Tonight:

Chapter five on economic analyses and chapter seven on fossil fuels and energy.

Combustion notes online give theoretical background for combustion results; this reading is optional

Next two classes: Chapter four on environmental effects and chapter six on sustainability.

Homework

Second homework assignment due tonight.

Download problem set due next Tuesday, February 10. Problems more like those in typical engineering course. If you have any questions we can discuss them in Thursday' s class (February 5), or you can send an email with your question(s).

Office hour at 2 pm cancelled for February 5.

Today's Class

- Review last class
- Modeling general fuels
- Air/fuel ratio and λ = relative ratio
- Products for complete combustion
- Combustion efficiency
- Time value of money
  - Present and future worth
  - Series of payments

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Two different topics will be considered tonight. Both of these topics can be covered in detail in separate courses. Engineering economic analysis is covered in the Engineering Economics course (MSE 304) required of all engineering majors. Combustion analysis is one of the main topics in the second thermodynamics course (ME 470).

The material covered in this lecture will summarize the important points of this material and provide equations that can be used for simple computations in each of these areas.

Review Properties and First Law

- Real fluid properties and ideal gas law
- Heat and work definitions and signs
- Closed system first law: $Q = \Delta U + W = m\Delta u + \int_{path} PdV$
- Open system first law:

$$\frac{dE_{cv}}{dt} = \dot{Q} - \dot{W}_U + \sum_{inlets} \dot{m}_{inlet}\left(h_{inlet} + \frac{\vec{V}^2_{inlet}}{2} + gz_{inlet} \right)$$

$$- \sum_{outlets} \dot{m}_{outlet}\left(h_{outlet} + \frac{\vec{V}^2_{outlet}}{2} + gz_{outlet} \right)$$

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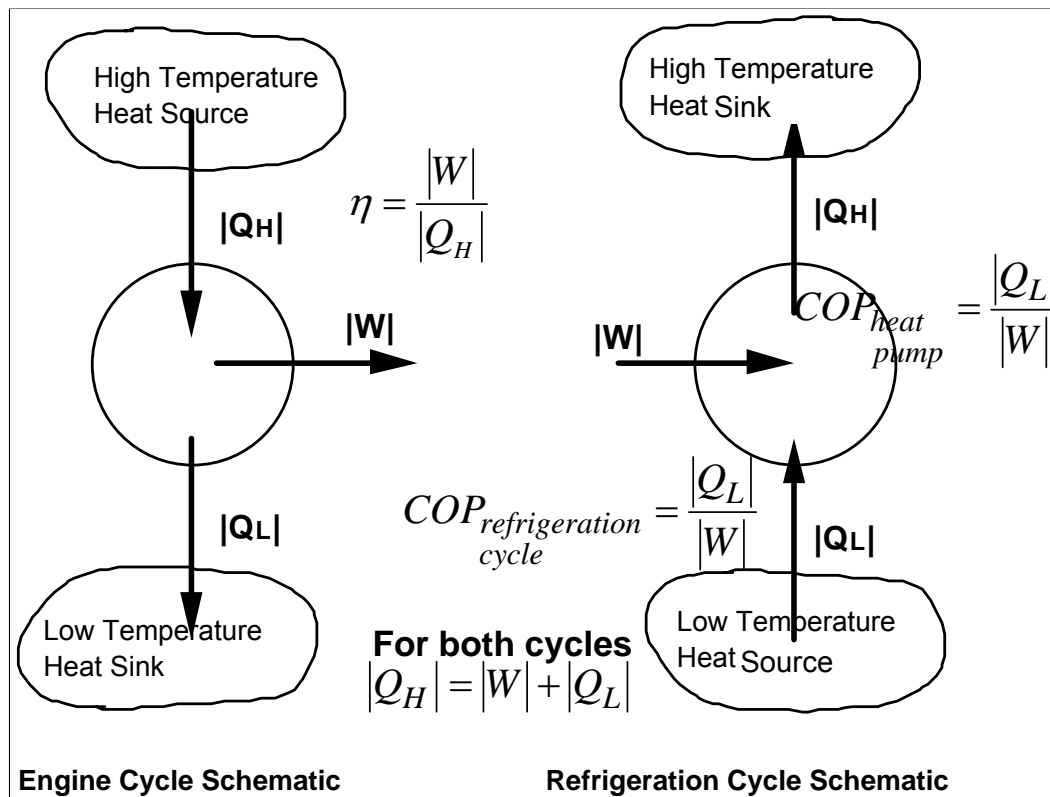Ideal gas: $PV = nR_uT$ where R_u, the universal gas constant, 8.31557 kJ/kgmol·K = R_u = 8.31557 kPa·m^3/kgmol·K = 10.7316 psia·ft^3/lbmol·R = 1.98588 Btu/lbmol·R. Engineering gas constant = R_u/M so PV = mRT.

Ideal gas relations apply at pressures that are low compares to the critical pressure and at temperatures that are high compared to the critical pressure. For real fluids we have to consider different phases, typically only liquid and gas, as well as mixtures of phases. Find properties from tables and compute mixed region properties from quality, x, the mass fraction of vapor in the liquid-vapor mixture.

Sign conventions: heat added to a system is positive; work done by a system is positive; heat rejected from a system is negative; work done on a system is negative.

Have different forms of the first law for closed (fixed mass) systems and open systems (sometimes called control volumes) that allow mass to enter and leave.

$$\eta = \frac{|W|}{|Q_H|}$$

$$COP_{heat\ pump} = \frac{|Q_L|}{|W|}$$

$$COP_{refrigeration\ cycle} = \frac{|Q_L|}{|W|}$$

For both cycles

$$|Q_H| = |W| + |Q_L|$$

Engine Cycle Schematic   **Refrigeration Cycle Schematic**

Cycles are a fundamental concept in energy production and use.

In an engine cycle the device gets heat $|Q_H|$ from a high temperature source, performs a certain amount of work, $|W|$, then rejects heat $|Q_L|$ to a low temperature sink.

In a refrigeration cycle the device gets heat $|Q_L|$ from a low temperature source, has an input of a certain amount of work, $|W|$, then rejects heat $|Q_H|$ to a high temperature sink. In your home refrigerator the low temperature source is as the inside of the refrigerator. Work is done by an electric motor and the high temperature heat transfer is done by the coils in the back of the refrigerator.

Note that traditional cycle analysis does not use the usual sign conventions for heat and work; instead it uses quantities that are always positive. For both the engine and refrigeration cycles we can write $|Q_H| = |Q_L| + |W|$.

An engine cycle is rated by its efficiency, η, the ratio of work output to heat input. For a refrigeration cycle we would like to remove as much heat as possible from the low temperature source while doing the least amount of work. Thus the figure of merit for a refrigeration cycle, called the coefficient of performance, COP, is the ratio of the heat removed from the low temperature heat source to the work input.

The efficiency of an engine cycle is between zero and one. The COP for a refrigeration cycle may be greater than one.

The notation $|q_H|$ and $|q_L|$ are used for heat transfer per unit mass.

Second Law

- There exists an extensive thermo-dynamic property called the entropy (with the symbol, S) defined as follows:
- dS = (dU + PdV)/T
- For any process in a system dS ≥ dQ/T, and, for an isolated system
- $\Delta S_{\text{isolated system}} \geq 0$
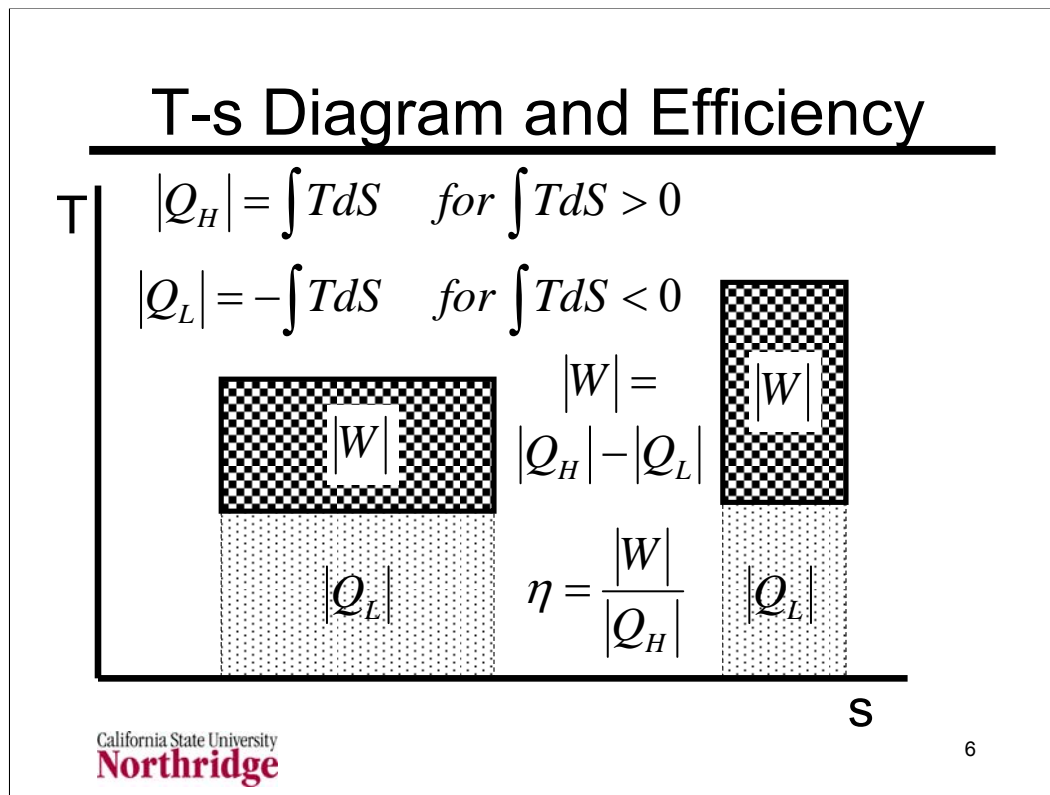- **Impossible:** 100% efficient engine cycle and refrigeration cycle with |W| = 0

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The second law provides a qualitative statement about limitations on cycles and it provides a mathematical tool, the entropy, to compute the efficiency of ideal cycles. We can use this tool, with the inequality relation that dS ≥ dQ/T, to determine the ideal case as the case in which dS = dQ/T. This is known as the reversible cycle. The maximum efficiency occurs in a reversible cycle.

For reversible heat transfer, dQ = TS so that Q = ∫Tds. If we can plot a reversible process on a diagram that has entropy as the abscissa and temperature as the ordinate (T-s coordinates or a T-s diagram) then the heat transfer is the area under the plot for that process.

No actual cycle is truly reversible, but we can try to approach reversibility as closely as possible within the constraints of cost. At some point the extra cost of making a device that is more nearly reversible outweighs the cost of the energy saved.

T-s Diagram and Efficiency

$$\left|Q_H\right| = \int TdS \quad for \int TdS > 0$$

$$\left|Q_L\right| = -\int TdS \quad for \int TdS < 0$$

$$|W| = |Q_H| - |Q_L|$$

$$\eta = \frac{|W|}{|Q_H|}$$

T

$|W|$

$|Q_L|$

$|W|$

$|Q_L|$

S

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The temperature-entropy or T-s diagram is often used to plot cycles because it shows provides a visual way of comparing cycle efficiency, once you are familiar with the underlying relations.

Recall that for a reversible process Q = ∫TdS. When we draw an ideal (reversible) cycle on a T-s diagram we can apply this equation. When the integral is positive, we have a heat input giving $|Q_H|$. Then the integral is negative we have the heat rejected so that $|Q_L|$ = –∫TdS. An engine cycle always operates in a clockwise manner. Each cycle can be viewed as stating in the upper left corner, then proceeding to the upper right corner and so on until the cycle is complete.

The chart uses the Carnot cycle, shown as the dark checked rectangles, as an example. There are only two parts of the cycle in which there is a heat transfer. Along the top part of the cycle, where the temperature is constant at a value T_H the integral gives $|Q_H|$ = $T_H\Delta S$. The lower portion gives $|Q_L|$ = –$(T_H)(-\Delta S)$ = $T_L\Delta S$. The difference between $|Q_H|$ and $|Q_L|$ is the net cycle work, $|W|$.

The area corresponding to $|Q_H|$ is the sum of two different areas shown on the diagram: the dark checkered area for the original cycle and the lower area. The lower area corresponds to $|Q_L|$. The difference between the two, which is the area in the cycle, is the work. The ratio of the cycle area to the total area (cycle area plus area beneath the cycle) is the efficiency.

Which of the two cycles has a greater efficiency?

Cycle Analysis

- The following assumptions define idealized versions of practical cycles
  - There are no line losses; the outlet state (i.e. thermodynamic properties) from one device is the same as the inlet state to the next device.
  - work devices are reversible and adiabatic so they have constant entropy (isentropic).
  - Heat transfer devices have no pressure loss and are reversible so Q = ∫Tds
  - Outlet states from devices with two phases are saturated liquids or vapors.

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These assumptions give the highest efficiency for a given set of cycle conditions. In practice they are not met and the degree to which they are not met gives the difference between the actual or maximum cycle efficiency and the actual cycle efficiency.

These assumptions can also be applied to the analysis of a refrigeration cycle to compute the maximum coefficient of performance.

Last class period we looked at a variety of cycles:

The **Rankine cycle** and its variants are used to model the process in a steam-electric power plant. Higher temperatures and pressures in the steam generator provide higher efficiencies, but reheating has to be used to ensure that there is not an excessive amount of water in the final stages of the turbine. Feedwater heaters are used to increase efficiency.

The **Otto cycle** models the operation of gasoline engines. The simple analysis shows that the efficiency is related to the compression ratio, CR, which is the ratio of the maximum cylinder volume to the minimum cylinder volume. This equation, $\eta = 1 - 1 / (CR)^{k-1}$, overstates the efficiency, but does show a correct trend of efficiency with compression ratio.

The **Brayton cycle** models gas turbine engines. The simple analysis shows that the efficiency is related to the pressure ratio, PR, which is the ratio of the engine pressure in the combustor to the minimum engine pressure at the compressor inlet and turbine outlet This equation, $\eta = 1 - 1 / (PR)^{(k-1)/k}$, overstates the efficiency, but does show a correct trend of efficiency with pressure ratio.

Introduction to Combustion

- Have several levels of analysis
  - Balanced chemical equation to determine species
    - Assume complete combustion
  - Energy balance to include chemical energies
  - Chemical equilibrium calculations
  - Chemical kinetics calculations
  - Computational fluid dynamics integrates flow, heat transfer, and chemical kinetics

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There is a range of analyses that can be done on combustion processes. At a basic level we know that chemical elements are conserved so we can write a simple chemical balance equation for the reaction of a fuel molecule with air. We can consider complex fuels by allowing non-integer amounts of atoms in our fuel "molecule". This allows us to represent the combustion of several fuels by a single chemical balance equation.

The assumption of complete combustion, where all the fuel carbon reacts to CO_2, all the fuel hydrogen reacts to H_2O, all the fuel sulfur reacts to SO_2, and all the fuel nitrogen reacts to N_2 is usually a reasonable one for well maintained lean combustion processes. It is a useful first approximation to the species balance and energy balance.

More extensive calculations can consider the thermochemical equilibrium. Computer codes are available to make these computations. These show that the combustion products at high temperatures have significant concentrations of other species such as CO and NO.

Chemical kinetics calculations use a set of ordinary differential equations to determine the rate of change of the species in an air-fuel mixture. Such calculations are limited to the simplest fuels.

Combustion processes usually occur in flow systems where there is a significant amount of turbulence. Sophisticated computer programs, known as computational fluid dynamics or CFD, can analyze such processes in principle, but a large amount of data are required.

Basic Fuel Analysis

- Apply to any fuel with any amount of the following elements: C, H, O, N, and S
- Covers most fossil fuels
  - Some natural gases have components such as helium and argon not covered
  - Ultimate analysis for liquid and solid fuels gives weight percent of each element, including mineral matter that forms "ash"
  - Gaseous fuels have molar analysis of each component in gas

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Fossil fuels, particularly coals, contain some amount of mineral matter that does not enter into the combustion process. The ultimate analysis of fuels, discussed on the next chart, gives the relative amounts, by mass, of carbon, hydrogen, oxygen, and mineral matter. The mineral matter does not provide any energy, but forms solids that either fall to the bottom of the combustion region (slag) or are emitted with the exhaust gas (fly ash).

The analysis of the combustion process deals with the conversion of the main fuel elements, C, H, O, N, and S into combustion products: CO_2, H_2O, SO_2, and N_2. The combustion products also contain excess O_2 and unreacted components of air such as N_2, Ar, and other trace species.

The goal of the analysis is to find the relative amounts of combustion products and determine combustion efficiencies.

Basic Fuel Analysis II

- General fuel formula: $C_xH_yS_zO_wN_v$
- Determine values of x, y, z, w, and v from ultimate analysis or analysis of gas mixtures
- Mineral matter included in ultimate analysis represented as %Ash or %MM
- For ultimate analysis x = wt%C/12.0107, y = wt%H/1.00794, z = wt%S/32.065, w = wt%O/16.0004, v = wt%N/14.0067

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When using data for an ultimate analysis we can arbitrarily set the mass equal to 100 kg or 100 lb_m depending on the units we are using. This arbitrary choice is called the basis of the calculation. We can use this arbitrary basis because we will state all results in terms of product species or energy release per unit mass of fuel. Hence arbitrary value of 100 (or any other value we choose) will cancel when we obtain per unit mass values.

Once we choose this basis we know that the mass of each element in the generic fuel formula is the weight percent from the ultimate analysis times 100 so simply the weight percent expressed as a number. For example a fuel with 85%wt carbon would have 85 kg of carbon in the assumed 100 kg of fuel. If we divide this 85 kg of carbon by the atomic mass of carbon (12.0107) we get the amount, x = 7.077, kilogram atoms of carbon atoms in one "mole" of our fuel formula. We can repeat this for each component in the ultimate analysis.

Note that the subscripts are usually not integers here. This is correct since we are representing a mixture, which has a non-integer composition, by a fuel formula that looks like a molecule. This is not really a molecule, but provides an approach to analyzing fuel mixtures that is exactly the same as our usual operations for balancing a chemical equation.

An example of converting a set of data on the ultimate analysis of a fuel to a fuel formula is shown on the following notes page.

Gas Mixture Analysis

Gas	Mole Fraction	Carbon	Hydrogen
CH_4	0.88	0.88	3.52
C_2H_6	0.07	0.14	0.42
C_3H_8	0.03	0.09	0.24
C_4H_{10}	0.02	0.08	0.2
Mixture	1	1.19	4.38

- Sum product of mole fraction times number of atoms in fuel (*e.g.*: $C_{1.19}H_{4.38}$)[11]

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Gas mixtures can also be analyzed by the general fuel formula, $C_xH_yS_zO_WN_v$ where the relative elemental amounts are computed as the mole fraction weighted sums of the elements in each species. In the example shown in the table above, the carbon content in the mixture is computed as follows:

1(.88) + 2(.07) + 3(.03) + 4(.02) = 1.19

and the hydrogen content is found as

4(.88) + 6(.07) + 8(.03) + 10(.02) = 4.38

An example of converting an ultimate analysis to a fuel formula is shown below:

Atom	Weight Percent	Atomic Weight	%wt / Atom Wt	Symbol
C	85.4	12.0107	7.110	x
H	14.4	1.00794	14.287	y
S	0.005	32.065	0.0002	z
O	0.19	15.9994	0.012	w
N	0.004	14.0067	0.0003	v
Ash	0.001	Not included in fuel "molecule" but part of fuel mass		

The resuting fuel formula is $C_{7.110}H_{14.287}S_{0.0002}O_{0.012}N_{0.0004}$. The minor components can be neglected in a simple analysis but the sulfur and nitrogen in the fuel play a role in pollutant emissions.

Combustion Air

- Complete combustion converts C to CO_2, H to H_2O, S to SO_2 and N to N_2
    - Stoichiometric O_2 is minimum to give this
- Stoichiometric O_2 for $C_xH_yS_zO_wN_v$ is A = $x + y/4 + z - w/2$ moles O_2
- Usually have extra O_2 so total is λA
    - λ is ratio of actual O_2 to stoichiometric O_2
- Also have other dry air components: N_2, Ar, and CO_2 plus H_2O from humidity

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Composition of Dry Air (Molar mass = 28.966) from http://ic.ucsc.edu/~wxcheng/envs23/lecture5/air_compo.htm (accessed February 5, 2007)

Gas	Mole %	Mass %	Moles/mole O_2
Oxygen	20.947	23.20	1
Nitrogen	78.084	75.47	3.7277
Carbon Dioxide	0.036	0.046	0.0017
Hydrogen	0.00005	~ 0	0.000002
Argon	0.934	1.28	0.0446
Neon	0.0018	0.0012	0.0001
Helium	0.0005	0.00007	0.000024
Krypton	0.0001	0.0003	0.0000025
Xenon	9×10^{-6}	0.00004	4×10^{-7}

There 3.774 moles of other species per mole of O_2 in dry air. In the simplest combustion analyses these additional moles are assumed to be all nitrogen that is an inert. Other analyses will include argon, and sometimes CO_2, as a separate species. When N_2 is the only other air species in the analysis it can be assigned a fictitious molar mass of 28.163 (compared to the correct value of 28.0134) to have the correct mass of all other species in air. This is called "atmospheric" nitrogen.

The mass of air per mole of O_2 = 28.966 /0.20947 = 138.28

Air/Fuel Ratio for $C_xH_yS_zO_wN_v$

- Given λ and data to find x, y, z, w, and v
- First compute $A = x + y/4 + z - w/2 =$ moles O_2/mole fuel
- $m_{fuel} = M_{fuel}$ / (1 – %Mineral in fuel)
  - $M_{fuel} = 12.0107x + 1.00794y + 32.065z + 15.9994w + 14.0067v$
  - $m_{fuel} = M_{fuel} = 100$ for %Mineral = 0
- $m_{air} = 138.28\lambda A$
- Air/fuel ratio = m_{air}/m_{fuel}

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Air fuel ratio is commonly expressed on a mass basis. (For most liquid hydrocarbon fuels the stoichiometric air/fuel ratio is about 14.7.) Note that approach used to compute x, y, z, w, and v for an ultimate analysis essentially assumes that the chemical formula is based on 100 mass units. If there is no mineral matter (ash) in the fuel, his is equivalent to assuming a molar mass of 100, so it is not necessary to compute M_{fuel} in this case. If the ultimate analysis contains a value for %Ash and you use 100 mass units to convert the ultimate analysis to a fuel formula, then the fuel mass m_{fuel} = 100. Regardless of the number of mass units you chose to use in the ultimate analysis you can always compute $m_{fyel} = M_{fuel}/(1 - \%Ash)$.

Note the subtle difference between complete combustion and stoichiometric combustion. Complete combustion is when all the fuel C forms CO_2, all the fuel H forms H_2O, all the fuel S forms SO_2 and all the fuel N forms N_2. This cannot possibly occur unless the oxygen is equal to or greater than stoichiometric.

Although we can define a stoichiometric oxygen supply and have actual combustion with just this amount of oxygen, the stoichiometric oxygen supply does not guarantee complete combustion. Usually excess air is added. This excess air is usually expressed as a ratio to the stoichiometric oxygen requirement, λ. (For combustion with air the stoichiometric air requirement is called the theoretical air and λ, expressed as a percentage, is called the percent theoretical air.)

Complete Combustion Products

- $C_xH_yS_zO_wN_v + \lambda A(O_2 + 3.77\ N_2) \rightarrow$
  $xCO_2 + (y/2)H_2O + zSO_2 + (\lambda - 1)AO_2 + 3.77\lambda A + v/2)N_2$

- Measurements on wet/day basis done with/without product water

- Relate λ and product O_2

$$\frac{\%O_2|_{dry}}{100} = \frac{(\lambda - 1)A}{x + 4.77\lambda\,A\ - A + z + \dfrac{v}{2}}$$

$$\lambda = \frac{A + \dfrac{\%O_2|_{dry}}{100}\left[x - A + z + \dfrac{v}{2}\right]}{A\left(1 - 4.77\dfrac{\%O_2|_{dry}}{100}\right)}$$

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The balanced chemical equation shown above uses the simple approach where all other constituents of air are assumed to be N_2. Recall that when we do this, we have to use a fictitious molar mass of 28.163 for molecular nitrogen (N_2).

This equation can be checked to show that all chemical elements are conserved. This is simple to do for C, H, N, and S. To see that it is correct for O, we have to use the definition of $A = x + y/4 + z - w/2$. The elemental balance for oxygen can be done for O_2. We first note that both sides of the equation have λA moles of O_2 which cancel. We are then left with the following sum of O_2 for all species on the right side: $x + y/4 + z - A = w/2$, which is the amount of O_2 left on the right side of the equation after cancelling the λAO_2.

Many analytical instruments require water in the combustion products to be removed prior to analysis. Because of this, the exhaust measurements are commonly made on a dry basis. The equations on this slide show how the exhaust mole fraction can be used to determine λ.

The equation for the dry oxygen mole fraction can be seen to be the ratio of the moles of oxygen in the exhaust $(\lambda - 1)A$ divided by the total number of dry moles, $D = x + z + (\lambda - 1)A + 3.77\lambda A + v/2$.

Note that the SO_2 dry mole fraction can be expressed by the following equation, analogous to the equation for the oxygen mole fraction: $y_{SO2} = z/[x + z + (\lambda - 1)A + 3.77\lambda A + v/2]$

Regulatory Measurements

- Correct measured value, C_{meas}, to concentration, C_{std}, at standard exhaust O_2 concentration $[\%O_2]_{std}$ to prevent compliance by dilution

$$C_{std} = C_{meas} \frac{20.9 - [\%O_2]_{std}}{20.9 - [\%O_2]_{meas}}$$

- Typical values for $[\%O_2]_{std}$ are 0, 3 (for boilers) and 15 (diesel engines and gas turbines)

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When emission standards are stated on a concentration (or mass or mole fraction basis) they are often corrected to some standard oxygen concentration that is typical of the device in question. A zero oxygen concentration is used to determine the actual flow rate as shown in the following slides.

Boilers in a range of sizes typically operate at a small amount of excess oxygen that is characterized for regulatory purposes as the amount that produces an exhaust concentration of 3% O_2. Diesel engines are operated much leaner and gas turbines operate even leaner than diesel engines. The correction to 15% O_2 is generally used for gas turbines. It is sometimes used for diesel engines, but other levels are used here as well.

Emission Standards

- Emission standards, E, mass of pollutant per unit heat input

$$E_i = \rho_{i,d} F_d \frac{20.9}{20.9 - \%O_{2,d}}$$

- Calculation method uses F-Factor, F_d
  - F_d is exhaust volume flow / heat input
  - E is emissions in ng/J or lb/MMBtu
  - $\rho_{i,d}$ is dry mass partial density ng/m^3 or lb_m/ft^3
  - $\%O_{2,d}$ is dry mole percent O_2 in exhaust
- F_d = (8710, 9190) ft^3/MMBtu for (gas, oil)

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The volume measurements shown above are at standard conditions of 68^OF = 20°C and atmospheric pressure.101.325 kPa = 14.696 psia. Such standard conditions are commonly abbreviated as scf for standard cubic feet or scm for standard cubic meters. To emphasize the use of dry measurements, the abbreviations dscf or dscm are sometimes used to denote dry standard cubic feet or dry standard cubic meters.

Some values of F_d from http://www.epa.gov/ttn/emc/promgate/m-19.pdf (accessed February 6, 2007) are shown below

Fuel	dscm/J	dscf/MMBtu
Anthracite Coal	2.71×10^{-7}	10,100
Bituminous Coal	2.63×10^{-7}	9,780
Lignite	2.65×10^{-7}	9,860
Oil	3 2.47×10^{-7}	9,190
Natural Gas	2.34×10^{-7}	8,710
Propane	2.34×10^{-7}	8,710
Butane	2.34×10^{-7}	8,710
Wood	2.48×10^{-7}	9,240
Wood Bark	2.58×10^{-7}	9,600

Emission Standards II

- Values for F_d for typical fuels found from EPA method 19 (reference below)
    - http://www.epa.gov/ttn/emc/promgate/m-19.pdf
- Can also be computed from ultimate analysis (%C, %H, etc.)

$$F_d = \frac{K\left(K_C\%C + K_H\%H + K_O\%O + K_S\%S + K_N\%N\right)}{Q_c}$$

- Q_c is higher heating value
- K values in notes page

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The constants in the equation for computing the factor, F_d, from the ultimate analysis are shown below. Two sets of values, one in SI units the other in engineering units, are given. Note that in the equation the values of the ultimate analysis are expressed as a percentage, not as a decimal. Thus a value for %C = 84% would be entered in the formula as 84 **not as .84**.

The units for the higher heating value (Q_c) are Btu/lb$_m$ or kJ/kg.

K = Conversion factor, 10^{-3} (kJ/J)/(%) [10^6 Btu/million Btu].

K_C = (9.57 scm/kg)/% [(1.53 scf/lb)/%].

K_H = (22.7 scm/kg)/% [(3.64 scf/lb)/%].

K_N = (0.86 scm/kg)/% [(0.14 scf/lb)/%].

K_O = (2.85 scm/kg)/% [(0.46 scf/lb)/%].

K_S = (3.54 scm/kg)/% [(0.57 scf/lb)/%].

The value for C_d on the previous chart is stated as ng/m^3 or lb$_m$/ft^3. Typically the emission measurements are mole fractions such as y_i for species i. To convert this to the partial mass density ρ_i use the following calculation: $\rho_{d,I}$ = $y_{d,i}M_iP/R_uT = y_{d,i}P/R_iT$ where P is the standard pressure of 101.325 kPa = 14.696 psia, R_u is the universal gas constant = 8.31447 kPa·m3/kgmol·K = 10.7316 psia·ft3/lbmol·R, T = standard temperature = 288.15 K = 518.67 R, M_i is the molar mass of species i, and R_i is the engineering gas constant = R_u/M_i. (The standard temperature used here is 15°C = 59°F; other standard temperatures can be used; a standard pressure of 14.3 psia is sometimes used.)

Calculation Summary

- Need $\rho_{i,d}$, F_d and %$O_{2,d}$ to compute E_i

$$E_i = \rho_{i,d} F_d \frac{20.9}{20.9 - \%O_{2,d}}$$

- Measured dry mole fractions of O_2 and species i, $y_{i,d}$, ($y_i = 10^{-6} ppm_i$)
  - $\rho_{i,d} = y_{i,d} M_i P_{std}/RT_{std}$
- F_d computed from ultimate analysis or default values are used
- If %O_2 not measured

$$\frac{\%O_2|_{dry}}{100} = \frac{(\lambda - 1)A}{x + 4.77\lambda\,A\,-\,A + z + \dfrac{v}{2}}$$

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This slide recapitulates the equations provided on previous slides to outline the steps in calculating the pollutant emissions rate in mass per unit heat input, E. The three parts to the formula from slide 16 are found by various ways as outlined here.

The partial mass density of the pollutant species is found from the ideal gas law as discussed on the previous notes page. Note that pollutant concentrations are often given in parts per million (ppm) which is a mole fraction multiplied by 10^6.

The F_d factor can be taken from the default values on the notes page for slide 16 or can be computed from an ultimate analysis using the formula on slide 17 with the associated K values on the notes page for that slide.

The exhaust oxygen concentration is typically measured. If measurements are not available or you are making a design calculation, the dry exhaust concentration of oxygen can be found from the formula on slide 14 which is copied here. The items in that formula are the ultimate analysis calculation results x, y, z, w, v found from the formulas on slide 10. The stoichiometric oxygen moles per fuel mole, A = x + y/4 + z – w/2, is found on slide 13. The relative air/fuel ratio, λ, is assumed to be known if the exhaust oxygen is not measured.

Example Calculation

- The exhaust from a combined cycle power plant has exhaust concentrations (dry) of 2.8% O_2 and 9 ppm NOx. What is the NOx rate in lb_m/MMBtu.
  - $\rho_{i,d} = y_{i,d}M_iP_{std}/R_uT_{std}$ $y_i = 10^{-6}ppm_i$
- $F_d = 8710$ ft³/MMBtu for gas

$$E_i = \rho_{i,d}F_d \frac{20.9}{20.9 - \%O_{2,d}} = \frac{0.011\, lb\, NOx}{MMBtu}$$

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See calculation details in notes page   19

We compute the partial density from the mole fraction (after multiplying the ppm by 10⁻⁶ to get $y_{i,d}$.)

$$\rho_{i,d} = \frac{y_{i,d}M_iP_{std}}{R_uT_{std}} = \frac{\dfrac{9x10^{-6}\,lbmol\,NOx}{lbmol}\dfrac{46.0065\,lb\,NOx}{lbmol\,NOx}(14.696\,psia)}{\dfrac{10.7316\,psia\cdot ft^3}{lbmol\cdot R}(518.67\,R)} = \frac{1.0832x10^{-6}\,lb\,NOx}{ft^3}$$

Note the convention that the molar mass used for NOx is that of nitrogen dioxide (NO_2).

Note also that the volume used here is the hypothetical volume of the dry exhaust at standard conditions. The units for cubic feet at standard conditions are often specified as SCF. The abbreviation DSCF for (dry standard cubic feet) is also used to emphasize that the measurements are made for the dry exhaust.

Once we find the partial density we use the standard value that F_d= 8710 ft³/MMBtu (sometimes written as 8710 DSCF/MMBTU as noted above) for natural gas to get the emission rate per unit heat input.

$$E_i = \rho_{i,d}F_d\frac{20.9}{20.9 - \%O_{2,d}} = \frac{1.0832x10^{-6}\,lb\,NOx}{ft^3}\frac{8710\,ft^3}{MMBtu}\frac{20.9}{20.9 - 2.8} = \frac{0.011\,lb\,NOx}{MMBtu}$$

Simplified Analyses

- Simple analysis to find mass of sulfur, SO_2, carbon, or CO_2 per unit fuel mass or heat input

$$\frac{m_S}{m_{fuel}} = \frac{wt\% S}{100} \qquad \frac{m_{SO_2}}{m_{fuel}} = \frac{wt\% S}{100} \frac{M_{SO_2}}{M_S} = 1.9979 \frac{wt\% S}{100}$$

$$\frac{m_C}{m_{fuel}} = \frac{wt\% C}{100} \qquad \frac{m_{CO_2}}{m_{fuel}} = \frac{wt\% C}{100} \frac{M_{CO_2}}{M_C} = 3.6642 \frac{wt\% C}{100}$$

$$\frac{m_C}{Q_{fuel}} = \frac{1}{Q_c} \frac{m_C}{m_{fuel}} \quad \frac{m_{CO_2}}{Q_{fuel}} = \frac{m_{CO_2}}{m_{fuel}} \quad \frac{m_S}{Q_{fuel}} = \frac{1}{Q_c} \frac{m_S}{m_{fuel}} \quad \frac{m_{SO_2}}{Q_{fuel}} = \frac{m_{SO_2}}{m_{fuel}}$$

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Simplified calculations of the mass of pollutant species can be made for SO_2 and CO_2 by assuming that all the sulfur in the fuel reacts to SO_2 and that all the carbon in the fuel reacts to CO_2. These are reasonable assumptions, with only a small (~1%) error.

The weight percent of sulfur or carbon (divided by 100 to give a weight fraction) gives the proportion of these elements in the fuel. Multiplying the fraction of sulfur in the fuel by the ratio of the molar mass of SO_2 to the molar mass of sulfur (64.0638 / 32.065) gives the result shown above. For practical purposes this molar mass ratio can be set to 2.

In a similar fashion, multiplying the fraction of carbon in the fuel by the ratio of the molar mass of CO_2 to the molar mass of carbon (44.0095 / 12.0107) gives the result shown above for the mass of CO_2 pre unit mass of fuel.

If the equations for the mass of carbon, sulfur, CO_2 or SO_2, per unit mass of fuel, are divided by the heat of combustion of the fuel, the result is the mass of carbon, sulfur, CO_2 or SO_2, per unit heat input from the fuel. Combining the equations on the chart gives the following results.

$$\frac{m_{CO_2}}{Q_{fuel}} = \frac{3.6642}{Q_c} \frac{wt\% C}{100} \qquad \frac{m_{SO_2}}{Q_{fuel}} = \frac{1.9979}{Q_c} \frac{wt\% S}{100}$$

Natural gas, with a higher value of Q_c and a lower value of wt% C compared to coal has lower emissions of CO_2 per unit heat input.

Combustion Efficiency

- How much heat of the amount possible in the fuel is actually used?

$$\eta_{comb} = \frac{|q|}{|q|_{max}} = 1 - \frac{\left[1 + \frac{Air}{Fuel}\right]}{Q_c} \int_{T_{in}}^{T_{out}} c_{P\,Air} \, dT' - \frac{xf\Delta h_{CO}}{M_{fuel}Q_c}$$

  – Air/fuel is the air to fuel (mass) ratio
  – $C_{p,air}$ = 0.24 Btu/lb$_m$·R = 1.005 kJ/kg·K
  – f = molar exhaust ratio CO/(CO + CO_2)
  – x = carbon atoms in fuel formula, C_xH_y…
  – Q_c = heat of combustion (Btu/lb$_m$ or kJ/kg)
  – Δh_{CO} 282,990 kJ/kgmol = 121,665 Btu/lbmol

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The combustion efficiency analysis, whose results are shown here, is based on the assumption that the heat capacity of the fuel plus air is the same as the heat capacity of the exhaust, both of which are taken to be the heat capacity of air. This is not such a bad assumption since the fuel/air mixture is about 94% air and the main component of exhaust gases is nitrogen.

The Δh_{CO} term is the enthalpy difference that could have been obtained by burning one mole of CO in the exhaust to CO_2. It's value is 282,990 kJ/kgmol = 121,665 Btu/lbmol.

Either higher or lower heating values can be used for Q_c and the combustion efficiency should be stated as a percent of the HHV or LHV as appropriate. Usually the lower heating value is used since the product water is in the vapor phase.

The heat capacity values for air shown in the slide are room temperature values. The assumption of a constant heat capacity is consistent with the assumption that the heat capacity of air applies to both the reactants and products. However, if there is a large temperature difference between the inlet and exit temperatures, a set of air tables can be used to find the integrated heat capacity.

Economic Analysis

- Consider time value of money
- Simplest idea is interest on a loan with a single payment at the end of the loan
  - $F = P(1 + i)^n$
    - P = present value = amount of loan
    - F = future value = amount to be repaid
    - n = number of years for the loan
    - i = annual interest rate on the loan
  - Formula implies that loan is compounded annually

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The key component of engineering economic analysis is recognizing the time value of money. Most of use are familiar with this through the interest charged on loans or credit cards. In investment, companies look for a desired rate of return, which is similar to an interest rate.

A key component of interest is compounding. Even if there is only a single payment at the end of the loan, the interest is quoted as an annual interest. In addition, the interest is applied each year (or more frequently). Future interest is based on the original loan amount plus the already incurred interest. For example, a loan of $10,000 with a 10% per year interest rate would have the following interest accumulations each year:

Year 0: $10,000

Year 1: $10,000 + 10%($10,000) = $11,000

Year 2: $11,000 + 10%($11,000) = $12,100

Year 3: $12,100 + 10%($12,100) = $13,310

Without compounding the interest of 10% per year for three years would be $3,000; with compounding, the total interest is $3,310. Note that the formula shown above predicts this result: $10,000(1 + 0.1)^3 = $10,000(1.331) = $13,310.

Interest Rate

- Can be compounded at greater frequency than annual
  - However, interest rate is still quoted as an annual rate
    - If interest is compounded k time a year the interest rate for each period is i/k
    - Value at the end of the year $(1 + i/k)^k$ times the value at the start of the year
    - As $k \rightarrow \infty$, $(1 + i/k)^k \rightarrow e^{i(1)}$
    - For multiple (or partial) years, t, $F = Pe^{it}$
    - Text uses e^{it} and computes $i = \ln(1 + i'/k)^k$

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Loans can be compounded at a frequency greater than an annual frequency. Home mortgages and credit card debt are compounded monthly. The ultimate compounding rate is instantaneous. In the limit as the number of compounding periods approaches infinity, the formula for the future worth becomes exponential: $F = Pe^{it}$.

Consider an interest rate of 6% per year. If there is no compounding during the year the value at the end of the year is 1.06 times the value at the start. If there is semi annual compounding, the value at the end of the year is $(1 + .06/2)^2 = 1.0609$ times the value at the start of the year. Continuing the progression we have the following results for the end/start ratio as a function of compounding periods:

3	1.06121	10	1.06146
4	1.06136	20	1.061741
6	1.06152	100	1.061817

We see that even with 10 compounding periods we are quickly approaching the instantaneous value of $e^{i(1)} = e^{0.06} = 1.061837$

The text always uses the formula $F = Pe^{it}$ where t is the time in years or partial years. This can be compared to a discrete interest rate, i', with k compounding periods in one year (t = 1): $e^{i(1)} = (1 + i'/k)^k$. Taking the natural logarithm of both sides of this equation gives the result shown on the chart. For i' = 6% and k = 1, $i = \ln(1 + .06) = 5.83\%$

Annualized Cost

- This is like the payments on a loan over the lifetime of the object purchased
  - Typical engineering economic analysis looks at cash flows at the end of a year
  - Equivalent annual cash flow for present worth, P, at interest rate i, lifetime n

$$A\!\!\Big/\!_P = \frac{i}{1-(1+i)^{-n}}$$

  - *E.g.*: i = 10%, n = 30, A/P = .1/[1 − (1 + .1)$^{-30}$]

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The ratio A/P can be found in tables in textbooks on engineering economics and is present on many calculators and in the Excel function pmt(interest rate, number of periods, present value). To compute the A/P ratio a value of -1 must be entered for the present value; the pmt function has additional arguments that can be ignored for the purposes of the A/P formula.

This formula allows one to compute the annual costs of an operation such as an electric power plant, including the annual operating and maintenance costs and fuel costs, plus the annualized cost of the initial plant construction.

This formula is sometimes called the capital recovery factor. In applications of the inverse of this formula, finding the present worth of a series of future payments, the interest rate is sometimes called the discount rate. This meaning is that an individual or company would "discount" future cash flows to compute their present value.

The analysis of projects with an initial cost and recurring costs must consider the time value of money. This can be done by computing the present worth, P, of the annual recurring costs, A, by the formula: $P = A[1 - (1 + i)^{-n}]/i$. This value is then added to the initial cost to obtain the total cost at present value.

An alternative approach is to convert the initial cost to an equivalent set of annual costs and add the annual cost to the recurring cost to get the total cost for each year over the life of the project.

Average Annualized Cost

- Text approach: Present worth of costs of $\overline{A}$ dollars/year spent continuously

$$P = \int_0^T \overline{A}e^{-it}\,dt = -\overline{A}\,\frac{e^{-it}}{i}\bigg|_0^T = -\frac{\overline{A}}{i}\left(e^{-iT}-1\right) = \frac{\overline{A}}{i}\left(1 - e^{-iT}\right)$$

- No exact comparison to formula for discrete case

$$\overline{A}\!\!\Big/_{\!P} = \frac{i}{1-e^{-iT}} \qquad A\!\!\Big/_{\!P} = \frac{i'}{1-(1+i')^{-T}} \qquad (1+i')^{-T} \neq e^{-iT}$$

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The text approach is to define a payment rate, $\overline{A}$, that is continuous and measured in units of dollars per year. Thus the total payment would be the integral over the lifetime of the investment (in years) from 0 to T years. To get the present worth we would have to discount the future payments back to the present worth by the formula that $P = Fe^{-it}$, the inverse of the formula for future worth, $F = Pe^{it}$.

Note that there is a difference in the meaning of A in each formula. The continuous formula assumes that the annual payments are done continuously. The discrete formula assumes that there is a single, end-of-year payment. Thus it is not possible to compare the two results.

The previous formula for comparing the interest rate in the discrete formula, i', with that in the continuous formula, i was given $i = \ln(1 + i'/k)^k$ where k is the number of compounding periods in one year. If k = 1, as implied in the discrete formula if n is the number of periods, then we get the equation that $i = \ln(1 + i')$ or $i' = e^i = 1 + i'$. This appears to give a direct comparison in the denominator of the two formulae, but it does not account for the different interest rates in the numerator.

The continuous formula can be used as can the discrete one to convert an initial cost into a series of equivalent ongoing costs. It can also be used to compute the present worth of a series of ongoing costs that can be added to an initial cost.

Considering Inflation

- What is i in equation $F = P(1 + i)^n$?
  - Real interest rate accounts for inflation
  - Market interest rate, i_m, paid by banks or charged by lenders, includes inflation
  - Inflation rate, f
- If i is real interest rate, F is in terms of constant dollars at time of investment
- If we use i_m, the market rate, F is in terms of then-current dollars

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We are all aware that inflation reduces the purchasing power of money over time. One thousand dollars in year zero has a purchasing power of $1000/(1.03) = $970.87after one year; after two years it is = $970.87/1.03 = $1000/(1.03)^2 = $942.60, *etc.* In general the purchasing power of a year zero dollar is $1/(1 + f)^n$ of the original dollar.

The actual price that we pay includes the effect of inflation; this approach is said to use current dollars. When we use this accounting we want to consider the market interest rate that includes the effects of inflation.

The real interest rate, which does not consider the effect of inflation is used for internal economic analyses. In this case we say that we are using constant dollars (as opposed to currency that loses its value due to inflation.).. It is useful for comparing options, but it will not give results that match future marketplace prices that change due to inflation.

The decision of which analysis to use (a) market interest rate and current dollars or (b) real interest rate and constant dollars, is a matter of choice, convention, or specifications determined by some government agency or standard-setting body.

Although the text by Tester *et al.* discusses various options it generally uses current dollars in its analyses. This uses a combination of the real interest rate (noted as x) and the inflation rate (with the symbol y).

Considering Inflation II

- For the market rate, i_m, the future worth in then-current dollars, $F = P(1 + i_m)^n$
- The future worth in then constant dollars, F', will be less than F due to inflation:
  $F' = F/(1 + f)^n = P(1 + i_m)^n/(1 + f)^n$
- The future worth in constant dollars is found by using the real interest rate, i
  - $F' = P(1 + i)^n = P(1 + i_m)^n/(1 + f)^n$
  - $i_m = i + f + if$

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The formulas on this chart are based on using discrete formulas. Starting with an initial present worth, P, the market interest rate, i_m (the actual rate you would get from a bank or pay to a lender), would product a future worth, $F = P(1 + i_m)^n$, in then current dollars. This is how many dollars it would produce, but what is the purchasing power of these future dollars compared to the purchasing power they would have if they existed at the time the process started?

The future F dollars would only be worth F' dollars using a constant dollar measure. The relation between F and F' is given by the inflation rate, f. If we had F' dollars at the start of the investment (when we really had P dollars) the inflation rate would produce $F = F'(1 + f)^n$ dollars (called constant or non-inflated dollars.

Combining these results gives $F' = F/(1 + f)^n = P(1 + i_m)^n/(1 + f)^n$. The real interest rate, i, produces these same F' dollars by the usual formula for future worth: $F' = P(1 + i)^n$. Comparing the two equations for F' gives:

$F' = P(1 + i)^n = P(1 + i_m)^n/(1 + f)^n$

$P(1 + i)^n (1 + f)^n = P[(1 + i) (1 + f)]^n = P[1 + i + f + if]^n = P(1 + i_m)^n$

Comparing the last two equations above shows that the market interest rate is the following combination of the actual interest rate and the inflation rate.

$i_m = i + f + if$

This is often approximated by ignoring the if term.

Other Factors

- Choice of index to account for inflation
- Taxes and depreciation may be considered
- Rate depends on source of funds
  - Borrowed money is tax deductible
  - Equity funding depends on desired rate of return on capital (not tax deductible)
- "Year zero" initial construction costs actually spread over several years

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Current year dollars account for inflation, typically using the consumer price index. See http://www.bls.gov/cpi/ (last accessed February 7, 2007) for the consumer price index.   This is a general index. Other possible inflation indices are available for specific items. For example, the inflation rate for fuel costs may be different from that for the general consumer price index.

The application of the previous formula for A/P and adding in a constant annual cost for maintenance, operations, and supplies is equivalent to doing the analysis in constant dollars. (Assuming a constant annual cost for these items ignores inflation.) In this case the correct interest rate to use in the real interest rate.

Advanced considerations include sources of cash and the tax implications of those sources. Analyses that consider tax also consider the impact of depreciation on the project accounting.

The example on pages 216-217 (with details on page 245 and 246) shows the application of inflation to the cost analysis of a power plant. (In that analysis the factor of 100 converts dollars to cents and the factor of 8766 is the average hours per year for a four year period. The last two homework problems ask you to apply this analysis to a combined-cycle gas turbine power plant and a solar photovoltaic collector. You can compare your results to those in the text for a nuclear power plant (light-water reactor).

Payback Period

- Defined as initial cost in dollars divided by annual savings (or income) in dollars per year
- Simplified analysis of fixed cost versus annual savings
- Engineering economics texts recommend **not** using this measure
- But – it is easier to understand than the discount rate

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If you are choosing between two possibilities in the purchase of a new appliance, with a cost difference D, between the two and an estimated annual savings S for the more expensive appliance. It is easy to compute the payback period D/S and then make a decision if the savings to you are worth it.

In a formal engineering economic analysis you would have to decide what a reasonable discount (or interest) rate, i, you would want to earn on the extra initial cost, D. You would also have to estimate how long you would own the appliance. You could then compute the present worth of the savings, P, from the reciprocal of the A/P formula:

$$P\big/_A = \frac{1-(1+i)^{-n}}{i}$$

For example if you were to keep the appliance for ten years and you wanted a discount rate of 3% the value of P/A would be 8.53 so the initial cost difference, D, would have to be less than 8.53 times the annual savings S. If the initial cost difference were exactly this figure (D = 8.53S) then the payback period, D/S, would be 8.53 years. If you wanted a 6% discount rate, your cost difference, D, would have to be less than 6.14 times the savings. If you kept the appliance for only three years your would want D < 2.8S for a 3% discount rate and D < 2.58S for a 10% rate.