Solutions Manual
for
Introduction to Internal Combustion Engines

Richard Stone

Springer

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PREFACE

The popularity of *Introduction to Internal Combustion Engines* during the last ten years or so, has prompted me to prepare this set of worked solutions for the *3rd Edition*. I have used many of the questions as exam questions, so during the marking of the scripts, I hope that I will have removed any errors. None the less, readers may encounter some errors, in which case I would be very grateful to hear about them.

So as to make this manual self-contained, I have included the questions, and for clarity these have been written **in bold type**. The questions in the 2nd Edition have been denoted by a superscript asterisk (*). At the end of many questions I have added a **Discussion**. This contains material that is strictly speaking beyond the scope of the question, but is intended to be useful supplementary information. This manual provides a useful means of adding supplementary material, as occasionally some of the discussion material, (especially in the discussion-type questions) is not in the book.

All Figure numbers and Equation numbers refer to the *3rd Edition* of the book, and to avoid any confusion, letters have been used in this *Manual* to define equations. The nomenclature and abbreviations are consistent with the book, with the exception of time derivatives for which it has not been possible to include the 'dot'. This means, for example, that work and power are both denoted by W, but it should be clear from the comments, units and context what is being used. ***Bold italics*** are used on occasion to indicate entries in the index for topics that are treated in the book, and do not form a core part of the solution. The final answers to each part of a question are shown in **bold font**.

In order to make this manual self contained, the Appendix contains thermodynamic tables for combustion calculations; this should also ensure consistency in the answers if these tables are made available to students. The tables contain equilibrium constants, and molar thermodynamic property data (internal energy, enthalpy, Gibbs Energy, and Entropy) for the species to be found in the reactants and products. The datum for enthalpy adopted here, is a datum of ***zero enthalpy for elements when they are in their standard state at a temperature of 25°C***. The enthalpy of any molecule at 25°C will thus correspond to its enthalpy of formation, ΔH_f°. This choice of datum (although not used to my knowledge in any other tables) will be seen to facilitate energy balances in combustion. Unlike tables that use an identical datum for reactant and product species, there is no need to include enthalpies or internal energies of reaction. Since the first publication of *Introduction to Internal Combustion Engines* the preferred practice for denoting molar quantities is to use a lower case letter (to emphasise that it is a specific quantity) with a tilde above, for example $\tilde{n}$. However, for consistency with the book (and in common with many other publications) molar quantities will be denoted here by upper case letters. This requires the reader to decide whether the symbol refers to a molar specific quantity, or a property value of the complete system.

Some of the combustion problems have been generated using the equilibrium solving package STANJAN, developed by Prof W C Reynolds of Stanford University.

Richard Stone

Summer 1999

CONTENTS

1 Introduction

1.1 What are the key technological developments for spark ignition engines in the first half of the 20th century.

1) Ricardo 1919 Patent for (side valve) turbulent combustion chamber. With the comparatively low octane rating fuel available for normal use (say 60-70), the compression ratio was limited to about 4:1. The Ricardo chamber allowed an increase in compression ratio to 5:1, and when this was combined with the faster burn, there was about a 20% improvement in both the output and the efficiency.

2) Work by Ricardo (for Shell) showed in 1917 that gasoline distilled from Borneo crude oil contained high levels of aromatics (notably: benzene, toluene and xylene). This fuel had a higher octane rating that permitted a unity increase in the compression ratio, with a 10% increase in power and slightly greater reduction in the fuel consumption. It was this fuel that enabled Alcock and Brown to cross the Atlantic in 1919 - they used a modified Rolls Royce Eagle engine, in which the compression ratio was increased from 5:1 to 6:1.

3) In 1922 Midgley and Boyd used tetra ethyl lead [$Pb(C_2H_5)_4$] to increase the octane rating of conventional gasolines (Journal of Industrial and Engineering Chemistry, 1922). This in due course led to the widespread availability of high octane rating fuels (above say 90) with the possibility of compression ratios of 8:1 and higher. This led to the demise of side valve engines since this type of geometry was limited to compression ratios in the region of 5:1. The only sensible way to obtain high compression ratios was to have the combustion chamber above the piston and an overhead valve arrangement.

2 Thermodynamic Principles

2.1* For the ideal air standard Diesel cycle with a volumetric compression ratio of 17:1 calculate the efficiencies for cut-off ratios of 1, 2, 4, 9. Take $\gamma = 1.4$. The answers can be checked with figure 2.2.

Using equation 2.10, we can first evaluate the term that is common to the Otto cycle efficiency:

with $r_v = 17$ and $\gamma = 1.4$, then $1/r_v^{\gamma-1} = 1/17^{1.4-1} = 0.322$

Next we need to evaluate the term in square brackets for each of the cut-off ratios (α), adopting a tabular approach:

α	$\dfrac{\alpha^\gamma - 1}{\gamma(\alpha-1)}$	$\dfrac{1}{r_v^{\gamma-1}}\dfrac{\alpha^\gamma-1}{\gamma(\alpha-1)}$	η_{Diesel}
1	1	0.322	0.678
2	1.171	0.377	0.623
4	1.420	0.457	0.543
9	1.846	0.594	0.406

Discussion: It will be seen later (question 5.6) that the values of the cut-off (or load ratio) are usually 3 or less. There is thus not much difference compared to the Otto cycle efficiency, and a difference that is reduced further in practice because Diesel engine combustion does not occur at constant pressure. (Nor of course is combustion in the spark ignition engine at constant volume).

2.2* Outline the shortcomings of the simple ideal cycles, and explain how the fuel-air cycle and computer models overcome these problems.

The Otto cycle assumes heat addition at constant volume, while the Diesel cycle assumes heat addition at constant pressure. Of course the spark ignition engine does not have instantaneous combustion (which would be equivalent to heat addition at constant volume), and nor does the diesel engine have combustion occurring at constant pressure. It is for these reasons that the Dual cycle (see section 2.2.3 and Figure 2.4) is sometimes considered. This allows some heat addition at constant volume, and the remainder to occur at constant pressure. However, the efficiencies predicted by the Otto cycle and Diesel cycle are not that different (see the discussion of the previous question), so the assumptions about the nature of heat addition are not the reasons for a difference of a factor of about 2 in the efficiencies of any engine compared to a simple cycle analysis.

To identify the shortcomings of the simple ideal cycles, we need to review the assumptions in the analyses (which will be identified here by italic script), and comment how the behaviour of a real engine differs. We will do this in an order that starts with the most significant shortcomings.

The working fluid is assumed to be air. In all engines there will be products of combustion during expansion, and in the case of engines with external mixture preparation, then there is compression of an air fuel mixture. For these mixtures, the specific heat capacities at constant pressure (c_p) and constant volume (c_v) are higher, and increase significantly with temperature (see Figure 2.9). The semi-perfect gas assumption is quite acceptable (in which c_p and c_v are only dependant on temperature, and the difference between them is constant - the specific gas constant [$c_p - c_v = R$]). The increase in the specific heat capacities as the temperature rises, means that the ratio of the specific heat capacities ($c_p/c_v = \gamma$) will fall. This is allowed for in both the fuel-air cycle analyses and computer models. As the air fuel ratio is richened then gamma (γ - the ratio of the heat capacities) will fall for two reasons. Firstly, the more fuel (which will have a higher heat capacity than air) then the lower the value of gamma, and then after combustion there will be relatively more water vapour and carbon dioxide than nitrogen in the products which will also lead to a lowering of gamma. Secondly, the more fuel present, then the higher the temperatures during and after combustion, so again the lower the value of gamma.

Fuel-air cycles and computer models allow for the real behaviour of the gases. Computer models usually make the semi-perfect gas assumption, that is to say the pressure dependency of the specific heat capacities is ignored, and the specific gas constant is invariant. The simple ideal cycles would give much more realistic predictions if a lower value of gamma was used, for a compression ratio of 10:1, then

gamma, γ	1.4	1.3	1.2
η_{Otto}	0.602	0.499	0.369

for which the fuel-air cycle predicts an efficiency of about 0.47 for stoichiometric (chemically correct for complete combustion in the absence of dissociation) octene/air mixtures.

It has already been explained how richening the mixture increases the departure from ideal gas behaviour, however, once mixtures are richened beyond stoichiometric there is insufficient oxygen for the complete combustion of fuel, and the efficiency falls rapidly (see figure 2.10).

The compression and expansion processes are assumed to be reversible and adiabatic. The assumption of reversibility is acceptable, since all frictional losses can be assigned to the mechanical efficiency of the engine. The mechanical efficiency can be incorporated into computer models, and falls from 90% or so at full load, to zero at no load. Heat transfer is ignored by the fuel-air cycle, and this is probably the most significant omission from the fuel-air cycle.

Consider a spark ignition engine with a compression ratio of 10, operating at full throttle with a stoichiometric mixture. The Otto cycle predicts an efficiency of 60% and the fuel-air cycle predicts an efficiency of 47%. In reality such an engine might have a full throttle brake efficiency of 30%, and this means there are 17 percentage points to be accounted for, perhaps as follows:

		percentage points
mechanical losses		3
finite speed of combustion:		2
20 degree 10-90% burn	1, or	
40 degree 10-90% burn	3	
blow-by and unburnt fuel in the exhaust		1
dissociation		1
cycle-by-cycle variations in combustion		2
exhaust blow-down and gas exchange		1
heat transfer		7

This breakdown has been produced by a computer model, and serves to summarise the losses that are not accounted for in either the simple air standard cycles or the fuel-air cycle analysis. It should also be added, that in general computer models do not allow for cycle-by-cycle variations in combustion.

Instantaneous heat input or combustion. Only computer models can allow for the 'rounding of the indicator diagram' or 'finite piston speed losses', and it is perhaps surprising how low the loss is for a contemporary fast burn combustion system (20 degree burn duration for the 10-90% mass fraction of the fuel to be burnt).

Instantaneous heat rejection or blowdown, and no gas exchange losses. The cycles by definition do not require any gas exchange, and the 'rounding of the indicator diagram' at the end of expansion caused by the exhaust valve opening before bottom dead centre is even smaller than the loss due to the finite speed of combustion. At full throttle the gas exchange losses are almost negligible, but at no load in a homogeneous charge spark ignition engine, the frictional losses and gas exchange work (in particular the throttle work) are almost equal to one another.

Leakage and incomplete combustion. The cycles by definition do not allow for any leakage from the cylinder, while for a typical engine this amounts to about 1% of the trapped cylinder mass. In the case of spark ignition engines this will be mostly unburnt mixture, which is normally returned to the inlet manifold by the crankcase ventilation system. Unburnt fuel will be emitted in the exhaust, and its origin depends on the engine type. With diesel engines operating close to full load, then there is insufficient mixing of the air and fuel to permit complete oxidation. The outer extremities of the spray may also become over-diluted and fail to burn - a problem that is most significant at light load. For spark ignition engines, unburned hydrocarbons are a consequence of fuel being absorbed in oil films and crevices as the pressure is rising, and then being released too late in the expansion stroke for complete combustion.

Dissociation is only significant for spark ignition engines, and perhaps surprisingly it is most significant at stoichiometric where it might account for a few per cent of the initial chemical energy (in a 3 way catalyst that provides complete oxidation of a stoichiometric mixture, then there is a temperature rise of about 50K). Away from stoichiometric dissociation is less significant, because either the excess air (for weak mixtures) or excess fuel (for rich mixture) moves the equilibrium in a way to minimise the effect of the excess species (see ***Le Châtelier***)

2.3* A 2 litre four-stroke indirect injection diesel engine is designed to run at 4500 rpm with a power output of 45 kW; the volumetric efficiency is found to be 80 per cent. The bsfc is 0.071 kg/MJ and the fuel has a calorific value of 42 MJ/kg. The ambient conditions for the test were 20 °C and 1 bar. Calculate the bmep, the arbitrary overall efficiency and the air fuel ratio.

We can start by calculating the bmep, by rearrangement of equation 2.38:

$$\text{bmep} = \text{brake power}/(V_s \text{x} N^*)$$

where: V_s = swept volume, and
N^* = number of times the swept volume is exchanged per second, remembering that this is a four-stroke engine, in which the volume is swept in alternate revolution.

$$\text{bmep} = 45 \text{ x } 10^3/(2\text{x}10^{-3} \text{ x } [4500/120]) = 6.0\text{x}10^5$$

$$\text{bmep} = \mathbf{6\ bar}$$

Equation 2.16 can be rearranged to calculate the arbitrary overall efficiency (η_o)

$$\eta_o = 1/(\text{bsfc x CV})$$

where: bsfc is the brake specific fuel consumption, and
CV is the calorific value of the fuel

$$\eta_o = 1/(0.071\text{x}10^{-6} \text{ x } 42\text{x}10^6) = 0.32$$

$$\eta_o = \mathbf{32\%}$$

Finally, to calculate the air fuel ratio we can employ equation 2.45

$$\text{bmep} = \eta_o \times \eta_v \times \rho_a \times \text{CV/AFR}$$

Alternatively, we can from first principles calculate the air flow rate and the fuel flow rate.

The fuel mass flow rate, m_f, is given by

$$m_f = \text{power}/(\eta_o \times \text{CV})$$

$$= 45\times10^3/(0.32 \times 42\times10^6) = 0.0032 \text{ kg/s}$$

To determine the air mass flow rate, we first need to determine its density (ρ_a), by means of the equation of state:

$$\rho_a = p/RT = 1\times10^5/(287 \times 293) = 1.189 \text{ kg/m}^3$$

where the specific gas constant (R) for air is 287 J/kgK

We evaluate the volumetric air flow rate (V_a) from the definition of the volumetric efficiency (equation 2.42):

$$V_a = V_s \times N^* \times \eta_v = 2\times10^{-3} \times [4500/120] \times 0.80 = 0.060 \text{ m}^3/\text{s}$$

The air fuel ratio (AFR) is a gravimetric ratio:

$$\text{AFR} = m_a/m_f = \rho_a \times V_a/m_f = 1.189 \times 0.060/0.0032 = \mathbf{22.3}$$

Discussion The AFR of 22.3 implies a load close to full load, perhaps the load (or bmep) for maximum efficiency, which is in accordance with the bmep of 6 bar. An efficiency of 32% is likely to be close to the maximum of an indirect injection engine, since this type is inherently less efficient than a direct injection engine.

2.4* A twin-cylinder two-stroke engine has a swept volume of 150 cm^3. The maximum power output is 19 kW at 11 000 rpm. At this condition the bsfc is 0.11 kg/MJ, and the gravimetric air/fuel ratio is 12:1. If the ambient test conditions were 10°C and 1.03 bar, and the fuel has a calorific value of 44 MJ/kg, calculate: the bmep, the arbitrary overall efficiency and the volumetric efficiency.

We can start by calculating the bmep, by rearrangement of equation 2.38:

$$\text{bmep} = \text{brake power}/(V_s \times N^*)$$

where: V_s = swept volume, and
N^* = number of times the swept volume is exchanged per second, remembering that this is a two-stroke engine, in which the volume is swept every revolution

$$\text{bmep} = 19\times10^3/(150\times10^{-6} \times [11\,000/60]) = 6.91\times10^5$$
$$\text{bmep} = \mathbf{6.91 \text{ bar}}$$

Equation 2.16 can be rearranged to calculate the arbitrary overall efficiency (η_o)

$$\eta_o = 1/(\text{bsfc} \times \text{CV})$$

where: bsfc is the specific fuel consumption, and
CV is the calorific value of the fuel

$$\eta_o = 1/(0.11\text{x}10^{-6} \text{ x } 44\text{x}10^{6}) = 0.207$$

$$\eta_o = \mathbf{20.7\%}$$

Finally, to calculate the volumetric efficiency, we can rearrange equation 2.42

$$\text{bmep} = \eta_o \text{ x } \eta_v \text{ x } \rho_a \text{ x CV/AFR}$$

Alternatively, we can from first principles calculate the fuel mass flow rate into the engine, and thence determine the air flow rate since we are given the air fuel ratio.

The fuel mass flow rate, m_f, is given by

$$m_f = \text{power x bsfc}$$

$$= 19\text{x}10^{3} \text{ x } 0.11\text{x}10^{-6} = 0.00209 \text{ kg/s}$$

The air fuel ratio (AFR) is a gravimetric ratio:

$$\text{AFR} = m_a/m_f \text{ or } m_a = \text{AFR x } m_f$$

$$12 \text{ x } 0.00209 = 0.0251 \text{ kg/s}$$

To determine the air volume flow rate, we first need to determine its density (ρ_a), by means of the equation of state:

$$\rho_a = p/RT = 1.03\text{x}10^{5}/(287 \text{ x } 283) = 1.268 \text{ kg/m}^3$$

where the specific gas constant (R) for air is 287 J/kgK

We can now evaluate the volumetric air flow rate (V_a)

$$V_a = m_a/\rho_a = 0.0251/1.268 = 0.0198 \text{ m}^3\text{/s}$$

Using the definition of the volumetric efficiency (equation 2.21):

$$\eta_v = V_a/(V_s \text{ x } N^*) = 0.0198/(150\text{x}10^{-6} \text{ x } [11\,000/60])$$

$$\eta_v = 0.720, \text{ or } \mathbf{72.0\%}$$

Discussion: This is evidently a small two-stroke engine, so it is likely to have under-piston scavenging, and a significant short-circuiting loss, in which some of the inducted charge flows directly into the exhaust system. This accounts for the low efficiency. The bmep (corresponding to full load) is lower than a four-stroke engine because of the residuals (exhaust gases not displaced from the cylinder), and the trapped volume being significantly less than the swept volume. The volumetric efficiency is lower than a four-stroke (for which over 90% would be expected at full load), since there is no separate induction stroke.

2.5* **A four-stroke 3 litre V6 spark ignition engine has a maximum power output of 100 kW at 5500 rpm, and a maximum torque of 236 Nm at 3000 rpm. The minimum bsfc is 0.090 kg/MJ at 3000 rpm, and the air flow rate is 0.068 m^3/s. The compression ratio is 8.9:1 and the mechanical efficiency is 90 per cent. The engine was tested under ambient conditions of 20 °C and 1 bar; take the calorific value of the fuel to be 44 MJ/kg.**

(a) Calculate the power output at 3000 rpm and the torque output at 5500 rpm.
(b) Calculate for both speeds the bmep and the imep.
(c) How does the arbitrary overall efficiency at 3000 rpm compare with the corresponding air standard Otto cycle efficiency?
(d) What is the volumetric efficiency and air/fuel ratio at 3000 rpm?

(a) The equation for relating power (*W*) to torque (*T*) is:

$$W = T \times \omega$$

where ω is the angular velocity (rad/s, or 2xπ rev/s)

Thus at 3000 rpm, $W = 236 \times 2\pi \times 3000/60 =$ **74.14 kW**

At 5500 rpm, $T = W/\omega = 100\text{x}10^3/(5500 \times 2\pi/60) =$ **173.6 Nm**

(b) Next we can calculate the bmep, by rearrangement of equation 2.38:

$$\text{bmep} = \text{brake power}/(V_s \text{x} N^*)$$

where: V_s = swept volume, and
N^* = number of times the swept volume is exchanged per second, remembering that this is a four-stroke engine, in which the volume is swept in alternate revolutions

Once the bmep is known, then the definition of mechanical efficiency (η_{mech}) in equation 2.19 will yield the imep:

$$\eta_{\text{mech}} = \text{bmep/imep}$$

At 3000 rpm bmep = $74.14\text{x}10^3/(3000\text{x}10^{-6} \times [3000/\{2 \times 60\}]) = 9.89\text{x}10^5$
bmep = **9.89 bar**

and imep = bmep/η_{mech} = 9.89/0.9 = **10.98 bar**

At 5500 rpm bmep = $100\text{x}10^3/(3000\text{x}10^{-6} \times [5500/\{2 \times 60\}]) = 7.27\text{x}10^5$
bmep = **7.27 bar**

and imep = bmep/η_{mech} = 7.27/0.9 = **8.08 bar**

(c) Equation 2.16 can be rearranged to calculate the arbitrary overall efficiency (η_o)

$$\eta_o = 1/(\text{bsfc} \times \text{CV})$$

where: bsfc is the specific fuel consumption, and
CV is the calorific value of the fuel

$\eta_o = 1/(0.09\text{x}10^{-6} \text{ x } 44\text{x}10^6) = 0.253$

$\eta_o = \mathbf{25.3\%}$

The expression for the Otto cycle efficiency (equation 2.22) is:

$$\eta_{Otto} = 1 - \frac{1}{r_v^{\gamma-1}}$$

Substitution of the values:

compression ratio, $r_v = 8.9$, and
ratio of heat capacities, $\gamma = 1.4$, gives

$$\eta_{Otto} = 1 - \frac{1}{8.9^{1.4-1}} = 0.583$$

$$\eta_{\text{Otto}} = \mathbf{58.3\%}$$

(d) Using the definition of the volumetric efficiency (equation 2.42), for the volumetric air flow rate (V_a):

$\eta_v = V_a /(V_s \text{ x } N^*) = 0.068/(3000\text{x}10^{-6} \text{ x } [3000/\{2 \text{ x } 60\}])$

$\eta_v = 0.907$, or 90.7%

To calculate the air/fuel ratio, we need to convert the volumetric air flow into a mass flow rate (m_a), and then calculate the fuel mass flow rate (m_f).

The equation of state can be written as:

$pV_a = m_aRT$, or $m_a = pV_a/(RT) = 1.0\text{x}10^5 \text{ x } 0.068/(287 \text{ x } 293) = 0.08086$ kg/s

where the specific gas constant (R) for air is 287 J/kgK

The fuel mass flow rate, m_f, is given by rearrangement of equation 2.15:

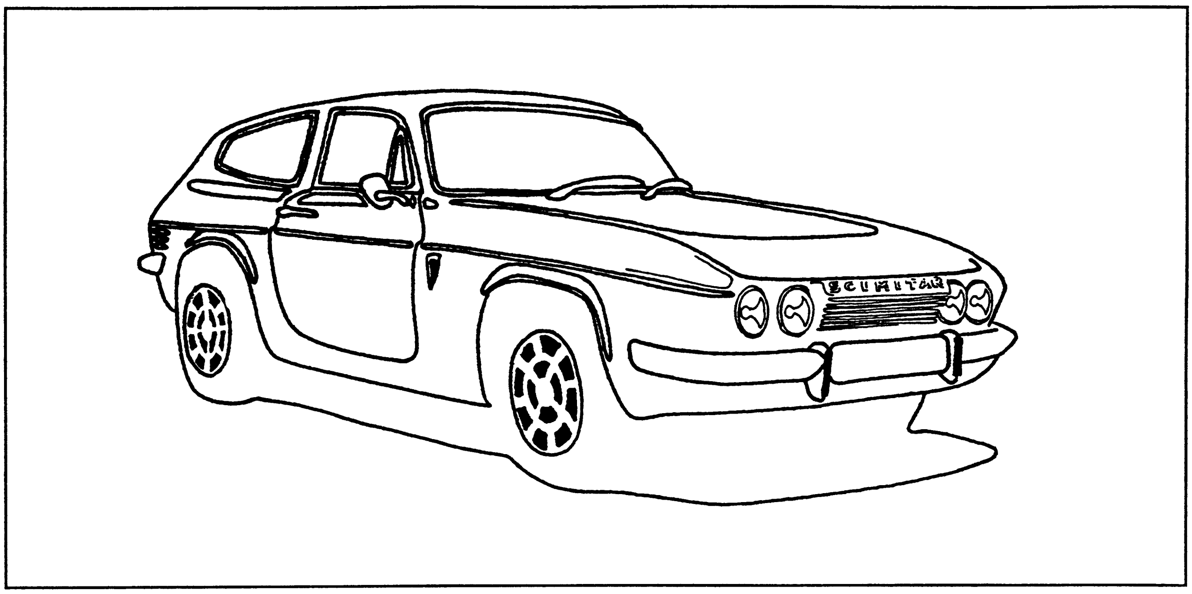
$m_f = \text{power x sfc}$

$= 74.14\text{x}10^3 \text{ x } 0.090\text{x}10^{-6} = 0.006673$ kg/s

The air fuel ratio (AFR) is a gravimetric ratio:

$\text{AFR} = m_a/m_f = 0.08086/0.006673 = \mathbf{12.12}$

Discussion: This question is based around the published compression ratio, torque and power data for the Ford Essex engine. This was used in British Ford vehicles from the 1960s to the 1980s (being used last in the Transit van), but it was also popular for sports car use, such as in the Reliant Scimitar. The assumption of a constant mechanical efficiency is unrealistic, and the mechanical efficiency is likely to fall to about 75% at 5500 rpm. A paper '*Turbocharging the 3 litre V6 Ford Essex Engine*' by E R R Fuchs, K G Parker and B T Pritchard Lovell (Proc. Instn Mech. Engrs, vol 188, pp33-47, 1974, provides some useful data for comparison with the assumptions in this paper. In particular, the sfc is almost constant at 0.083 kg/MJ between 2500 and 5000 rpm. Problem 9.17 is based on the turbocharged performance of this engine.



Reliant Scimitar - SE5a

2.6 Show that the air standard Dual cycle efficiency is given by:

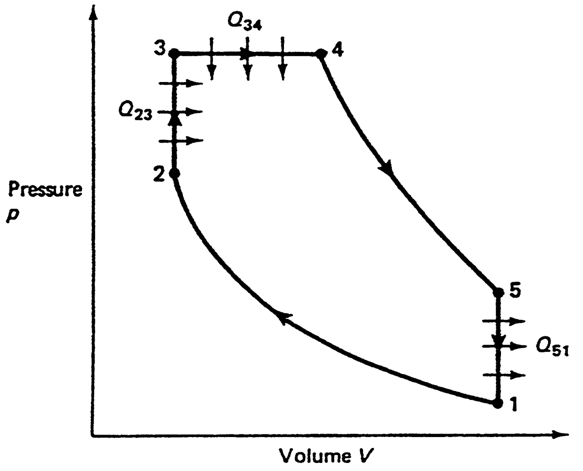
$$\eta = 1 - \frac{1}{r_v^{\gamma-1}}\left[\frac{r_p\alpha^\gamma - 1}{(r_p-1) + \gamma r_p(\alpha-1)}\right]$$

where r_v = volumetric compression ratio

r_p = pressure ratio during constant-volume heat addition

α **= volumetric expansion ratio during constant-pressure, heat addition**

With reference to Figure 2.4:



$$r_p = p_3/p_2 \qquad (A$$

$$\alpha = V_4/V_3 \qquad (B$$

$$V_5 = V_1 = r_v V_3$$

and $$V_4 = V_5 \alpha / r_v = V_1 \alpha / r_v \qquad (C$$

Figure 2.4 Ideal Air Standard Dual Cycle

For any cycle, the First Law of Thermodynamics can be applied:

$$\eta_{\text{Dual}} = 1 - Q_{\text{out}}/Q_{\text{in}} = 1 - Q_{51}/(Q_{23} + Q_{34}) \qquad (D$$

Next we can evaluate the heat flows in terms of the temperatures around the cycle, but to do so we need to invoke the assumption of having a Perfect Gas (with constant specific heat capacities), and a fixed mass (m):

$$Q_{51} = m \text{ x } c_v (T_5 - T_1) \qquad (E$$

$$Q_{23} = m \text{ x } c_v (T_3 - T_2) \qquad (F$$

$$Q_{34} = m \text{ x } c_p (T_4 - T_3) \qquad (G$$

Substitution of equations E, F, and G into equation D gives:

$$\eta_{Dual} = 1 - \left[\frac{T_5 - T_1}{(T_3 - T_2) + c_p / c_v (T_4 - T_3)} \right] \qquad (H$$

or

$$\eta_{Dual} = 1 - \left[\frac{T_5 - T_1}{(T_3 - T_2) + \gamma (T_4 - T_3)} \right] \qquad (I$$

We now need to work around the cycle, so as to evaluate all the temperatures in terms of a single temperature. We will start with T_1 and proceed in a clockwise direction. It would of course be possible to start at any temperature, and proceed in either direction, and sometimes it is expedient to work clockwise and anti-clockwise from the initial temperature, when it is not possible to complete the cycle in any other way.

1 → 2 assumed to be reversible and adiabatic, and thus isentropic: $T_2 = T_1 r_v^{\gamma-1}$ (J

2 → 3 heat addition at constant volume, so application of the equation of state ($pV = mRT$) gives

$$T_3 = T_2 p_3/p_2$$

substitution for T_2 from Equation (J) and for p_3/p_2 from Equation (A) gives:

$$T_3 = T_1 r_v^{\gamma-1} r_p \qquad \text{(K}$$

3 → 4 heat addition at constant pressure, so application of the equation of state ($pV = mRT$) gives

$$T_4 = T_3 V_4/V_3$$

substitution for T_3 from Equation (K) and for V_4/V_3 from Equation (B) gives:

$$T_4 = T_1 r_v^{\gamma-1} r_p \alpha \qquad \text{(L}$$

4 → 5 assumed to be reversible and adiabatic, and thus isentropic: $T_5 = T_4 (V_4/V_5)^{\gamma-1}$

substitution for T_4 from Equation (L) and for V_4/V_5 from Equation (C) gives:

$$T_5 = T_1 r_v^{\gamma-1} r_p \alpha (\alpha/r_v)^{\gamma-1} = T_1 r_p \alpha^\gamma \qquad \text{(M}$$

Substitution for T_2, T_3, T_4 and T_5 in terms of T_1 (using equations J, K, L and M), into equation (I) gives

$$\eta_{Dual} = 1 - \left[\frac{r_p \alpha^\gamma - 1}{r_v^{\gamma - 1}(r_p - 1) + \gamma r_p r_v^{\gamma - 1}(\alpha - 1)} \right]$$

or

$$\eta_{Dual} = 1 - \frac{1}{r_v^{\gamma-1}} \left[\frac{r_p \alpha^\gamma - 1}{(r_p - 1) + \gamma r_p (\alpha - 1)} \right] \qquad \text{(O}$$

Extra questions

2.7 Explain why air-standard cycles are used to represent the performance of real internal combustion engines.

Although internal combustion engines follow a mechanical cycle, they do not follow a thermodynamic cycle - the incoming reactants self-evidently have a different thermodynamic state from the products of combustion, both in terms of composition and temperature. None the less, there is some justification in using the air standard cycles for a comparison. Firstly, they predict the correct trends, namely that increasing the compression ratio normally increases the efficiency, and that increasing the fuelling level in a compression ignition engine decreases the efficiency. Secondly, the major constituent of the reactants and products is nitrogen (about 80% in both cases), and there is no reason why a heat exchanger can not be added so as to return the temperature of the exhaust products to the initial temperature.

Some internal combustion engines have been adapted to operate on a thermodynamic cycle, usually for underwater applications. The products of combustion are cooled and pressurised in the presence of water, to condense the water vapour, and dissolve the carbon dioxide in the water. Oxygen is then added to compensate for that used during combustion. Since not all of the carbon dioxide is removed there will be a lower ratio of specific heat capacities, but this can be compensated for by adding argon to the reactants[1].

2.8 A four-cylinder, four stroke petrol engine is to develop 40 kW at 40 rev/s when designed for a volumetric compression ratio of 10.0 to 1. The ambient air conditions are 1 bar and 18° C, and the calorific value of the fuel is 44 MJ/kg.

(a) Calculate the specific fuel consumption in kg per MJ of brake work if the indicated overall efficiency is 50% of the corresponding air-standard Otto cycle, and the mechanical efficiency is 90%. The specific heat capacity ratio for air is 1.4.

(b) The required gravimetric air-fuel ratio is 15.4 and the volumetric efficiency is 92%. Estimate the required total swept volume, and the cylinder bore if the bore is to be equal to the stroke. Calculate also the brake mean effective pressure.

The expression for the Otto cycle efficiency (equation 2.9) is:

$$\eta_{Otto} = 1 - \frac{1}{r_v^{\gamma-1}}$$

Substitution of the values:

compression ratio, $r_v = 10.0$, and
ratio of heat capacities, $\gamma = 1.4$, gives:

$$\eta_{Otto} = 1 - \frac{1}{10.0^{1.4-1}} = 0.602$$

$$\eta_{\mathrm{Otto}} = \mathbf{60.2\%}$$

$$\eta_{\mathrm{brake}} = \eta_{\mathrm{i}} \mathrm{x} \eta_{\mathrm{mech}} = 0.5 \mathrm{~x~} \eta_{\mathrm{Otto}} \mathrm{x} \eta_{\mathrm{mech}} = 0.5 \mathrm{~x~} 0.602 \mathrm{~x~} 0.9 = 0.271$$

Equation 2.6 can be used to calculate the specific fuel consumption (sfc):

$$\mathrm{sfc} = 1/(\eta_{\mathrm{brake}} \mathrm{~x~CV}) = 1/(0.271 \mathrm{~x~} 44\mathrm{x}10^6) = \mathbf{83.9\ g/MJ}$$

where: CV is the calorific value of the fuel

b)

The brake specific fuel consumption and the required power output, enable us to calculate the fuel mass flow rate. Since we have been told the gravimetric air/fuel ratio, we can also calculate the air flow rate:

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[1] A Fowler, 'Experimental Research in Closed-Cycle Diesel Technology', IMechE Seminar, *Experimental Methods in Engine Research and Development*, 1988

m_a = AFR x m_f = AFR x W_b x sfc = 15.4 x 40x10^3 x 83.9x10^{-6} = 51.7 g/s

The equation of state can be used to find the density of the air, and the volumetric efficiency can then be used to determine the swept volume rate.

The equation of state can be written as:

$pV_a = m_aRT$, or $V_a = m_aRT/p$ = 0.0517 x 287 x (18 + 273)/1.0x10^5 = 0.0432 m^3/s

swept volume rate = V_a/η_{vol} = V_s x (n/2) n being in rev/s, and the division by 2 as it is a 4-stroke engine

Rearrangement gives: V_s = (V_a x 2)/(n x η_{vol}) = (0.0432 x 2)/(40 x 0.92) = **2.35 litres**

Since this is a four cylinder engine, the volume per cylinder is (2.35/4 =) 587 cm^3 = $\pi B^3/4$

B = 9.07 cm^3

Next we can calculate the bmep from equation 2.38:

bmep = brake power/(V_sxN^*)

where: V_s = swept volume, and
N^* = number of times the swept volume is exchanged per second, remembering that this is a four-stroke engine, in which the volume is swept in alternate revolutions.

bmep = 40x10^3/(2.35x10^{-3} x [40/2]) = **8.51 bar**

2.9 A compression-ignition engine has a volumetric compression ratio of 15. Find the thermal efficiency of the following air-standard cycles having the same volumetric compression ratio as the engine. The specific heat capacity ratio for air is 1.4.

(a) an Otto cycle

(b) a Diesel cycle in which the temperature at the beginning of compression is 18°C, and in which the heat supplied per unit mass of air is equal to the energy supplied by the fuel (in terms of its calorific value). The gravimetric air: fuel ratio is 28:1; the calorific value of the fuel is 44 MJ/kg; assume the specific heat of air at constant pressure is 1.01 kJ/kgK and is independent of temperature.

a) The expression for the Otto cycle efficiency (equation 2.22) with substitution for the compression ratio, (r_v = 10.0), and the ratio of heat capacities, (γ = 1.4), gives:

$$\eta_{Otto} = 1 - \frac{1}{r_v^{\gamma - 1}} = 1 - \frac{1}{15.0^{1.4-1}} = 0.661$$

b) Figure 2.3 defines the Diesel cycle. For isentropic compression:

$T_2 = T_1 r_v^{\gamma-1}$ = 291 x 15$^{1.4-1}$ = 860 K

Using the basis of the equivalent heat input defined in the question:

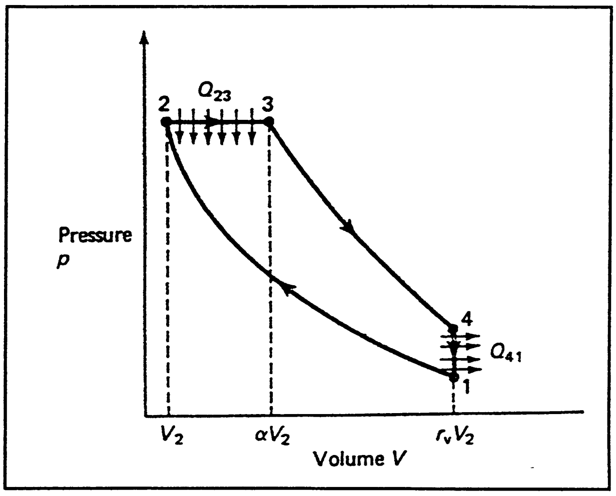
q_{23} = CV/AFR = $c_p\,(T_3 - T_2)$ or

$T_3 = T_2$ + CV/(AFR x c_p)

= 860 + 4x10^6/(28 x 1.01x10^3) = 2416 K

For isobaric expansion:

$$\frac{T_3}{T_2} = \frac{V_3}{V_2} = \alpha = \frac{2416}{860} = 2.81$$



We can now substitute this value of the load ratio (α) into the equation for Diesel cycle efficiency, or we can continue by finding the temperature at the end of the expansion stroke, and then determining the ratio of the heat supplied to the heat rejected.

For expansion 3 → 4 $V_3 = V_4\alpha/r_v = V_4 15/2.81 = 5.338V_4$

if the expansion is isentropic, then $T_4 = T_3(V_4/V_3)^{\gamma - 1} = 2416\,(1/5.338)^{1.4 - 1} = 1236$ K

$$\eta_{Diesel} = \eta_{cycle} = 1 - \frac{q_{out}}{q_i} = 1 - \left[\frac{c_v(T_4 - T_1\,)}{c_p(T_4 - T_3)}\right]$$

$$\eta_{Diesel} = 1 - \left[\frac{T_4 - T_1}{\gamma(T_4 - T_3)}\right] = 1 - \left[\frac{1236 - 291}{\gamma(2416 - 860)}\right] = 0.566$$

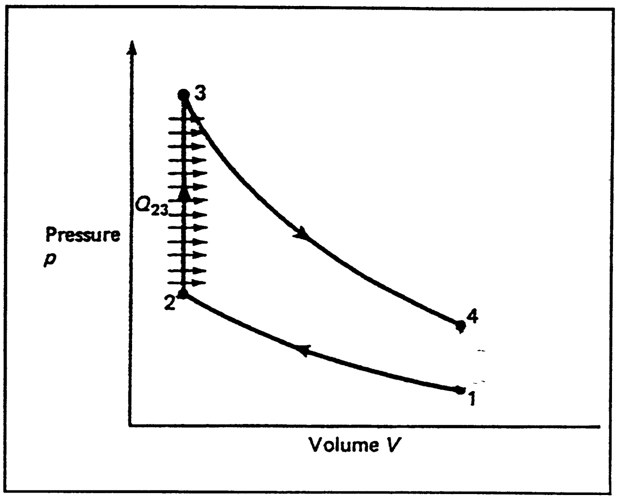
2.10 **A petrol engine of volumetric compression ratio 9 to 1 takes in a mixture of air and fuel in the ratio 17 to 1 by weight; the calorific value of the fuel is 44 MJ/kg. At the start of compression the temperature of the charge is 50°C. Assume that compression and expansion are reversible with pv^n constant, and n = 1.325 and 1.240 respectively, and that combustion occurs instantaneously at minimum volume. Combustion can be regarded as adding heat equal to the calorific value to the charge.**

However, there is a finite combustion efficiency, and heat transfer from the combustion chamber. Combustion is thus equivalent to a net heat input that corresponds to 75% of the calorific value of the fuel being burnt.

Calculate the temperatures: after compression, and at the start and end of expansion. Calculate the net work produced by the cycle and thus evaluate the indicated efficiency of the engine. Why is it inappropriate to calculate the indicated efficiency in terms of the heat flows?

Use the following thermodynamic data:

	Molar Mass kg	**Specific Heat Capacity at Constant Volume c_v kJ/kgK**
Air Fuel Mixture	**30**	**0.95**
Combustion Products	**28**	**0.95**



The accompanying figure shows the three linked, irreversible processes; there is clearly not a cycle.

For polytropic compression 1 → 2:

$$T_2 = T_1 r_v^{n-1} = (273 + 50) \text{ x } 9^{1.325 - 1} = 660 \text{ K}$$

Using the basis of the equivalent heat input defined in the question (remembering that there will be [AFR+1] kg of products or reactants, for every kg of fuel):

$$Q_{23} = \text{CV x } \eta_{\text{comb}} = c_v(\text{AFR} + 1)(T_3 - T_2)$$

or

$$T_3 = T_2 + (\text{CV x } \eta_{\text{comb}})/([\text{AFR} + 1] \text{ x } c_v)$$

$$= 660 + (44\text{x}10^6 \text{ x } 0.75)/(18 \text{ x } 0.95\text{x}10^3) = 2590 \text{ K}$$

For polytropic expansion 3 → 4:

$$T_4 = T_3/r_v^{n-1} = 2590/9^{1.240 - 1} = 1529 \text{ K}$$

To calculate the compression and expansion work, we need to evaluate $\int p\mathrm{d}V$. For a polytropic process pV^n is a constant (c). Thus:

$$W = \int p\mathrm{d}V = \int c/V^n \,\mathrm{d}V = -cV^{-n+1}/(n - 1) + \text{const1} = -(pV^n)\, V^{-n+1}/(n - 1) + \text{const1}$$

$$= -pV/(n - 1) + \text{const1}$$

If we now introduce integration limits (denoted by suffices 1 and 2), then: $W = (p_1V_1 - p_2V_2)/(n - 1)$

Using the equation of state ($pV = mRT$), this can be re-written as: $W = m(R_1T_1 - R_2T_2)/(n - 1)$

We can assume Perfect Gas behaviour, in which the gas constant is constant: $R_1 = R_2 = R_{12}$. Our next step is to evaluate the gas constants:

$$R_{12} = R_0/M_{12} = 8.3143/30 = 0.277 \text{ kJ/kgK} \quad \text{and} \quad R_{34} = R_0/M_{34} = 8.3143/28 = 0.297 \text{ kJ/kgK}$$

The compression work is thus: $w_{12} = R_{12}(T_1 - T_2)/n_{12} = 0.277(323 - 660)/(1.325 - 1) = -287$ kJ/kg_mixture

The expansion work is thus: $w_{34} = R_{34}(T_1 - T_2)/n_{34} = 0.297(2590 - 1529)/(1.240 - 1) = 1313$ kJ/kg_mixture

The net specific work , $w_{net} = w_{12} + w_{34} = -287 + 1313 = 1026$ kJ/kg_mixture

The energy supplied (per kg of mixture is): $q_{in} = CV/(1 + AFR) = 44x10^6/(1 + 17) = 2.44$ MJ/kg_mixture

The indicated efficiency is: $w_{net}/q_{in} = 1.026/2.444 = 0.42$ or $\eta_i = 42\%$

These processes do not form a cycle, so it is not possible (with the information given) to calculate properly the heat that would be 'rejected' to return the exhaust products at state 4 to state 1. It would also be necessary to calculate the heat flows in the compression and expansion processes. These can be evaluated by the change in internal energies and the work done in each process. Since there is a requirement to calculate the work flows, then this information might just as well be used directly.

DISCUSSION:

An indicated efficiency of 42% is clearly somewhat high for a spark ignition engine. However, no allowance has been made for:

the gas exchange work,
the non-instantaneous combustion leading to a rounding of the indicator diagram,
the exhaust valve opening before bottom dead centre,
incomplete combustion,
dissociation,
blowby, and other leakage from the cylinder
cycle-by-cycle variations in combustion, and
the compression process not starting until a little way after bottom dead centre.

None the less, this analysis has given a much more realistic estimate of performance than the Otto cycle analysis.

2.11 Derive the expression for the air standard Diesel cycle efficiency, in terms of the ratio of gas specific heat capacities (γ), the volumetric compression ratio (r_v) and the load ratio (α). State clearly the assumptions in your analysis.

Show that the indicated mean effective pressure ($\bar{p}_i$) of the air standard Diesel cycle is given by:

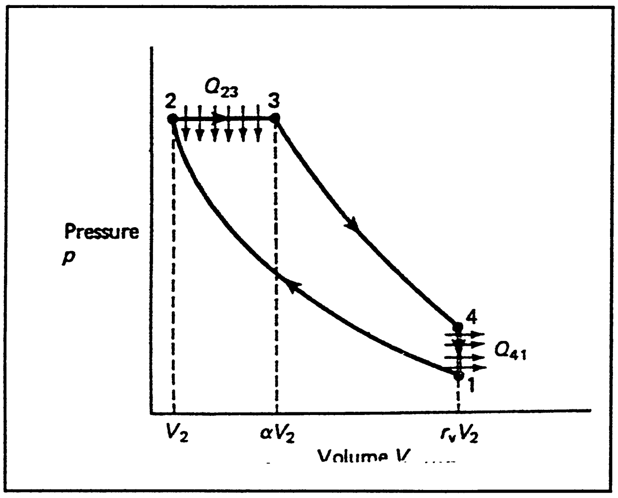
$$\bar{p}_i = \frac{P_1}{\gamma - 1} \times \frac{r_v}{r_v - 1} \left[\gamma r_v^{\gamma-1} (\alpha - 1) - (\alpha^\gamma - 1)\right]$$

where p_1 is the pressure at the start of compression.

With reference to Figure 2.3:

$\alpha = V_3/V_2$ (A

$V_4 = V_1 = r_v V_2$ (B



and $V_3 = \alpha V_1 / r_v$ (C

For any cycle, the First Law of Thermodynamics can be applied:

$$\eta_{Diesel} = 1 - Q_{out}/Q_{in} = 1 - Q_{41}/Q_{23} \qquad \text{(D}$$

Next we can evaluate the heat flows in terms of the temperatures around the cycle, but to do so we need to invoke the assumption of having a Perfect Gas (with constant specific heat capacities), and a fixed mass (m):

$$Q_{41} = m \; x \; c_v \; (T_4 - T_1) \qquad \text{(E}$$

$$Q_{23} = m \; x \; c_p \; (T_3 - T_2) \qquad \text{(F}$$

Substitution of equations E and F into equation D gives:

$$\eta_{Diesel} = 1 - \left[\frac{T_4 - T_1}{c_p \, / \, c_v (T_3 - T_2)} \right] \qquad \text{(G}$$

or

$$\eta_{Diesel} = 1 - \left[\frac{T_4 - T_1}{\gamma (T_3 - T_2)} \right] \qquad \text{(H}$$

We now need to work around the cycle, so as to evaluate all the temperatures in terms of a single temperature. We will start with T_1 and proceed in a clockwise direction. It would of course be possible to start at any temperature, and proceed in either direction. Sometimes it is expedient to work clockwise and anti-clockwise from the initial temperature, when it is not possible to complete the cycle conveniently in any other way.

1 → 2 assumed to be reversible and adiabatic, and thus isentropic: $T_2 = T_1 r_v^{\gamma-1}$ (I

2 → 3 heat addition at constant pressure, so application of the equation of state ($pV = mRT$) gives

$$T_3 = T_2 V_3 / V_2$$

substitution for T_2 from Equation (I) and for V_4/V_3 from Equation (B) gives:

$$T_3 = T_1 r_v^{\gamma-1} \alpha \qquad \text{(J}$$

3 → 4 is assumed to be reversible and adiabatic, and thus isentropic: $T_4 = T_3 (V_3/V_4)^{\gamma-1}$

substitution for T_3 from Equation (L) and for V_3/V_4 from Equation (C) gives:

$$T_4 = T_1 r_v^{\gamma-1} \alpha (\alpha / r_v)^{\gamma-1} = T_1 \alpha^{\gamma} \qquad \text{(K}$$

Substitution for T_2, T_3 and T_4 in terms of T_1 (using equations I, J and K), into equation (H) gives:
or

$$\eta_{Diesel} = 1 - \left[\frac{\alpha^{\gamma} - 1}{\gamma r_v^{\gamma - 1}(\alpha - 1)} \right]$$

$$\eta_{Diesel} = 1 - \frac{1}{r_v^{\gamma-1}} \left[\frac{\alpha^{\gamma} - 1}{\gamma(\alpha - 1)} \right]$$ (L

The imep of the engine is the indicated work divided by the swept volume (W_i/V_s). The indicated work is equal to the difference between the heat input and the heat output (which have been defined by Eqs E and F):

$$W_{net} = Q_{in} - Q_{out} = Q_{23} - Q_{41} = m \; [c_p \; (T_3 - T_2) - c_v \; (T_4 - T_1)]$$ (M

Substitution for T_2, T_3 and T_4 in terms of T_1 (using equations I, J and K), and division by c_v gives:

$$w_{net} = mc_v T_1 \left[\gamma(\alpha r_v^{\gamma-1} - r_v^{\gamma-1}) - (\alpha^{\gamma} - 1) \right]$$

or

$$w_{net} = mc_v T_1 \left[\gamma r_v^{\gamma-1}(\alpha - 1) - (\alpha^{\gamma} - 1) \right]$$ (N

The swept volume is: $V_s = V_1 - V_2 = V_2(r_v - 1)$ (O

We now need an expression for the trapped mass, and this can be obtained from the Equation of State, applied to state 1:

$$m = p_1 V_1 / RT_1 = p_1 r_v V_2 / RT_1$$ (P

Equation N has a term mc_v, so using Eq. P (and noting that $R = c_p - c_v$) this becomes

$$mc_v = p_1 V_1 c_v / RT_1 = p_1 r_v V_2 c_v / RT_1 = p_1 r_v V_2 c_v / (c_p - c_v) T_1 = p_1 r_v V_2 / (\gamma - 1) T_1$$ (Q

Dividing Eq N by V_s (from Eq. O) to give the imep, and substituting for mc_v from Eq. Q gives (since the V_2 and T_1 terms cancel):

$$\bar{p}_i = \frac{P_1}{\gamma - 1} \times \frac{r_v}{r_v - 1} \left[\gamma r^{\gamma - 1_v} (\alpha - 1) - (\alpha^{\gamma} - 1) \right]$$

2.12 The Lenoir engine operates without compression before ignition, and it can be modelled by the following processes in an air standard cycle:

1 → 2 heat addition at constant volume, to increase the temperature to ϕT_1,
2 → 3 reversible and adiabatic expansion through a volumetric expansion ratio r_e,
3 → 4 heat rejection at constant volume, to decrease the pressure to p_1, and
4 → 1 heat rejection at constant pressure, to decrease the temperature to T_1.

Draw the processes on a pV diagram, and show that the air standard cycle efficiency is given by:

$$\eta = 1 - \frac{(\gamma - 1)r_e^{\gamma} + \phi - \gamma r_e^{\gamma - 1}}{(\phi - 1)r_e^{\gamma-1}}$$

where: r_e = volumetric expansion ratio, and
ϕ = temperature ratio during constant-volume heat addition.

Show that the Atkinson cycle efficiency (see Example 2.3) reduces to this result when the compression ratio is set to unity. The Atkinson cycle efficiency (from example 2.3) is:

$$\eta_A = 1 - \frac{(\gamma - 1)r_e^{\gamma} + r_c(\theta - \gamma r_e^{\gamma - 1}) + r_c^{\gamma}}{\theta r_c r_e^{\gamma-1}}$$

The heat input is defined in terms of a temperature difference, so $T_3 = T_2 + \eta T_1$.

What is the air standard cycle efficiency when the expansion ratio (r_e) is 2, and the temperature ratio during constant-volume heat addition (ϕ) is 6?

For process 1 → 2: $T_2 = \phi T_1$

Process 2 → 3 is adiabatic and reversible, so it is also isentropic for which $TV^{\gamma - 1}$ is a constant, thus:

$$T_3 V_3^{\gamma - 1} = T_2 V_2^{\gamma - 1} \quad \text{or} \quad T_3 = T_2/r_e^{\gamma - 1} = \phi T_1/r_e^{\gamma - 1}$$

Process 4 → 1 is isobaric, so pV is a constant, thus: $T_4 = r_e T_1$

The heat input for process 1 → 2 is: $q_{12} = c_v(T_2 - T_1)$

The heat rejected for process 3 → 4 is: $q_{34} = c_v(T_3 - T_4)$

The heat rejected for process 4 → 1 is: $q_{41} = c_p(T_4 - T_1)$

$$\eta_{\text{Lenoir}} = 1 - q_{out}/q_{\text{in}} = 1 - (q_{34} + q_{41})/q_{12} = 1 - [c_v(T_3 - T_4) + c_p(T_4 - T_1)]/c_v(T_2 - T_1)$$

$$= 1 - [(T_3 - T_4) + \gamma(T_4 - T_1)]/(T_2 - T_1)$$

Substituting in for the temperatures in terms of T_1 (which then cancels out) gives:
Multiplying the numerator and denominator by $r_e^{\gamma - 1}$ gives:

$$\eta_{Lenoir} = 1 - \frac{\phi / r_e^{\gamma - 1} - r_e + \gamma(r_e - 1)}{(\phi - 1)} \qquad \text{(A}$$

$$\eta = 1 - \frac{(\gamma - 1)r_e^{\gamma} + \phi - \gamma r_e^{\gamma - 1}}{(\phi - 1)r_e^{\gamma - 1}}$$

The Atkinson cycle efficiency (from example 2.3) is:

$$\eta_A = 1 - \frac{(\gamma - 1)r_e^{\gamma} + r_c(\theta - \gamma r_e^{\gamma - 1}) + r_c^{\gamma}}{\theta r_c r_e^{\gamma - 1}}$$

Noting that the for the Lenoir cycle, there is no compression, so that the compression ratio (r_c) is unity. Also, the heat input is defined in terms of a temperature difference, so $\theta = \phi - 1$. Making these substitutions into the expression for the Atkinson cycle efficiency gives:

$$\eta = 1 - \frac{(\gamma - 1)r_e^{\gamma} + 1((\phi - 1) - \gamma r_e^{\gamma - 1}) + 1^{\gamma}}{(\phi - 1)1 r_e^{\gamma - 1}}$$

Which simplifies to the expression for the Lenoir cycle efficiency:

$$\eta = 1 - \frac{(\gamma - 1)r_e^{\gamma} + \phi - \gamma r_e^{\gamma - 1}}{(\phi - 1)r_e^{\gamma - 1}}$$

Substitution of the numerical values into Equation (A) gives:

$$\eta_{Lenoir} = 1 - \frac{\phi / r_e^{\gamma - 1} - r_e + \gamma(r_e - 1)}{(\phi - 1)} = 1 - \frac{6/2^{0.4} - 2 + 1.4(2 - 1)}{6 - 1} = 0.21$$

2.13 In an Otto cycle, the temperature rise during constant-volume heat addition is ϕT_1. If the conditions at the start of compression are defined as state 1, and the volumetric compression ratio is r_v, find expressions for the compression work, the expansion work, the net work, and the work ratio (net work divided by the expansion work).

For a closed reversible and adiabatic (and thus isentropic) process pV^{γ} = *constant*:

$W = \int p\mathrm{d}V = \int (\text{constant}/V^{\gamma})\mathrm{d}V = \int (\text{constant}V^{-\gamma})\mathrm{d}V = (1/[-\gamma + 1])(\text{constant}V^{-\gamma + 1})$ + integration constant

pV^{γ} can be substituted to eliminate the constant:

$W = (1/[-\gamma + 1])(pV^{\gamma}\ V^{-\gamma + 1})$ + integration constant $= (1/[-\gamma + 1])(pV)$ + integration constant

The integration constant can be eliminated by the use of integration limits:

$$W_{12} = (p_2V_2 - p_1V_1)/(1 - \gamma) \qquad \text{(A}$$

Using the equation of state $pV = mRT$, enables Equation A to be written in terms of temperatures:

$$W_{12} = mR(T_2 - T_1)/(1 - \gamma) \qquad \text{(B}$$

Noting that $R = c_p - c_v$, and $\gamma = c_p/c_v$, then:

$$W_{12} = m(c_p - c_v)(T_2 - T_1)/(1 - c_p/c_v) = -mc_v(T_2 - T_1) \qquad \text{(C}$$

a result that could have been obtained directly by applying the 1st Law of Thermodynamics and calculating the change in internal energy, since we know that the process is adiabatic.

For isentropic compression with a volumetric compression ratio of r_v, $T_2 = T_1r_v^{\gamma-1}$ (D

Thus $W_{12} = -mc_vT_1(r_v^{\gamma-1} - 1)$ (E

For isentropic expansion with a volumetric expansion ratio of r_v, $T_4 = T_3/r_v^{\gamma-1}$ (F

Thus $W_{34} = -mc_vT_3(1/r_v^{\gamma-1} - 1) = mc_vT_3(1 - 1/r_v^{\gamma-1})$ (G

The temperature rise during constant-volume heat addition is ϕT_1, so $T_3 = T_1(r_v^{\gamma-1} + \phi)$ (H

Equation G now becomes: $W_{34} = mc_vT_1(r_v^{\gamma-1} + \phi)(1 - 1/r_v^{\gamma-1})$ (I

The net work is: $W_{34} + W_{12} = mc_vT_1\{(r_v^{\gamma-1} + \phi)(1 - 1/r_v^{\gamma-1}) - (r_v^{\gamma-1} - 1)\}$

$$= mc_vT_1\{r_v^{\gamma-1}(1 - 1/r_v^{\gamma-1}) + \phi(1 - 1/r_v^{\gamma-1}) - (r_v^{\gamma-1} - 1)\}$$

$$= mc_vT_1\{\phi(1 - 1/r_v^{\gamma-1})\} \qquad \text{(J}$$

A result that could have been obtained directly by multiplying the Otto cycle efficiency $(1 - 1/r_v^{\gamma-1})$, by the heat input $(mc_vT_1\phi)$.

The work ratio is the net work divided by the expansion work, so using Equations I and J gives:

$$mc_vT_1\{\phi(1 - 1/r_v^{\gamma-1})\}/mc_vT_1(r_v^{\gamma-1} + \phi)(1 - 1/r_v^{\gamma-1}) = \phi/(r_v^{\gamma-1} + \phi) \qquad \text{(K}$$

3 Combustion and Fuels

In the following combustion calculations, values are needed for the molar masses of various species, and in the case of air, we also need to define its composition.

Table 3.1 Composition of Air, and the Molar Masses of its Constituents

Constituent	Mole Fraction	Molar Mass kg/kmol	Approximate Molar Mass kg/kmol
Nitrogen, N_2	0.7809	28.013	28
Oxygen, O_2	0.2095	31.999	32
Argon, Ar	0.0093	39.948	40
Carbon Dioxide, CO_2	0.0003	44.010	44

By multiplying the mole fraction of each species by its molar mass, and adding, we can determine the molar mass of air (M_{air})

$$M_{\text{air}} = 28.964 \simeq 29 \text{ kg/kmol}$$

In combustion calculations it is often taken that the oxygen forms 21% of the air, and the remaining constituents are referred to as atmospheric nitrogen (N_2^*), as a simple way of representing then argon, carbon dioxide and other trace gases. With this assumed composition, the molar mass of the atmospheric nitrogen(M_{N2*}) can be set so as to give the correct molar mass of air:

$$M_{N2*} = (28.964 - 0.21 \times 32)/0.79 = 28.16 \text{ kg/kmol}$$

Molar masses are also needed for carbon and hydrogen

Table 3.2 Molar Masses of Carbon and Hydrogen

Species	Molar Mass kg/kmol	Approximate Molar Mass kg/kmol
Hydrogen, H_2	2.016	2
Carbon, C	12.011	12

Care must be taken with the molar masses of oxygen and hydrogen, since the values here are for molecules, not atoms. In the subsequent calculations the approximate values for composition and molar masses will be used. The thermodynamic data necessary for energy balance and equilibrium calculations are explained and tabulated in Appendix A.

3.1* If a fuel mixture can be represented by the general formula C_xH_{2x}, show that the stoichiometric gravimetric air/fuel ratio is 14.8:1.

The molar (or volumetric) composition of air can be assumed to be 21% oxygen and 79% nitrogen. Thus for every kmol of oxygen there are (79/21=) 3.76 kmols of atmospheric nitrogen. Our reaction is thus:

$$C_xH_{2x} + z(O_2 + 3.76N_2^*) \rightarrow aCO_2 + bH_2O + 3.76zN_2^*$$

We have already applied an atomic balance for nitrogen, and we continue with the atomic balances for carbon and hydrogen:

C balance $a = x$

H balance $2b = 2x$

Next we can use the atomic oxygen balance:

O balance $2z = 2a + b$ or $2z = 2x + x$

So $z = 1.5x$

Assuming the following molar masses:

M_{H2} hydrogen (H_2)	2	kg/kmol
M_C carbon	12	kg/kmol
M_{N2*} nitrogen (N_2)	28.16	kg/kmol
M_{O2} oxygen (O_2)	32	kg/kmol
M_{air} air (21%O_2,79%N_2)	29	kg/kmol

Then the mass of 1 kmol of fuel is

$$xM_C + 2x(M_{H2}/2) = 12x + 2x(2/2) = 14x$$

1 kmol of fuel reacts with $z(O_2 + 3.76N_2)$, the mass of which is

$$z(M_{O2} + 3.76M_{N2}) = 1.5x(32 + 3.76\times28.16) = 206.82x$$

Division of the mass of air ($206.82x$) by the mass of fuel ($14x$), gives the stoichiometric gravimetric air/fuel ratio of (206.82/14=) **14.77.**

Note The mass of air could have been determined more simply by saying that 1 kmol of fuel reacted with $1.5x(4.76)$ kmols of air, (for which the molar mass is 29kg/kmol), so the mass of air reacting with 1 kmol of fuel is:

$$1.5x(4.76\times29) = 207.06x$$

For which the stoichiometric gravimetric air/fuel ratio is (207.06/14=) **14.79.**

3.2* A fuel has the following molecular gravimetric composition

pentane (C_5H_{12})	**10 per cent**
heptane (C_7H_{16})	**30 per cent**
octane (C_8H_{18})	**35 per cent**
dodecane ($C_{12}H_{26}$)	**15 per cent**
benzene (C_6H_6)	**10 per cent**

Calculate the atomic gravimetric composition of the fuel and the gravimetric air/fuel ratio for an equivalence ratio of 1.1

A tabular approach will lead to the most compact solution, and we can assume a 100kg of fuel:

COLUMN	1	2	3	4	5
Component	mass kg	molar mass kg/kmol	moles of component kmols	moles of C kmols	moles of H kmols
pentane (C_5H_{12})	10	72	0.1389	0.6945	1.6667
heptane (C_7H_{16})	30	100	0.3000	2.1000	4.8000
octane (C_8H_{18})	35	114	0.3070	2.4561	5.5263
dodecane ($C_{12}H_{26}$)	15	170	0.0824	1.0588	2.2941
benzene (C_6H_6)	10	78	0.1282	0.7692	0.7692
	100			7.0786	15.0563

Column 1 Since we have specified 100 kg, then the masses of each component (i) correspond to their percentages.

Column 2 The molar mass of each component (C_xH_y) in the fuel is

$$xM_C + y(M_{H2}/2) = 12x + y(2/2) = 12x + y$$

Column 3 The number of kmols (n) of each species is:

$$n = (\text{Column 1})/(\text{Column 2})$$

Column 4 For each component, the number of kmols of carbon atoms (n_C) is given by the number of kmols of each component (n), multiplied by the number of carbon atoms in each molecule:

$$n_C = nx$$

Column 5 For each component, the number of kmols of hydrogen atoms (n_C) is given by the number of kmols of each component (n), multiplied by the number of hydrogen atoms in each molecule:

$$n_H = ny$$

Adding up each of Columns 4 and 5, gives us the relative atomic composition of the fuel; this can be expressed as:

$$C_{7.0786}H_{15.0563}$$

(A typical molar mass for gasoline is 100kg/kmol, in which case we have also found the mean molecular composition of the fuel.)

A useful check at this stage is to check the mass of our fuel:

$$7.0786M_C + 15.0563(M_{H2}/2) = 7.0786x12 + 15.0563(2/2) = 84.9432 + 15.0563 = 99.9995 \text{ kg}$$

a perfectly satisfactory check on our arithmetic)

The mass of hydrogen in our fuel is given by:

$$15.0563(M_{H2}/2) = 15.0563(2/2) = 15.0563 \text{ kg}$$

By difference, we know that from our initial 100 kg of fuel, that the mass of carbon will be:

$$100 - 15.0563 = 84.9437$$

so that the gravimetric composition of the fuel is : C:0.849, H:0.151

To find the air fuel ratio, we first need to establish the stoichiometric air fuel ratio.

The molar (or volumetric) composition of air can be assumed to be 21% oxygen and 79% nitrogen. Thus for every kmol of oxygen there are (79/21=) 3.76 kmols of atmospheric nitrogen. Our reaction is thus:

$$C_xH_y + z(O_2 + 3.76N_2^*) \rightarrow aCO_2 + bH_2O + 3.76zN_2^*$$

We have already applied an atomic balance for nitrogen, and we continue with the atomic balances for carbon and hydrogen:

C balance $a = x$

H balance $2b = y$

Next we can use the atomic oxygen balance:

O balance $2z = 2a + b$ or $2z = 2x + y/2$

So $z = x + y/4$

For our fuel ($C_{7.0786}H_{15.0563}$), $z = 7.0786 + 15.0563/4 = 10.8427$.

Our 100 kg of fuel reacts with $z(O_2 + 3.76N_2)$, the mass of which is

$$z(M_{O2} + 3.76M_{N2}) = 10.8427(32 + 3.76\times28.16) = 1495.01$$

In other words, the stoichiometric gravimetric air fuel ratio is (1495.01/100=) 14.95.

When the equivalence ratio is 1.1, then the air fuel ratio (AFR) is given by:

$$\mathbf{AFR} = \mathrm{AFR_s}/\phi = 14.95/1.1 = \mathbf{13.59}$$

An alternative approach would have been to calculate the gravimetric composition of each component of the fuel, and to then sum the masses of carbon and hydrogen for each component of the mixture. The gravimetric composition of the fuel could then be converted to a molar composition, and the stoichiometric equations completed as above.

3.3* The dry exhaust gas analysis from an engine burning a hydrocarbon fuel is as follows: CO_2 0.121, O_2 0.037, N_2^* 0.842. Determine the gravimetric composition of the fuel, the equivalence ratio of the fuel/air mixture, and the stoichiometric air fuel ratio.

Assume that the hydrocarbon (C_xH_y), reacts with z kmols of oxygen to produce 100 kmols of dry products of combustion, (there will of course be water present in the exhaust, so that our specified quantity of reactants produces more than 100 kmols of products).

The molar (or volumetric) composition of air can be assumed to be 21% oxygen and 79% nitrogen. Thus for every kmol of oxygen there are (79/21=) 3.76 kmols of nitrogen. Our reaction is thus:

$$C_xH_y + z(O_2 + 3.76N_2) \rightarrow \text{100 kmols of dry products and water vapour}$$

$$C_xH_y + z(O_2 + 3.76N_2) \rightarrow 12.1CO_2 + 3.7O_2 + 84.2N_2^* + wH_20$$

(Check: 12.1 + 3.7 + 84.2 = 100.0; the oxygen level implies a weak mixture, which is also consistent with there being no measurement of carbon monoxide.)

The four atomic balances are:

N balance $3.76 \times 2z = 2 \times 84.2,\ z = 22.39$ (A

C balance $x = 12.1$ (B

O balance $2z = 12.1 \times 2 + 3.7 \times 2 + w = 31.6 + w$ (C

Substituting for the value of z from Eqn A:

$2 \times 22.39 = 31.6 + w\ ,\ w = 13.18$ (D

H balance $y = 2w$ (E

Substituting for the value of w from Eqn D: $y = 26.36$ (F

The molar composition of the fuel is thus: $C_{12.1}H_{26.36}$. To find the gravimetric composition of the fuel, we need to find separately the mass of the carbon and hydrogen:

Mass of carbon - $xM_C = 12.1 \times 12 = 145.2$

Mass of hydrogen - $yM_{H2} = 26.36 \times 1 = 26.36$ Total Mass = 171.56 (G

Mass fraction of carbon 145.2/171.56 = **0.846**

Mass fraction of hydrogen 26.36/171.56 = **0.154**

To find the equivalence ratio, define z_s as the quantity of air required for stoichiometric combustion:

$$C_{12.1}H_{26.36} + z_s(O_2 + 3.76N_2) \rightarrow aCO_2 + bH_2O + cN_2$$

The atomic balances are:

C balance $\quad 12.1 = a$

H balance $\quad 26.36 = 2b$

$$C_{12.1}H_{26.36} + z_s(O_2 + 3.76N_2) \rightarrow 12.1CO_2 + 13.18H_2O + cN_2$$

O balance $\quad 2z_s = 2 \times 12.1 + 13.18, \; z_s = 18.69$ (4

The equivalence ratio (ϕ) is the ratio of the quantity of air required for stoichiometric combustion (z_s) compared to that actually used (z, evaluated in Eq A)

$$\phi = z_s/z = 18.69/22.39 = 0.835$$

The stoichiometric air/fuel ratio can be found from the mass of fuel (Eq G), and the mass of the stoichiometric quantity of air (z_s).

Mass of Air $z_s(O_2 + 3.76N_2)$ - $z_s(M_{O2} + 3.76M_{N2}) = 18.69(32 + 3.76 \times 28.15) = 2576.3$

$$\mathbf{AFR_s} = 2576.3/171.56 = \mathbf{15.02}$$

The hydrogen/carbon ratio is slightly high for most hydrocarbon fuels; the equivalence ratio could refer to combustion from either a diesel engine or a spark ignition engine.

3.4* An engine with a compression ratio of 8.9:1 draws in air at a temperature of 20 °C and pressure of 1 bar. Estimate the temperature and pressure at the end of the compression stroke. Why will the temperature and pressure be less than this in practice?

The gravimetric air/fuel ratio is 12:1, and the calorific value of the fuel is 44 MJ/kg. Assume that combustion occurs instantaneously at the end of the compression stroke. Estimate the temperature and pressure immediately after combustion. (This is a continuation of Eq 2.5)

Let the start of compression be state 1, the end of compression be state 2, and the end of combustion be state 3.

Assuming the compression process to be adiabatic and reversible (and thus isentropic), then:

$$T_2 = T_1\,(V_1/V_2)^{\gamma-1} \quad \text{and } \mathrm{p}_2 = p_1\,(V_1/V_2)^{\gamma}$$

with $r_v = 8.9$, $T_1 = 293.15$ K and $\gamma = 1.4$, then $T_2 = 293.15 \times 8.9^{1.4-1} = \mathbf{720.8\ K}$

and $p_2 = 1.0 \times 8.9^{1.4} = \mathbf{21.34\ bar}$

(A more realistic value of γ might be 1.3, in which case: $T_2 = 293.15 \times 8.9^{1.3-1} = \mathbf{564.8\ K}$

and $p_2 = 1.0 \times 8.9^{1.3} = \mathbf{17.15\ bar}$

The estimate of the temperature and pressure at the end of compression is high because of heat transfer and to a lesser extent leakage from the cylinder. Taking γ as 1.4 is a value appropriate for air, the presence of fuel vapour, heat transfer and leakage make 1.3 a more realistic exponent for the polytropic compression process. (This still assumes a reversible process).

The question says to *estimate* the conditions after combustion so this invites us to undertake a very simple, calculation. Furthermore, being given only a calorific value of the fuel (without any details of its composition) further justifies the use of simple approximations. Applying a simple energy balance gives:

$$(m_a + m_f)c_p\Delta T_{2,3} = m_f\mathrm{CV} \qquad \text{or} \qquad \Delta T_{2,3} = m_f\mathrm{CV}/((m_a + m_f)c_p)$$

An upper estimate can be made by assuming $c_p = 1.01$ kJ/kgK, and recalling that the air/fuel ratio (AFR = m_a/m_f) is given as 12, then:

$$\Delta T_{2,3} = m_f\mathrm{CV}/((m_a + m_f)c_p) = 1 \times 44\mathrm{x}10^3/((12 + 1)1.01) = 3377 \text{ K}$$

and

$$T_3 = T_2 + \Delta T_{2,3} = 721 + 3377 = \mathbf{4098\ K}$$

A more realistic value for the specific heat capacity of the combustion products is $c_p = 1.20$ kJ/kgK, in which case:

$$\Delta T_{2,3} = 2842 \text{ K}$$

When this is combined with the lower estimate for the temperature at the end of compression (T_2 = 564. 8 K), then:

$$T_3 = T_2 + \Delta T_{2,3} = 565 + 2842 = 3407 \text{ K}$$

This still rather high, the main reason being that an AFR of 12 will correspond to a rich mixture, so that not all of the chemical energy from the reactants is released. Suppose the stoichiometric AFR is 14.4, in which case a revised estimate of the temperature rise would be:

$$\Delta T_{2,3} = 2842 \times (12/14.4) = 2368 \text{ K, giving } T_3 = T_2 + \Delta T_{2,3} = 565 + 2368 = \mathbf{2933\ K}$$

This is still about 800 K or so high, for a number of reasons: heat transfer (most significantly, and the effects of dissociation (least significantly), and combustion not occurring at constant volume.

To estimate the pressure after combustion we would strictly speaking need to know the change in the number of kmols as the reactants are converted to products during combustion. However, assuming no change will be a small source of error compared to the errors in calculating the temperatures. By applying the equation of state we can calculate the pressure.

Equation of state: $pV = nR_oT$, with n being the number of kmols. For constant volume combustion in which n is assumed constant:

$$p_3 = p_2(T_3/T_2)$$

First we will use the upper estimates of: p_2, T_3 *and* T_2: $p_3 = 21.34(3377/721) = $ **99.95 bar**

Secondly, we will use the lower estimates of: p_2, T_3 *and* T_2: $p_3 = 17.15(2933/565) = $ **89.03 bar**

The reasons for the over-estimation of T_3 have already been discussed, and it was noted that the estimate was about 800 K high. This would lead to an estimate of p_3 being 64.7 bar. If the maximum pressure occurs about 15 °atdc, then the piston will have moved less than 2% of the stroke, but the clearance volume will have increased by about 20%. For a polytropic expansion process with an index of 1.25 this piston movement would account for only about a 5% fall in temperature.

3.5* Compute the partial pressures of a stoichiometric equilibrium mixture of CO, O_2, CO_2 at (i) 3000 K and (ii) 3500 K when the pressure is 10 bar. Compare the answers with example 3.5. Are the results in accordance with Le Châtelier's Principle?

From Table A.6, the values of the equilibrium constant are:

	3000 K	3500 K (by interpolation)
$\text{Ln } K_p = \ln(P^*_{CO2}) - \ln(P^*_{CO}) - \frac{1}{2}\ln(P^*_{O2}) =$ (where P^* is a dimensionless quantity, numerically equal to the partial pressure in units of bar)	1.102	-0.445

We can introduce a variable a into the combustion equation to allow for the effect of dissociation:

$$CO + \tfrac{1}{2}O_2 \rightarrow (1 - a)CO_2 + aCO + a/2O_2$$

The partial pressure of a species is proportional to the number of moles of that species. Thus:

$P_{CO2} = P(1 - a)/[(1 - a) + a + \frac{1}{2}a] = P(1 - a)/[1 + \frac{1}{2}a]$,

$P_{CO} = Pxa/[(1 - a) + a + \frac{1}{2}a] = Pxa/[1 + \frac{1}{2}a]$,

$P_{O2} = P(\frac{1}{2}a)/[(1 - a) + a + \frac{1}{2}a] = P(\frac{1}{2}a)/[1 + \frac{1}{2}a]$ Where P is the system pressure

Using bar as our pressure units enables us to write:

$$K_p = \{(1 - a)/(a\surd[\tfrac{1}{2}a])\} \text{ x} \surd[(1 + \tfrac{1}{2}a)/P]$$

When the system pressure is 10 bar, and the temperature is 3000 K (for which Ln K_p = 1.102):

$\exp(1.102) = \{(1 - a)/(a\surd[\frac{1}{2}a])\} \text{ x} \surd[(1 + \frac{1}{2}a)/10]$

$3.0102 = \{(1 - a)/(a\surd[\frac{1}{2}a])\} \text{ x} \surd[(1 + \frac{1}{2}a)/10]$, rearranging gives

$3.0102(a\surd[\frac{1}{2}a])\surd(10) = (1 - a) \text{ x} \surd(1 + \frac{1}{2}a)$, squaring both sides gives

$45.306a^3 = (1 - 2a + a^2)(1 + \frac{1}{2}a) = (1 - 2a + a^2) + (\frac{1}{2}a - a^2 + \frac{1}{2}a^3)$

or

$$44.806a^3 + 1.5a - 1 = 0$$

This is a cubic equation which we can solve iteratively:

$$a_{n+1} = \sqrt[3]{[(1 - 1.5a_n)/44.806]}, \text{ where } n \text{ is the iteration number.}$$

We know that $0 < a < 1$, so we can make our first guess 0.5; the following table tracks the convergence:

n	1	2	3	4	5	6	7
x	0.5	0.1777	0.2540	0.2400	0.2426	0.2421	0.2422

Substituting the numerical values gives:

$P_{CO2} = P(1 - a)/[1 + \frac{1}{2}a] = 10(1 - 0.2422)/(1 + \frac{1}{2}0.2422) =$ **6.759 bar**

$P_{CO} = P \times a/[1 + \frac{1}{2}a] = 10 \times 0.2422/(1 + \frac{1}{2}0.2422) = \mathbf{2.160\ bar}$

$P_{O2} = P(\frac{1}{2}a)/[1 + \frac{1}{2}a] = 10 \times 0.5 \times 0.2422/(1 + \frac{1}{2}0.2422) = \mathbf{1.080\ bar}$

As a check, the partial pressures add to 9.999 bar, and

$$\text{Ln } K_p = \text{Ln}(P^*_{CO2}) - \text{Ln}(P^*_{CO}) - \tfrac{1}{2}\text{Ln}(P^*_{O2}) = \text{Ln}6.759 - \text{Ln}2.160 - \tfrac{1}{2}\text{Ln}1.080 = 1.1022$$

which are in very close agreement with the data.

When the temperature is increased to 3500 K (for which Ln $K_p = -0.445$):

$$\exp(-0.445) = \{(1 - a)/(a\sqrt{[\tfrac{1}{2}a]})\} \times \sqrt{[(1 + \tfrac{1}{2}a)/10]}$$

which as before expands into a cubic equation:

$$1.5533a^3 + 1.5a - 1 = 0$$

We can solve this equation iteratively, with a first guess of $a = 0.5$:

$$a_{n+1} = \sqrt[3]{[(1 - 1.5a_n)/1.5533]}, \text{ where } n \text{ is the iteration number.}$$

n	1	2	3	4
x	0.5	0.5440	0.4912	0.5534

Since this iterative solution is diverging, we need to try a different formulation:

$$a_{n+1} = (1 - 1.5533a^3_n)/1.5$$

With a first guess again of $a = 0.5$:

n	1	2	3	4	5	6	7	eventually
x	0.5	0.5372	0.5061	0.5324	0.5104	0.5290	0.5134	0.5206

Substituting the numerical values gives:

$P_{CO2} = P(1 - a)/[1 + \frac{1}{2}a] = 10(1 - 0.5206)/(1 + \frac{1}{2}0.5206) = \mathbf{3.804\ bar}$

$P_{CO} = P \times a/[1 + \frac{1}{2}a] = 10 \times 0.5206/(1 + \frac{1}{2}0.5206) = \mathbf{4.131\ bar}$

$P_{O2} = P(\frac{1}{2}a)/[1 + \frac{1}{2}a] = 10 \times 0.5 \times 0.5206/(1 + \frac{1}{2}0.5206) = \mathbf{2.065\ bar}$

As a check, the partial pressures add to 10.000 bar, and

$$\text{Ln } K_p = \text{Ln}(P^*_{CO2}) - \text{Ln}(P^*_{CO}) - \tfrac{1}{2}\text{Ln}(P^*_{O2}) = \text{Ln}3.804 - \text{Ln}4.131 - \tfrac{1}{2}\text{Ln}2.065 = -0.445$$

which are in exact agreement with the data.

Le Châtelier's Principle states that an equilibrium will be displaced in such a way as to minimise any changes imposed from outside the system. Increasing the temperature from 3000 K to 3500 K decreases the amount of carbon dioxide, since the dissociation of carbon dioxide to carbon monoxide and oxygen is an endothermic (heat absorbing) reaction - this can be seen by inspection of the absolute enthalpies at these temperatures:

	Molar Enthalpy (MJ/kmol)		
T(K)	O_2	CO	CO_2
3000	98.116	-16.969	-240.621
3500	118.312	1.706	-209.383

The effect of raising the pressure (compared to 1 bar in Example 3.5) has been to reduce the amount of carbon dioxide, since when this dissociates it leads to an increase in the number of moles. Thus decreasing the amount of carbon dioxide that dissociates will tend to reduce the pressure. These results are thus consistent with Le Châtelier's Principle.

3.6* In a test to determine the cetane number of a fuel, comparison was made with two reference fuels having cetane numbers of 50 and 55. In the test the compression ratio was varied to give the same ignition delay. The compression ratios for the reference fuels were 25.4 and 23.1 respectively. If the compression ratio for the test fuel was 24.9, determine its cetane number.

If we let the cetane number of the test fuel be x, we can summarise the data as follows:

cetane number	50	x	55
compression ratio	25.4	24.9	23.1

By linear interpolation we can say that:

$$\frac{50 - x}{25.4 - 24.9} = \frac{50 - 55}{25.4 - 23.1}$$

or

$$\frac{50 - x}{0.5} = \frac{-5.0}{2.3}$$

which can be multiplied out to give $2.3(50-x) = 0.5(-5.0) = -2.5$

and $x = 50 + 2.5/2.3 = \mathbf{51.1}$

3.7* Contrast combustion in compression ignition engines and spark ignition engines. What are the main differences in fuel requirements?

Combustion in compression ignition engines is normally dominated by *diffusion controlled combustion*, whilst combustion in spark ignition engines is normally *pre-mixed*.

Conventional spark ignition engines rely on mixture preparation before the charge enters the engine, either by means of ***fuel injection*** or a ***carburettor***. It is usually assumed that the mixture is homogeneous, although with some port injection systems there is the intention of stratifying the air/fuel mixture. None the less, by the time ignition occurs, the expectation is that the majority of the fuel will have vaporised and formed a (locally) homogeneous mixture. In pre-mixed combustion the flame front is assumed to propagate steadily throughout the combustion chamber, until all the mixture has been burnt. During combustion, the pressure will of course be rising, and this raises the temperature of the unburnt gas, as does heat transfer from hot components such as the exhaust valve. If the unburnt mixture is at a high enough temperature for sufficient time, then it can self-ignite or auto-ignite. Once self-ignition has occurred at one location, then the mixture at other locations will also be on the point of self-ignition: the pressure rise (and temperature rise) from the first site of self-ignition thus initiates an avalanche effect with wide-spread self-ignition throughout the remaining unburnt mixture and this leads to a rapid pressure rise. In all but the most mild cases, the rapid pressure rise initiates structural oscillations in the engine (at frequencies in the range 10-15 kHz), and these are audible and referred to as ***knock***.

Apart from its audible annoyance, knock can lead to overheating of components and structural damage. This is most likely to happen to the piston, since its full load opearting temperature will be above 200°C, and this is just below the temperature range at which aluminium alloys start to soften. The overheating occurs, because the pressure oscillations that follow the rapid pressure rise disrupt the thermal boundary layers, and thereby increase the heat flux into the combustion chamber components. Even if there is no immediate mechanical damage, the rise in the combustion chamber temperatures can lead to ***pre-ignition***. Pre-ignition is a surface ignition phenomena (in which the mixture is ignited through contact with a hot component such as the spark plug, combustion chamber deposits or the exhaust valve), in which ignition occurs *before* the spark. Obviously turning off the ignition stystem will not prevent pre-ignition, and since the ignition timing has been advanced, there will then be higher combustion pressures <u>and</u> temperatures. This in turn will make the self-ignition of the unburnt mixture occur earlier, and the larger quantity of mixture invloved will increase the intensity of the knock. The component temperatures will rise, and thereby making the pre-ignition occur earlier. This is a vicious circle (in which the knock makes the pre-ignition earlier, and the earlier pre-ignition makes the knock more severe) that leads to a phenomenon known as *runaway knock*. Turning off the ignition will is not likely to stop this (since ignition has been initiated before the spark), and the only hope is to close the throttle (turn off the fuel if possible). If runaway knock occurs during high speed driving, the noise may not be noticeable, and the driver may only be aware of trouble once molten piston material has been deposited in the sump.

In compression ignition engines the fuel is injected towards the end of the compression stroke. The fuel droplets vaporise and start to mix with the air. Once the mixture has been at a high enough temperature for sufficient time, then ignition occurs and combustion proceeds. The time between the start of injection and the start of combustion is called the ***ignition delay***, and at the end of the ignition delay, there is pre-mixed combustion of the flammable mixture that was prepared during the ignition delay. This is characterised by a very rapid pressure rise, because if it is hot enough for self-ignition at one point, then other parts of the mixture will also be on the point of self-ignition. However, the major part of combustion is diffusion controlled. ***Diffusion combustion*** is controlled by the rate at which air and fuel vapour mix to form a flammable mixture, and the rate at which the combustion products are dispersed. Although it is termed diffusion combustion, the presence of turbulence and mean flows means that convection is more important for mass transfer than diffusion.

Fuel Requirements

Self-Ignition Fuels for spark ignition engines must be resistant to self-ignition (so as to be able to operate at high compression ratios without the occurrence of knock), while fuels for compression ignition engines need to self-ignite readily (so that the engine can be started from cold and subsequently operate without excessively long ignition delays). Spark ignition engine fuels are characterised by their ***octane rating*** (the resistance to self-ignition), while compression ignition engine fuels are characterised by their ***cetane rating*** (the susceptibility to self-ignition). Thus a fuel with a high octane rating will have a low cetane rating and *vice versa* (Fig 3.14).

Volatility With mixture preparation in spark ignition engines occurring before the mixture enters the engine, the fuel has to be sufficiently volatile for a major part of the fuel to evaporate in the induction system. With compression ignition engines volatility is less important, but it is necessary for most of the fuel to vaporise below 350°C. When fuels with few components (such as vegetable oils) are used then they have a very narrow boiling point range, and a lower volatility may be needed; it is possible for the self-ignition temperature to be below the boiling point, and this can lead to the fuel decomposing in a way that leads to significant combustion deposits.

Viscosity Viscosity is only an issue with compression ignition engines. Increasing the viscosity leads to slightly poorer fuel atomisation. However diesel engines are able to operate on residual fuels, which have to be heated to enable the fuel to flow from the fuel tank to the injectors.

Surface Ignition Fuels for spark ignition engines must be resistant to surface-ignition. Otherwise they would be prone to pre-ignition. For example, although methanol has a very high octane rating (RON 106), its susceptibility to surface ignition limits the compression ratio of methanol fuelled engines. Hydrogen is also susceptible to surface ignition. Surface ignition is often a consequence of catalytic effects, that may be due to combustion chamber deposits or the materials used for building the engine.

3.8* What is the difference between 'knock' in compression ignition engines and spark ignition engines? How can knock be eliminated in each case?

During combustion in a spark ignition engine, the pressure will be rising, and this raises the temperature of the unburnt gas, as does heat transfer from hot components such as the exhaust valve. If the unburnt mixture ahead of the flame front is at a high enough temperature for sufficient time, then it can self-ignite or auto-ignite. Once self-ignition has occurred at one location, then the mixture at other locations will also be on the point of self-ignition: the pressure rise (and temperature rise) from the first site of self-ignition thus initiates an avalanche effect with wide-spread self-ignition throughout the remaining unburnt mixture and this leads to a rapid pressure rise. In all but the most mild cases, the rapid pressure rise initiates structural oscillations in the engine (at frequencies in the range 10-15 kHz), and these are audible and referred to as ***knock***.

In a compression ignition engine, the time between the start of injection and the start of combustion is called the ***ignition delay***, and at the end of the ignition delay, there is pre-mixed combustion of the flammable mixture that was prepared during the ignition delay. This is characterised by a very rapid pressure rise, because if it is hot enough for self-ignition at one point, then other parts of the mixture will also be on the point of self-ignition. During this rapid pressure rise, all of the flammable mixture formed during the ignition delay period will burn, and contribute to the pressure rise.

In the case of compression ignition engines, it could be argued that it is impossible to completely eliminate knock, but diesel knock can be minimised by:

1) a controlled injection that avoids injecting too much fuel during the ignition delay period. With common rail injection systems or unit injectors, it is possible to inject the fuel in two (or more) stages. the main part of the fuel is not injected until after the first fuel to be injected has ignited.

2) diesel knock will be reduced by anything that decreases the ignition delay period. This could be achieved by:

   injecting later, so that the in-cylinder gas temperature is higher.

   using a fuel that is more susceptible to self-ignition (in other words, it has a higher ***cetane rating***), or by adding an ignition improver to the fuel such as amyl nitrate or an ether.

   increasing the compression ratio of the engine

   pre-heating the air (if necessary by burning some fuel in the inlet manifold) or by using some form of in-cylinder heater (although these are usually only used for starting). Use recirculated exhaust gases.

Diesel knock is most severe at low load and speed operating points, and it can result in mechanical damage to engines. This is most likely to occur with highly turbocharged engines, in which the compression ratio has been reduced so as to limit the peak pressures. Such an engine is likely to be intercooled, and when this is in the engine coolant circuit, at low boost pressures there will be a very small temperature rise in the compressor, and the air will be heated by the engine coolant.

The ways of eliminating knock in spark ignition engines are the opposite to those required in compression ignition engines. The techniques for eliminating knock are:

1) Use a fuel that is more resistant to self ignition (in other word it has a higher ***octane rating***), or use additives that inhibit the self-ignition mechanism. The most notable additives being ***tetra methyl*** and ***tetra ethyl lead***.

2) Lower the compression ratio of the engine

3) Retard the ignition timing, reduce the coolant temperature.

4) Use air that is as cool as possible.

3.9* A dual fuel engine operates by aspirating a mixture of air and fuel, which is then ignited by the spontaneous ignition of a small quantity of diesel fuel injected near the end of the compression stroke. A dual fuel engine is operating with a gravimetric air fuel ratio of 20, and the effective atomic H:C composition of the fuel is 3.1:1.

(i) Write down the stoichiometric and actual combustion equations, and calculate the volumetric wet gas composition.
(ii) If the calorific value of the fuel is 46 MJ/kg, what percentage of this could be recovered by cooling the exhaust gas from 627°C to 77°C?
(iii) If the fuel consists of methane (CH_4) and cetane ($C_{16}H_{34}$), what is the ratio of the two fuel mass flowrates? What would the advantages be of cooling the exhaust below the dew-point temperature?

In a dual fuel engine, what determines the selection of the compression ratio? Explain under what circumstances emissions might be a problem.

(i)

The molar (or volumetric) composition of air can be assumed to be 21% oxygen and 79% nitrogen. Thus for every kmol of oxygen there are (79/21=) 3.76 kmols of atmospheric nitrogen. Our reaction is thus:

$$CH_{3.1} + z(O_2 + 3.76N_2^*) \rightarrow aCO_2 + bH_2O + 3.76zN_2^*$$

We have already applied an atomic balance for nitrogen, and we continue with the atomic balances for carbon and hydrogen:

C balance $a = 1$

H balance $2b = 3.1$

Next we can use the atomic oxygen balance:

O balance $2z = 2a + b$ or $2z = 2 + 3.1/2 =$

So $z = 1.775$
and our stoichiometric reaction is:

$$CH_{3.1} + 1.775(O_2 + 3.76N_2^*) \rightarrow CO_2 + 1.55H_2O + 6.677N_2^*$$

Assuming the following molar masses:

M_{H2} hydrogen (H_2)	2 kg/kmol
M_C carbon	12 kg/kmol
M_{N2*} nitrogen (N_2)	28.16 kg/kmol
M_{O2} oxygen (O_2)	32 kg/kmol
M_{air} air (21%O_2,79%N_2)	29 kg/kmol

Then the mass of 1 kmol of fuel is:

$$M_C + 3.1(M_{H2}/2) = 12 + 3.1(2/2) = 15.1$$

1 kmol of fuel reacts with $z(O_2 + 3.76N_2^*)$, the mass of which is

$$z(M_{O2} + 3.76M_{N2*}) = 1.775(32 + 3.76\times28.16) = 244.74$$

Division of the mass of air (244.74) by the mass of fuel (15.1), gives the stoichiometric gravimetric air/fuel ratio of (244.74/15.1=) **16.21**.

For the AFR of 20:1, the combustion equation becomes:

$$CH_{3.1} + 1.775(20/16.21)(O_2 + 3.76N_2^*) \rightarrow CO_2 + 1.55H_2O + 8.234N_2^* + cO_2$$

notice how the quantity of nitrogen has increased, and the use of a temporary variable (c) to account for the presence of oxygen in the combustion products; this can now be evaluated by an atomic oxygen balance.

O balance: $1.775(20/16.21)2 = 2 \text{ x } 1 + 1.55 + 2c$ or $c = 0.415$

The number of kmols of wet (that is, including the water vapour) Products (n_P),

$$n_P = 1 + 1.55 + 8.234 + 0.415 = 11.20$$

The exhaust gas composition on a wet basis is thus:

$\%CO_2 = 1 \text{ x } 100/n_P = 100/11.2 =$ **8.93%**

$\%H_{2O} = 1.55 \text{ x } 100/n_P = 155/11.2 =$ **13.84%**

$\%N_2^* = 8.234 \text{ x } 100/n_P = 823.4/11.2 =$ **73.52%**

$\%O_2 = 0.415 \text{ x } 100/n_P = 41.5/11.2 =$ **3.71%** (which add up to 100%)

(ii)

Consider 1 kmol of fuel ($CH_{3.1}$), for which the molar mass (M_f) is 15.1 kg.

Combustion energy (Q_c) is: $M_f \text{ x CV} = 15.1 \text{ x } 46 = 694.6$ MJ/kmol_fuel

The exhaust products are being cooled from 627°C (900 K) to 77°C (350 K), the change in enthalpy for each component in the exhaust:

$\Delta H_p = \Sigma n_i(H_{900} - H_{350})_i$, where n is the number of kmols of species i, i = CO_2, H_2O, $4N_2^*$, O_2

$$\Delta H_p = 1(-365.477 - \tfrac{1}{2}[-389.509 - 393.443]) + 1.55(-219.899 - \tfrac{1}{2}[-238.371 - 241.761]) \\ + 8.234(18.219 - \tfrac{1}{2}[2.969 + 0.053]) + 0.415(19.244 - \tfrac{1}{2}[3.028 + 0.054])$$

$$\Delta H_p = 25.999 + 31.259 + 137.574 + 7.347 = 202.179 \text{ MJ/kmol\_fuel}$$

The potential heat recovery is $\Delta H_p/M_f \times$ CV = 202.179/694.6 = 0.291, or **29.1%**

(iii)

We can start by finding the molar ratio of the fuels, by introducing a temporary variable y:

$$y\text{CH}_4 + \text{C}_{16}\text{H}_{34} = (16 + y)\text{CH}_{3.1}$$

The carbon balance has been used in writing the equation above, but we can evaluate y by determining the hydrogen balance:

Atomic H balance: $4y + 34 = (16 + y)3.1$

$4y + 34 = 49.6 + 3.1y$ $\quad y = 17.33$

The gravimetric ratio of methane to cetane is:

$$17.33M_{\text{CH4}}:M_{\text{C16H34}}$$

where:

$$M_{\text{CH4}} = M_\text{C} + 4M_\text{H} = 12 + 4 \times (2/2) = 16$$

$$M_{\text{C16H34}} = 16M_\text{C} + 34M_\text{H} = 16 \times 12 + 34 \times (2/2) = 226$$

The gravimetric ratio of methane to cetane is:

17.33 x 16 : 226 or **1.227kgCH$_4$:1kgC$_{16}$H$_{34}$**

Comment The exhaust temperature and air fuel ratio both indicate that the engine is close to full load, at which point the gravimetric ratio of methane to cetane could be 4:1 or higher. Perhaps in this particular case there was a shortage of methane.

Cooling the exhaust below the dewpoint temperature would mean that the enthalpy of condensation of the water vapour (Hfg) would be added to the heat transferred during the cooling process (this is sometimes called the sensible heat). There is 13.84% water vapour in the exhaust, so if ambient pressure is 1 bar, the partial pressure of the water vapour will be 0.1384 bar, and the water vapour will start to condense at the temperature when the partial pressure of the water vapour equals the saturation pressure. Inspection of steam tables indicates that the dew point temperature will be about 52°C, and that if the exhaust was cooled to 25°C, then the partial pressure of the water vapour would fall to 0.01704 bar.

Of the original 1.55 kmols of water vapour, the number condensing is:

1.55(0.1384 - 0.01704)/0.1384 = 1.36 (kmols water vapour/kmol fuel)

The enthalpy of condensation for water vapour at this temperature is 43.990 MJ/kmol, so the heat transfer would be increased by (1.36 x 43.99 =) 59.83 MJ/kmol_fuel. This compares to a calorific value of 694.6 MJ/kmol_fuel (8.6%), an increase of (59.83/202.179 =) 30%.

A dual fuel engine operates by compression ignition of (diesel) fuel sprayed into the combustion chamber, which then ignites fuel which has been admitted with the air. The compression ratio thus has to be high enough to enable the engine to ignite the pilot fuel sprayed into the combustion chamber, for which the most critical condition is when the engine is being started from cold. On the other hand, the compression ratio must not be so high as to cause self-ignition of the fuel admitted with the air, before the flame front initiated by the pilot fuel has ignited the air/fuel mixture.

Dual fuels normally operate weak of stoichiometric, since otherwise there would be significant emissions of particulates from the partial combustion of the pilot fuel. At full load the air fuel ratio would normally be just weak of stoichiometric, so the emissions of carbon monoxide would be negligible, but the NOx emissions would be significant. The measures for controlling NOx would be the same as for diesel engines, namely:

(i) retard the injection timing
(ii) use exhaust gas recirculation
(iii) employ some form of post engine treatment, either a trap or some form of catalyst.
(iv) operate the engine significantly weak of stoichiometric (lambda of 1.5), and if necessary increase the turbocharger boost pressure so as to maintain the engine output.

Unburnt hydrocarbon emissions are also broadly in-line with diesel engine emissions. At low loads, it is possible that the air/fuel mixture inducted will be sufficiently weak to cause partial burns, despite the multiplicity and the intensity of ignition sites associated with the pilot fuel ignition. At full load, there is also the possibility of particulate emissions (as mentioned above), which of course contain unburnt hydrocarbons.

3.10* Some combustion products at a pressure of 2 atm are in thermal equilibrium at 1400 K, and a volumetric gas analysis yielded the following data:

CO_2	**0.065**
H_2O	**0.092**
CO	**0.040**

(i) Deduce the concentration of H_2 from the equilibrium equation.
(ii) If the fuel was octane, calculate the approximate percentage of the fuel chemical energy not released as a percentage of the partial combustion.
(iii) Sketch how engine exhaust emissions vary with the air/fuel ratio, and discuss the shape of the nitrogen oxides and unburnt hydrocarbon curves.

(i)

The presence of water vapour in the data implies that these data are from a wet gas analysis. We need to convert the system pressure to bar, and then determine the partial pressures of each constituent (by multiplying the system pressure by the mole fraction):

system pressure: 2 atm = 2 x 1.01325 = 2.0265 bar

species	mole fraction	partial pressure (bar)
CO_2	0.065	0.1317
H_2O	0.092	0.1864
CO	0.040	0.081

By definition:

$$(\mathrm{Ln}\ K_p)_{1400K} = \mathrm{Ln}(P^*_{H2O}) + \mathrm{Ln}(P^*_{CO}) - \mathrm{Ln}(P^*_{CO2}) - \mathrm{Ln}(P^*_{H2}) = 0.768$$

Substitution of numerical values gives:

$$\mathrm{Ln}(0.1864) + \mathrm{Ln}(0.081) - \mathrm{Ln}(0.1317) - \mathrm{Ln}(P^*_{H2}) = 0.768$$

$$-1.680 + (-2.513) - (-2.027) - \mathrm{Ln}(P^*_{H2}) = 0.768$$

or

$$\mathrm{Ln}(P^*_{H2}) = 2.027 - 0.768 - 1.680 - 2.513 = -2.934$$

$$P^*_{H2} = \exp(-2.934) = 0.05318 \text{ bar}$$

The partial pressure can be converted to a mole fraction of hydrogen by division with the system pressure (0.5318/2.0265 =) 0.0262 (or 2.62% H_2).

(ii)

If we let the wet products of combustion be 100 kmol, we can find out how many kmols of fuel have been burnt:

$$yC_8H_{18} + z(O_2 + 3.76N_2) \rightarrow 6.5CO_2 + 9.2H_2O + 4.0CO_2 + 2.62H_2 + 3.76zN_2$$

Since we are only interested in the quantity of fuel, we only need one atomic balance (either for hydrogen or carbon), but using two atomic balances will provide a check on the consistency of the data:

C balance $8y = 6.5 + 4.0$, $y = 1.3125$

or

H balance $18y = 9.2 \times 2 + 2.62 \times 2$ $y = 1.3133$

This is a satisfactory check, and we will take: $y = 1.313$.

The calorific value of iso-octane is 5100.50 MJ/kmol_fuel, so when 1.313 kmols of iso-octane are burnt, then:

$$1.313 \times 5100.5 = 6696.96 \text{ MJ}$$

are converted to heat.

If the partial products of combustion were subsequently oxidised (using data for 25°C), then:

2.62 kmols of H_2 would be oxidised, releasing $2.62(H_{H2} - H_{H2O})_{298.15K} = 2.62(0 - [-241.824]) = 633.58$ MJ

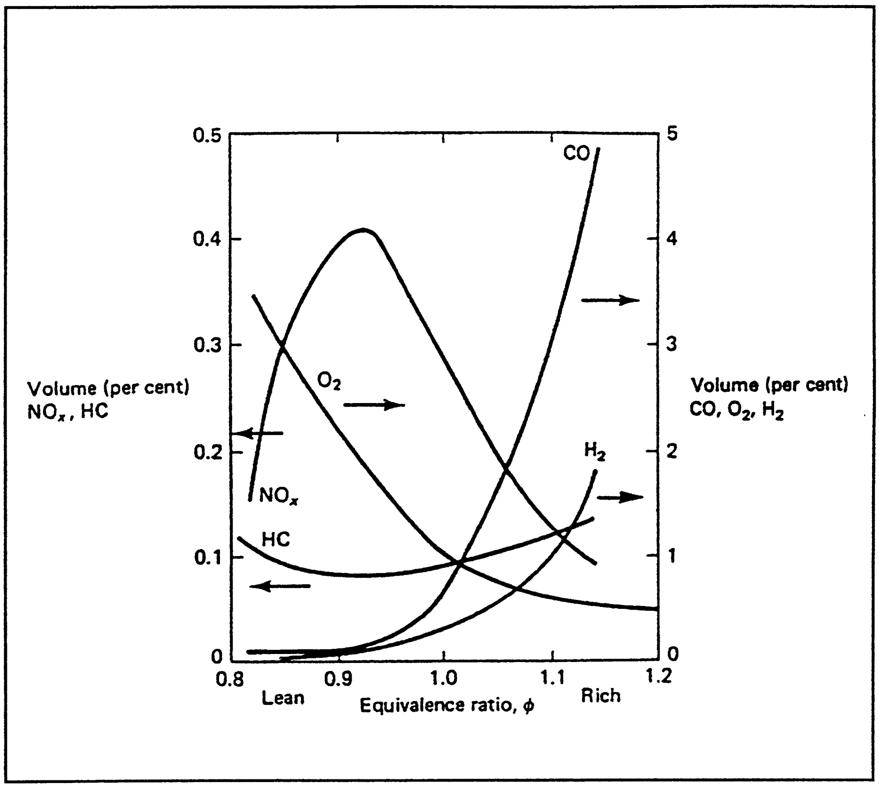
4.0 kmols of CO would be oxidised, releasing $4(H_{CO} - H_{CO2})_{298.15K} = 4(-110.525 - [-393.512]) = 1131.95$ MJ

which added together make 1765.53 MJ, which is **26.4%** of the 6696.96 MJ originally available in the fuel.

(iii)

Figure 3.18 shows the dependence of the emissions on the air/fuel ratio.

The NOx emissions require both oxygen and high temperatures for their formation. The highest temperatures will occur with mixtures just rich of stoichiometric, and then fall as the mixture is weakened. However, it is only with weak mixtures that there will be significant quantities of uncombined oxygen present. Thus as the mixture is weakened from stoichiometric, there is a trade-off between the increasing level of oxygen, and the falling temperature, and the maximum NOx emissions occur about 10% rich of stoichiometric.



The hydrocarbon emissions are lowest just weak of stoichiometric, and remain low until incipient mis-fire occurs as the weak mixture limit of combustion is reached. Some cycles will only burn very slowly, so that combustion is incomplete before the exhaust valve opens, and in other cycles the flame will be extinguished during the expansion stroke, because of mixture motion and the fall in temperature. On the rich side of stoichiometric there will be a gradual rise in the unburnt hydrocarbon emissions. Hydrocarbons from the unburnt mixture are absorbed into oil films and crevices whilst the cylinder pressure is rising. When the pressure falls the hydrocarbons are released, often into burnt mixture. With rich mixtures there is less scope for oxidation of these hydrocarbons that are desorbed. Also in the flame front of rich mixtures, the radicals formed during hydrocarbon decomposition are more likely to recombine to form other hydrocarbon molecules than to take part in oxidation reactions.

3.11* The results of a dry gas analysis for a Diesel engine exhaust are as follows:

Carbon dioxide, CO_2	**10.1 per cent**
Atmospheric nitrogen, N_2	**82.6 per cent**

Stating any assumptions, calculate:

(i) the gravimetric air/fuel ratio.
(ii) the atomic and gravimetric composition of the fuel
(iii) the stoichiometric gravimetric air fuel ratio
(iv) the actual equivalence ratio.

Why are the results derived from an exhaust gas analysis likely to be less accurate, when the mixture is rich or significantly weak of stoichiometric? What other Diesel engine emissions are significant?

We know that this is a diesel engine, which we can expect to be operating weak of stoichiometric, in which case we can assume there to be oxygen in the exhaust, but no carbon monoxide. Examination of the data shows that the emissions do not add up to 100% (10.1 + 82.6 = 93.7), so the balance of 6.3% can be assumed to be oxygen.

Assume that the hydrocarbon (C_xH_y), reacts with z kmols of oxygen to produce 100 kmols of dry products of combustion, (there will of course be water present in the exhaust, so that our specified quantity of reactants produces more than 100 kmols of products).

The molar (or volumetric) composition of air can be assumed to be 21% oxygen and 79% nitrogen. Thus for every kmol of oxygen there are (79/21=) 3.76 kmols of nitrogen. Our reaction is thus:

$$C_xH_y + z(O_2 + 3.76N_2) \rightarrow \text{100 kmols of dry products and water vapour}$$

$$C_xH_y + z(O_2 + 3.76N_2) \rightarrow 10.1CO_2 + 7.3O_2 + 82.6N_2^* + wH_20$$

The four atomic balances are:

N balance $3.76 \times 2z = 2 \times 82.6,\ z = 21.97$ (A

C balance $x = 10.1$ (B

O balance $2z = 10.1 \times 2 + 7.3 \times 2 + w = 34.8 + w$ (C

Substituting for the value of z from Eqn A:

$2 \times 21.97 = 34.8 + w\ ,\ w = 9.14$ (D

H balance $y = 2w$ (E

Substituting for the value of w from Eqn D: $y = 18.28$ (F

The molar composition of the fuel is thus: $C_{10.1}H_{18.28}$.

To find the molar mass of the fuel, we need to add the mass of the carbon and hydrogen:

Mass of carbon :- $\mathrm{x}M_C = 10.1 \times 12 = 121.2$

Mass of hydrogen :- $\mathrm{y}M_{H2} = 18.28 \times 1 = 18.28$ Total Mass = 139.48 (G

(i) To find the gravimetric air fuel ratio, we need to find the mass of the air that combines with our 1 kmol of fuel.

There are 21.97 kmols of oxygen, so there are (21.97 x 4.76 =) 104.58 kmols of air. The molar mass of air is 29 kg/kmol, so we have (104.58 x 29 =) 3032.7 kg. Division by the molar mass of fuel (143.7 kg/kmol) gives us the air fuel ratio:

The **gravimetric AFR** = 3032.7/139.48 = **21.74**

(ii) To find the atomic and gravimetric composition of the fuel, we need to use the ratio x:y from equations B and E:

atomic hydrogen/carbon ratio of the fuel (y/x) - 18.28/10.1 = **1.81**

The gravimetric composition of the fuel requires rearrangement of equation G:

Mass fraction of carbon 121.2/139.48 = **0.869**

Mass fraction of hydrogen 18.28/139.48 = **0.131**

or (0.869/0.131 =) **6.63** kg_C per kg_H

(iii) The stoichiometric gravimetric air fuel ratio is found by determining the quantity of air required for stoichiometric combustion:

Define z_s as the quantity of air required for stoichiometric combustion:

$$C_{10.1}H_{18.28} + z_s(O_2 + 3.76N_2) \rightarrow aCO_2 + bH_2O + cN_2$$

The atomic balances are:

C balance $10.1 = a$

H balance $18.28 = 2b$

Thus, $C_{10.1}H_{18.28} + z_s(O_2 + 3.76N_2) \rightarrow 10.1CO_2 + 9.14H_2O + cN_2$

O balance $2z_s = 2 \times 10.1 + 9.14,\ z_s = 14.67$

The stoichiometric air/fuel ratio can be found from the mass of fuel (Eq G), and the mass of the stoichiometric quantity of air (z_s).

Mass of Air $z_s(O_2 + 3.76N_2)$:- $z_s(M_{O2} + 3.76M_{N2}) = 14.67(32 + 3.76 \times 28.15) = 2022.2$

AFR_s = 2022.2/139.48 = **14.5**

(iv) The equivalence ratio (ϕ) is the ratio of the quantity of air required for stoichiometric combustion (z_s) compared to that actually used (z, evaluated in Eq A)

$$\phi = z_s/z = 14.67/21.97 = \mathbf{0.67}$$

Comment: The exhaust emissions are only ratios, so we are only able to determine ratios, for example the hydrogen/carbon ratio, or the air/fuel ratio. The molar composition of the fuel is also only a ratio, since our choice of 100 kmols of dry products of combustion was arbitrary. If we had specified 10 kmols of dry products of composition, then the molar composition of the fuel would have been: $C_{10.1}H_{18.28}$.

3.12* A four-stroke engine is running on methane with an equivalence ratio of 0.8. The air and fuel enter the engine at 25°C, the exhaust is at 527°C, and the heat rejected to the coolant is 340 MJ/kmol fuel. Write the equations for stoichiometric combustion and the actual combustion.

(i) By calculating the enthalpy of the exhaust flow, deduce the specific work output of the engine, and thus the overall efficiency.

(ii) If the engine has a swept volume of 5 litres and a volumetric efficiency of 72 per cent (based on the air flow), calculate the power output at a speed of 1500 rpm. The ambient pressure is 1 bar.

State clearly any assumptions that you make, and comment on any problems that would occur with a rich mixture.

The molar (or volumetric) composition of air can be assumed to be 21% oxygen and 79% nitrogen. Thus for every kmol of oxygen there are (79/21=) 3.76 kmols of atmospheric nitrogen. Our reaction is thus:

$$CH_4 + z(O_2 + 3.76N_2^*) \rightarrow aCO_2 + bH_2O + 3.76zN_2^*$$

We have already applied an atomic balance for nitrogen, and we continue with the atomic balances for carbon and hydrogen:

C balance $a = 1$

H balance $2b = 4$

Next we can use the atomic oxygen balance:

O balance $2z = 2a + b$ or $2z = 2 + 4/2 = 4$

So $z = 2$

and our stoichiometric reaction is:

$$CH_4 + 2(O_2 + 3.76N_2^*) \rightarrow CO_2 + 2H_2O + 7.52N_2^*$$

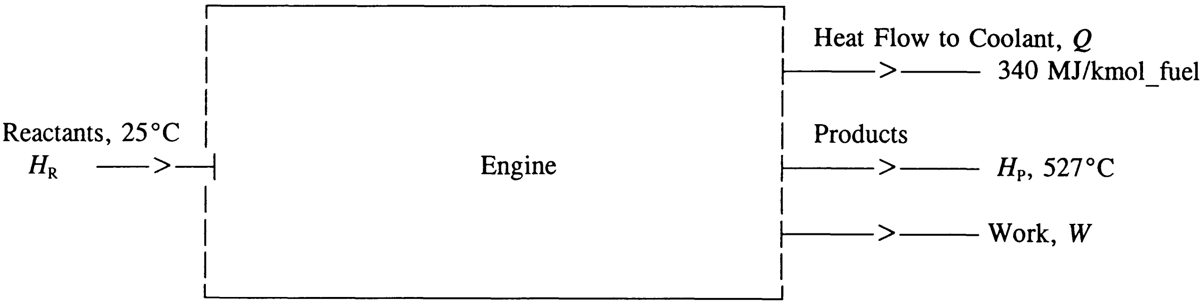
The equivalence ratio is 0.8, so the actual combustion equation is:

$$CH_4 + (2/0.8)(O_2 + 3.76N_2^*) \rightarrow CO_2 + 2H_2O + (2/0.8)7.52N_2^* + (2/0.8 - 1)O_2$$

In writing this equation we have revised the atomic balances for oxygen and nitrogen, and after some simple arithmetic we get:

$$CH_4 + 2.5(O_2 + 3.76N_2^*) \rightarrow CO_2 + 2H_2O + 9.4N_2^* + 0.5O_2$$

i) We can treat the engine as a 'black box', in which there are various flows as shown below; we will use a basis of 1 kmol of fuel. But in order to solve the question we need to assume complete combustion of the fuel (as in the above equation), with no unburnt hydrocarbons, and if there is any blowby, it has to be assumed that this will returned to the inlet manifold.



In order to find the work flow, we need to apply the Steady Flow Energy Equation:

$$H_R = H_P + Q + W$$

which requires us to determine H_R and H_P.

$$H_R = (H_{CH4} + 2.5(1 + 3.76)H_{air})_{298.15K}$$

$$H_P = (H_{CO2} + 2H_{H2O} + 9.4H_{N2} + 0.5H_{O2})_{800K}$$

using the tables gives:

$$H_R = -74.520 + 11.9x0 = -74.520 \text{ MJ/kmol\_fuel}$$

$$H_P = -370.699 + 2x(-223.831) + 9.4 \text{ x } 15.042 + 0.5 \text{ x } 15.837 = -669.048 \text{ MJ/kmol\_fuel}$$

$$W = H_R - H_P - Q = -74.520 - (-669.048) - 340 = \mathbf{254.528 \text{ MJ/kmol\_fuel}}$$

The **overall efficiency** is W/CV = 254.528/802.64 = **0.317**

ii) To determine the power output we need to find the flowrate of fuel into the engine, and since we know the air fuel ratio, then we can find the fuel flowrate from the air flowrate. As we are given the volumetric efficiency (η_v), the air flowrate (V_a) is:

$V_a = \eta_v \; V_s \; (1500/120)$ assuming that the engine operates on a 4 stroke cycle.

for which the swept volume (V_s) is 5 litres:

$$V_a = 0.72 \text{ x } 5x10^{-3}(1500/120) = 45x10^{-3} \text{ m}^3/\text{s}$$

The ratio of the air flowrate to the fuel flowrate (V_f) is 2.5x(1 + 3.76):1, so the methane flowrate is:

$$V_f = 45x10^{-3}/(2.5 \text{ x } 4.76) = 3.78x10^{-3} \text{ m}^3/\text{s}$$

The flowrate of the fuel (in terms of kmols/s) can be found fro a rearrangement of the equation of state:

$$n = pV/(R_oT) = 10^5 \text{ x } 3.78x10^{-3}/(8314.3 \text{ x } 298.15) = 0.1525x10^{-3} \text{ kmol\_fuel/s}$$

The power output now comes from multiplying the molar flowrate (n) by the molar specific work output (W)

Power Output = $0.1525x10^{-3} \text{ x } 254.528 = 38.8$ kW

Note that there is no need to find either the mass flowrate of the air or the gravimetric air fuel ratio, if the analysis uses a molar basis.

If a rich mixture was used, it would be necessary to assume no oxygen in the exhaust, and estimate the relative proportions of hydrogen and carbon monoxide from the water gas equilibrium equation. The chemical energy associated with these species would be automatically accounted for in the tabulations of absolute molar enthalpy.

3.13* The results of a dry gas analysis of an engine exhaust are as follows:

Carbon dioxide, CO_2	**10.7 per cent**
Carbon monoxide, CO	**5.8 per cent**
Atmospheric nitrogen, N_2^*	**83.5 per cent**

Stating any assumptions, calculate:

(i) the gravimetric air/fuel ratio.

(ii) the gravimetric composition of the fuel
(iii) the stoichiometric gravimetric air fuel ratio.

Discuss some of the means of reducing engine exhaust emissions.

The level of carbon monoxide indicates that this is a spark ignition engine. The quoted emissions add up to 100%, which is perhaps surprising since some hydrogen would also be expected to be present. This also mean that there is no oxygen in the exhaust. However, we have to solve the problem with the stated data.

Assume that the hydrocarbon (C_xH_y), reacts with z kmols of oxygen to produce 100 kmols of dry products of combustion, (there will of course be water present in the exhaust, so that our specified quantity of reactants produces more than 100 kmols of products).

The molar (or volumetric) composition of air can be assumed to be 21% oxygen and 79% nitrogen. Thus for every kmol of oxygen there are (79/21=) 3.76 kmols of nitrogen. Our reaction is thus:

$$C_xH_y + z(O_2 + 3.76N_2) \rightarrow 100 \text{ kmols of dry products and water vapour}$$

$$C_xH_y + z(O_2 + 3.76N_2) \rightarrow 10.7CO_2 + 5.8CO + 83.5N_2^* + wH_20$$

The four atomic balances are:

N balance $3.76 \times 2z = 2 \times 83.5,\ z = 22.21$ (A

C balance $x = 10.7 + 5.8 = 16.5$ (B

O balance $2z = 10.7 \times 2 + 5.8 + w = 27.2 + w$ (C

Substituting for the value of z from Eqn A: $2 \times 22.21 = 27.2 + w,\ w = 17.22$ (D

H balance $y = 2w$ (E

Substituting for the value of w from Eqn D: $y = 34.44$ (F

The molar composition of the fuel is thus: $C_{16.5}H_{34.44}$.

i)

To find the gravimetric air fuel ratio, we need to find the mass of fuel ($C_{16.5}H_{34.44}$), and the mass of air that this reacts with.

Mass of carbon :- $xM_C = 16.5 \times 12 = 198.0$

Mass of hydrogen :- $yM_{H2} = 34.44 \times 1 = 34.44$ Total Mass = 232.44 (G

There are 22.21 kmols of oxygen, so there are (22.21 x 4.76 =) 105.72 kmols of air. The molar mass of air is 29 kg/kmol, so we have (105.72 x 29 =) 3065.88 kg. Division by the mass of fuel (232.44 kg) gives us the air fuel ratio:

The **gravimetric AFR** = 3065.88/232.44 = **13.19**

(ii) To find the gravimetric composition of the fuel, we need to rearrange equation G:

Mass fraction of carbon 198.0/232.44 = **0.852**

Mass fraction of hydrogen 34.44/232.44 = **0.148**

or (0.852/0.148 =) **5.76** kg_C per kg_H

(iii) The stoichiometric gravimetric air fuel ratio is found by determining the quantity of air required for stoichiometric combustion:

Define z_s as the quantity of air required for stoichiometric combustion:

$$C_{16.5}H_{34.44} + z_s(O_2 + 3.76N_2) \rightarrow aCO_2 + bH_2O + cN_2$$

The atomic balances are:

C balance $16.5 = a$

H balance $34.44 = 2b$

Thus, $C_{16.5}H_{34.44} + z_s(O_2 + 3.76N_2) \rightarrow 16.5CO_2 + 17.22H_2O + cN_2$

O balance $2z_s = 2 \times 16.5 + 17.22,\ z_s = 25.11$

The stoichiometric air/fuel ratio can be found from the mass of fuel (Eq G), and the mass of the stoichiometric quantity of air (z_s).

Mass of Air $z_s(O_2 + 3.76N_2)$:- $z_s(M_{O2} + 3.76M_{N2}) = 25.11(32 + 3.76 \times 28.15) = 3461.26$

AFR$_s$ = 3461.26/232.44 = **14.89**

Reduction of Exhaust Emissions

Addressing each pollutant in turn, we will answer this question in terms of emissions from spark ignition engines.

Carbon Monoxide (CO) Carbon monoxide is minimal when engines are running more than 10% weak of stoichiometric; at stoichiometric the emissions might rise to 1% carbon monoxide. An oxidising catalyst is effective way of further reducing CO, but oxygen needs to be present, so for mixtures rich of stoichiometric it is necessary to add air to the exhaust stream.

Unburnt Hydrocarbons (UHC) Unburnt hydrocarbon emission are minimal, except when engines are operating close to either the rich or lean combustion limit. Oxidising catalysts are an effective way of reducing UHCs, but oxygen needs to be present, so for mixtures rich of stoichiometric it is necessary to add air to the exhaust stream.

Nitrogen Oxides (NOx) NOx emissions are most severe when engines are running about 10% weak of stoichiometric, but fall rapidly as the mixture is either richened or weakened. The engine out emissions of NOx can be reduced by anything that lowers the combustion temperature, such as:

a) retarding the ignition timing,

b) adding diluents (such as exhaust gas or water vapour) to the incoming charge.

A reducing catalyst is only effective in decreasing NOx when mixtures are rich or very close (within 1%) to stoichiometric. Catalysts or traps (using materials such as zeolites) have only a limited effectiveness in reducing NOx with lean mixture products of combustion. This limited effectiveness is manifest in both the conversion efficiency and the durability.

3.14* The following equation is a simple means for estimating the combustion temperature (T_c) of weak mixtures (that is, equivalence ratio, $\phi<1.0$):

$$T_c = T_m + k\phi \qquad \phi<1.0$$

where T_m is the mixture temperature prior to combustion, and k is a constant.

By considering the combustion of an air/octane (C_8H_{18}) mixture with an equivalence ratio of 0.9 at a temperature of 25°C, calculate a value for k (neglect dissociation).

For rich mixtures the following equation is applicable:

$$T_c = T_m + k - (\phi - 1.0) \times 1500 \qquad \phi \geq 1.0$$

Plot the combustion temperature rise for weak and rich mixtures, and explain why the slopes are different each side of stoichiometric. Sketch how the results would be modified by dissociation.

The molar (or volumetric) composition of air can be assumed to be 21% oxygen and 79% nitrogen. Thus for every kmol of oxygen there are (79/21=) 3.76 kmols of atmospheric nitrogen. Our stoichiometric reaction is thus:

$$C_8H_{18} + z(O_2 + 3.76N_2^*) \rightarrow aCO_2 + bH_2O + 3.76zN_2^*$$

We have already applied an atomic balance for nitrogen, and we continue with the atomic balances for carbon and hydrogen:

C balance $a = 8$

H balance $2b = 18$

Next we can use the atomic oxygen balance:

O balance $2z = 2a + b$ or $2z = 2 \times 8 + 18/2$

So $z = 12.5$

The stoichiometric reaction is thus:

$$C_8H_{18} + 12.5(O_2 + 3.76N_2^*) \rightarrow 8CO_2 + 9H_2O + 47.0N_2^*$$

When the equivalence ratio is 0.9:

$$C_8H_{18} + 12.5/0.9(O_2 + 3.76N_2^*) \rightarrow 8CO_2 + 9H_2O + (47.0/0.9)N_2^* + dO_2$$

We can use the atomic oxygen balance:

O balance $2 \times 12.5/0.9 = 2 \times 8 + 9 + 2d \quad d = 1.39$

So the combustion equation is:

$$C_8H_{18} + 12.5/0.9(O_2 + 3.76N_2^*) \rightarrow 8CO_2 + 9H_2O + 1.39O_2 + 52.22N_2^*$$

We are considering 1 kmol of fuel, and we can start the combustion temperature calculations by computing the enthalpy of the reactants, using the data from Tables A.4 and A.5:

$H_r = \Sigma n_i(H_{298.15})_i$, where n is the number of kmols of species i, $i = C_8H_{18}$, $52.22N_2^*$, $13.89O_2$

$H_r = (1 \times -224.0101) + (52.22 \times 0.0) + (13.89 \times 0.0) = -224.010$ MJ/kmol_fuel

We need to guess the temperature of the products of combustion, and as a first guess we will assume 2500 K:

$H_{p,2500} = \Sigma n_i(H_{2500})_i$, where n is the number of kmols of species i, and: $i = 8CO_2$, $9H_2O$, $1.39O_2$, $52.22N_2^*$

$H_{p,2500} = 8 \times (-271.587) + 9 \times (-142.883) + 1.39 \times 78.381 + 52.22 \times 74.308 = 530.67$

A comparison with H_r (-224.010 MJ) shows that the guess of 2500 K was too high, so we can make a second guess of 2000 K:

$H_{p,2000} = 8 \times (-302.128) + 9 \times (-169.146) + 1.39 \times 59.171 + 52.22 \times 56.114 = -926.82$

Now that we have made two estimates of the temperature we can use linear interpolation to make the third estimate:

$$\frac{530.67-(-926.82)}{2500 - 2000} = \frac{-224.010-(-926.82)}{T - 2000}$$

Rearranging gives: $(T - 2000)1457.49 = 500 \times 702.81$ or $T = 2241.1$ K

Substitution into the original equation:

$$T_c = T_m + k\phi \qquad \phi<1.0$$

gives: $2241.1 = 298.15 + 0.9k$, or $k = 2159$

Figure A shows a comparison between the computed combustion temperatures, for iso-octane air mixtures at an initial temperature of 350 K, using:

a) the equations developed here,

b) An equilibrium calculation with STANJAN, allowing for the presence of CO and H_2 rich of stoichiometric, and

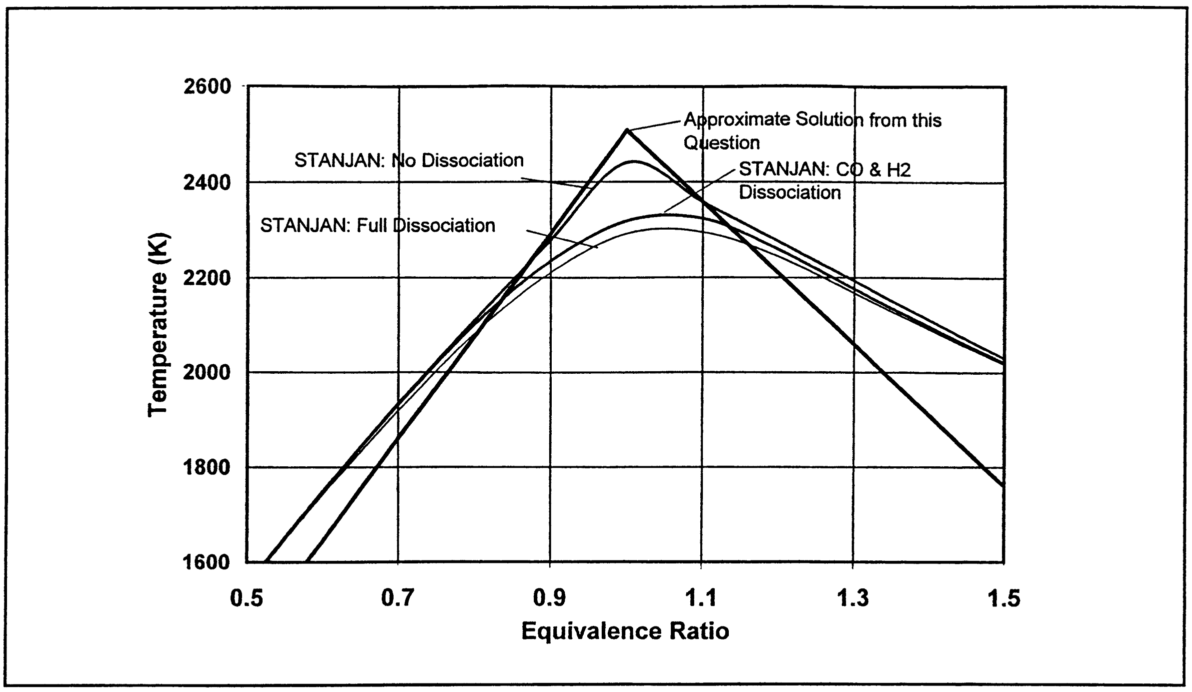


Figure A **Comparison of Computed Combustion Temperatures**

c) An equilibrium calculation using STANJAN that allows for the presence of CO, CO_2, H_2O, H_2, 0_2, O, OH, NO and H.

c) An calculation using STANJAN with no dissociation.

Weak of stoichiometric the differences between cases (a) and (b) are due to the dependence of the heat capacities of the constituents on temperature, whilst rich of stoichiometric there are changes in the position of the CO, CO_2, H_2O, and H_2 equilibrium. The differences between cases (b) and (c) reduce as the mixture strength moves away from stoichiometric; the difference is only 16 K at an equivalence ratio of 0.7, and only 15K at an equivalence ratio of 1.2. The largest differences occur at stoichiometric, for which there is a difference of about 210 K between cases (a) and (c), about 60 K is due to the underestimation of the heat capacities, and 150K is due to dissociation. At an equivalence ratio of 0.9, the overestimate of about 80 K is solely due to dissociation.

3.15 Equations are required to calculate: the air fuel ratio, the hydrogen/carbon ratio, the stoichiometric air fuel ratio, and the equivalence ratio, from the exhaust emissions readings obtained from a 4 gas analyser. The 4 gas analyser measures the following emissions on a dry gas basis:

carbon monoxide (%CO),
carbon dioxide (%CO_2),
oxygen (%O_2), and
unburnt hydrocarbons (as ppm of hexane - C_6H_{14})

The fuel may be assumed to be a pure hydrocarbon (that is, there are no oxygenates such as ethanol present), and it is also acceptable to ignore the presence of hydrogen in the exhaust products for the rich mixtures. Assume the following molar masses:

M_{H2} hydrogen (H_2)	**2 kg/kmol**
M_C carbon	**12 kg/kmol**
M_{N2} nitrogen (N_2)	**28 kg/kmol**
M_{O2} oxygen (O_2)	**32 kg/kmol**
M_{air} air (21%O_2,79%N_2)	**29 kg/kmol**

A convenient way to proceed, is to assume that a hydrocarbon (C_xH_y), reacts with z kmols of oxygen to produce 100 kmols of dry products of combustion, (there will of course be water present in the exhaust, so that our specified quantity of reactants produces more than 100 kmols of products). In these calculations we are only ever dealing with ratios, so when we evaluate the hydrogen/carbon ratio the mean molar mass of the fuel will be unknown. We could have specified that r kmols of C_sH_y react with our z kmols of oxygen, in which case:

$$x = rs \text{ and } y = rt.$$

The hydrogen/carbon ratio would be the same, and the only difference is an extra variable r, that we are not able to determine.

The molar (or volumetric) composition of air can be assumed to be 21% oxygen and 79% nitrogen. Thus for every kmol of oxygen there are (79/21=) 3.76 kmols of nitrogen. Our reaction is thus:

$$C_xH_y + z(O_2 + 3.76N_2) \rightarrow 100 \text{ kmols of dry products and water vapour}$$

By specifying 100 kmols of dry products, there is a direct correspondence between the measured percentages of each constituent of the exhaust and the number of kmols. Let:

a	be the percentage (or the number of kmols) of carbon monoxide (CO),
b	be the percentage (or the number of kmols) of carbon dioxide (CO_2),
c	be the percentage (or the number of kmols) of oxygen (%O_2), and
d	be the ppm (or $d/10^4$ of kmols) of unburnt hydrocarbons (C_6H_{14}).

Since we have specified 100 kmols of dry products, and we are ignoring any hydrogen, we can determine by difference the number of kmols of nitrogen:

$$100 - (a+b+c+d/10^4) \text{ kmols } N_2$$

If we introduce an additional variable (w), to specify the number of kmols of water vapour (H_20), our reaction becomes:

$$C_xH_y + z(O_2 + 3.76N_2) \rightarrow aCO + bCO_2 + cO_2 + d/10^4C_6H_{14} + (100\text{-}a\text{-}b\text{-}c\text{-}d/10^4)N_2 + wH_20$$

We have four unknowns (w, x, y and z), and since we can write 4 atomic balance equations, then it is possible to solve the equations. (As we only know the relative concentrations of the species in the exhaust, then we will only be able to determine the ratios of w to x to y to z. In other words we will be able to find the ratios (such as x/y the Hydrogen/Carbon ratio), but not the absolute values.

The four atomic balances are:

N balance $\quad 3.76z = 100 - a - b - c - d/10^4$ (1

C balance $\quad x = a + b + (6d/10^4)$

- noting that there are 6 carbon atoms in each molecule of hexane (2

O balance $2z = a + w + 2(b + c)$ (3

H balance $y = 2w + (14d/10^4)$ (4

The number of kmols of oxygen (z) is found directly from equation 1, whilst the number of kmols of carbon (x) is found directly from equation 2. In contrast, the number of kmols of hydrogen (y) requires solution of Eq. 3 to determine the number of kmols of water vapour (w).

Rearrangement of Eq. 1 gives:

$$z = (100 - a - b - c - d/10^4)/3.76 \quad (5$$

and rearrangement of Eq. 3 gives:

$$w = 2z - [a + 2(b + c)] \quad (6$$

Substitution for z from Eq. 5 into Eq. 6 gives:

$$\begin{aligned} w &= 2(100 - a - b - c - d/10^4)/3.76 - [a + 2(b + c)] \\ &= 53.19 - 1.532a - 2.532b - 2.532c - 0.532d/10^4 \quad (7 \end{aligned}$$

Finally, substitution for w from Eq. 7 into Eq. 4 gives:

$$\begin{aligned} y &= 2[53.19 - 1.532a - 2.532b - 2.532c - 0.532d/10^4] + (14d/10^4) \\ &= 1063.8 - 3.064a - 5.064b - 5.064c + 12.94d/10^4 \quad (8 \end{aligned}$$

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The hydrogen/carbon ratio is given by the combination of Eqs 2 and 8:

$$y/x = [1063.8 - 3.064a - 5.064b - 5.064c + 12.94d/10^4]/[a + b + (6d/10^4)] \quad (9$$

The gravimetric air fuel ratio is obtained by determining the mass of the reacting species:

Fuel, C_xH_y - $xM_C + yM_{H2} = 12[a+b+(6d/10^4)] + 2[1063.8-3.064a-5.064b-5.064c+12.94d/10^4]$ (10

$$\begin{aligned} \text{Air, } z(O_2 + 3.76N_2) - z(M_{O2} + 3.76M_{N2}) &= [(100 - a - b - c - d/10^4)/3.76](32 + 3.76 \times 28) \\ &= 36.51(100 - a - b - c - d/10^4) \quad (11 \end{aligned}$$

Thus the gravimetric air fuel ratio (AFR) is:

$$\frac{[36.51(100-a-b-c-d/10^4)]}{12[a+b\pm(6d/10^4)]+2[1063.8-3.064a-5.064b-5.064c+12.94d/10^4]} \quad (12$$

The equivalence ratio is found by comparing the quantity of air used (z), with that required (a new variable u) for the complete oxidation of the fuel (C_xH_y) to carbon dioxide and water vapour.

$$C_xH_y + u(O_2 + 3.76N_2) \rightarrow xCO_2 + \tfrac{1}{2}yH_20 \quad (13$$

The variable u can be eliminated by an atomic oxygen balance:

$$2u = 2x + \tfrac{1}{2}y \quad \text{or} \quad u = x + \tfrac{1}{4}y \qquad (14$$

The stoichiometric reaction (Eq. 13) thus becomes:

$$C_xH_y + (x + \tfrac{1}{4}y)(O_2 + 3.76N_2) \rightarrow xCO_2 + \tfrac{1}{2}yH_20 \qquad (15$$

The corresponding mass of air is obtained by substituting u (from Eq. 14) for z in Eq. 11

Air, $u(O_2 + 3.76N_2)$:- $u(M_{O2} + 3.76M_{N2}) = (x + \tfrac{1}{4}y)(32 + 3.76 \text{ x } 28) = 137.28(x + \tfrac{1}{4}y)$ (16

The corresponding mass of fuel is given by Eq. 10

Fuel, C_xH_y :- $xM_C + yM_{H2} = 12[a+b+(6d/10^4)] + 2[1063.8\text{-}3.064a\text{-}5.064b\text{-}5.064c+12.94d/10^4]$(10

So the stoichiometric air fuel ratio (AFRs) is given by:

$$\frac{137.28(x + \tfrac{1}{4}y)}{12[a+b+(6d/10^4)] + 2[1063.8-3.064a-5.064b-5.064c+12.94d/10^4]} \qquad (17$$

The equivalence ratio (ϕ) is the stoichiometric air fuel ratio (AFRs) divided by the actual air fuel ratio (AFR). Noting that the denominators in Eqs 12 and 17 cancel, then:

$$\begin{aligned} \phi &= 137.28(x + \tfrac{1}{4}y)/[36.51(100-a-b-c-d/10^4)] \\ &= 3.76(x + \tfrac{1}{4}y)/(100-a-b-c-d/10^4) \qquad (18 \end{aligned}$$

which is of course the ratio of u (Eq.14) to z (Eq.5). The non-dimensional air fuel ratio (often referred to as lambda, λ) is the reciprocal of the equivalence ratio (ϕ):

$$\lambda = (100-a-b-c-d/10^4)/[3.76(x + \tfrac{1}{4}y)] \qquad (19$$

3.16 A rigid and well insulated combustion vessel contains propane, oxygen and nitrogen; the initial composition is as indicated in the equation below. The initial pressure is 2 bar, and the initial temperature is 300 K. An equilibrium calculation restricted to the 6 principal combustion species, gives the quantities of products that are identified below, and a temperature of 2718 K.

$$C_3H_8 + 5O_2 + 18.8N_2 \rightarrow 3.87H_2O + 0.13H_2 + 2.47CO_2 + 0.53CO + 0.33O_2 + 18.8N_2$$

The enthalpy of formation for propane (C_3H_8) is -104.68 MJ/kmol, and the molar specific heat capacity at constant pressure for the temperature range 200 to 300 K may be taken as 0.0628 MJ/kmolK

Stating clearly any assumptions that you make:

a) What will the final pressure be ?

b) Demonstrate that the temperature of 2718 K is consistent with the computed composition, and the conservation of energy.

c) What other dissociation reactions are likely to be significant, and if they were to be included, what would the effect on the final temperature and pressure be.

Assuming that the vessel is adiabatic, there is no change in volume, the products of combustion are at a uniform temperature, and all the gases may be treated as semi-perfect.

a) The equation of state can be applied in molar form:

$$pV = nR_oT \qquad \text{or} \qquad V = (nR_oT/p)_R = (nR_oT/p)_P$$

$$\text{or} \qquad p_P = (n_P/n_R)*(T_P/T_R)*p_R \qquad (1$$

$$n_R = 1 + 5 + 18.8 = 24.8 \text{ kmols}$$

$$n_P = 3.87 + 0.13 + 2.47 + 0.53 + 0.33 + 18.8 = 26.13$$

Substituting numerical values into Eq 1 gives

$$p_P = (26.13/24.8)*(2718/300)*2 \quad \text{bar}$$
$$= \mathbf{19.09} \quad \textbf{bar}$$

b) There are two parts to this section, since energy has to be conserved, and the composition has to be compatible with the equilibrium constants.

We will consider the energy balance first, (remembering to use internal energy, as the volume is constant):

First, find the Internal Energy of the Reactants:

For the propane, $H_{300} = H_f^\circ + C_p\Delta T = -104.68 + 0.0628*(300 - 298.15) = -104.56$ MJ/kmol (2

for a semi-perfect gas, $H = U + R_oT$,
and $U_{300} = H_{300} - R_oT = -104.56 - 0.0083143*300 = -107.05$ MJ/kmol (3

both of which agree well with the values in Table A.5.

Using the values from Tables A.4 and A.5:

Species i	n kmols	U_{300} MJ/kmol	U_i MJ/kmol fuel
C_3H_8	1	-107.05	-107.05
O_2	5	-2.440	-12.20
N_2	18.8	-2.441	-45.89
			======
	TOTAL	Σn_iU_i	-165.14

The Internal Energy of the products, is found by using linear interpolation between the data tabulated at 2700K and 2800 K. This can be done in one of 2 ways (both are used here, as a way of checking the arithmetic). The preferred method (denoted by *) is to evaluate the internal energy of the mixture at each of 2700K and 2800 K, and then interpolate (this allows the totals to be used for interpolation to find the actual temperature at which the internal energy corresponds to that of the products). The alternative method (denoted by #) is to interpolate the data for each species at 2718 K, and then complete the summation - this method involves more operations and does not make it so easy to judge the significance of any imbalance:

Species i	n kmols	U_{2700} MJ/kmol	U_{2800} MJ/kmol	U_{2718} MJ/kmol	U_i MJ/kmol fuel
H_2O	3.87	-154.480	-149.825	-153.642	-594.59
H_2	0.13	55.242	58.060	55.749	7.25
CO_2	2.47	-281.688	-276.325	-280.722	-693.38
CO	0.53	-50.560	-47.683	50.042	-26.52
O_2	0.33	63.767	66.883	64.328	21.23
N_2	18.80	59.214	62.073	59.729	1122.90
				=======	
(MJ/kmol_fuel)	TOTALS $\Sigma n_i U_i$	-179.956	- 91.026	-163.95*	-163.11#

The two methods indicate a satisfactory energy balance with that of the original reactants (-165.14 MJ/kmol_fuel). The difference in the two methods for evaluating the internal energy of the products is due to either rounding errors, or a small arithmetic error. When linear interpolation is used to refine the estimate of the products temperature, the result is:

Product Temperature = 2700 + 100(-165.14 + 179.956)/(-91.026 + 179.956) = 2716.6 K

[Alternatively, the difference between the internal energy of the products and the reactants can be placed into perspective by remembering that:

a) the constant pressure calorific value of propane is about 2043 MJ/kmol, or

b) the heat capacity of the products at constant volume is about 0.75 MJ/kmol_fuel, so the discrepancy in the energy balance is equivalent to a 1 K temperature error.]

Now we can undertake the equilibrium checks:

Using the equation numbers of the equilibrium data in Table A.6 in the Appendix:

$\Sigma \nu i A i = 0$ where ν_i is the stoichiometric coefficient of species A_i (5

Reaction 7 $-CO - \frac{1}{2}O_2 + CO_2 = 0$

Reaction 9 $-CO - H_2O + CO_2 + H_2 = 0$

$$\text{Ln } K_p = \Sigma \nu_i \text{Ln} p^*_i \qquad (6$$

where p^*_i is numerically equal to the partial pressure of substance A_i

The relevant values of Ln K_p are:

Reaction	2700K	2800K	2718K
7	2.320	1.884	2.242
9	-1.884	-1.918	-1.890

The values at 2718K were obtained by linear interpolation, for example:

$\text{Ln } K_p = 2.320 + [(2718 - 2700)/(2700 - 2600)]*(1.884 - 2.320) = 2.242$

The partial pressures of each species are evaluated from:

$p^*_i = p \times n_i/\Sigma n_i$, remembering in this application to use units of bar

$\Sigma n_i = n_P = 26.13$ kmols, and $p = 19.09$ bar

Species i	n kmols	$\text{Ln}p^*_i$ bar
H_2O	3.87	1.039
H_2	0.13	-2.354
CO_2	2.47	0.591
CO	0.53	-0.949
O_2	0.33	-1.423

For reaction 7, $-CO - \tfrac{1}{2}O_2 + CO_2 = 0$

$\text{Ln } K_p = \Sigma\nu_i \text{Ln}p^*_i = -(-0.949) - \tfrac{1}{2}(-1.423) + 0.591 = 2.252$ (cf 2.242)

For reaction 9 $-CO - H_2O + CO_2 + H_2 = 0$

$\text{Ln } K_p = \Sigma\nu_i \text{Ln}p^*_i = -(-0.949) - 1.039 + 0.591 + (-2.354) = -1.853$ (cf -1.890)

In both cases this is a satisfactory agreement, since small changes in the lowest concentrations (O_2 in Reaction 7, and H_2 in Reaction 9) will lead to substantial changes in the values of Ln K_p.

c)

Other species that are likely to be present are (in order of decreasing concentration):
OH, NO, H, O, N. The temperature of the products will be lower, and the pressure will also be reduced, since the lower temperature has a larger effect than the slight increase in the number of kmols of the reactants.

This question was devised using **STANJAN**, which has also been used to quantify the effects discussed in part (c). The temperature is reduced to 2663 K (2718 K), the pressure is reduced to 18.75 bar (19.09 bar), and the number of kilomoles is increased to 26.19 (26.16). The concentrations of the minor species are:

OH 5938 ppm, NO 5824 ppm, H 786 ppm, O 633 ppm, and N 234 ppm.

It is of course unlikely that the equilibrium level of NO will be attained.

The final temperature is higher than for isobaric combustion, since no work has been done by the gases in increasing their volume against the ambient pressure. The assumption of uniform temperature is required, since in practice, the first gases burnt will be at a higher temperature than the last gas to be burnt.

3.17 A flow of methane at 1 bar and 298.15 K is divided into two equal flows. Flow 1 is mixed with a stoichiometric quantity of air (also at 1 bar and 298.15 K) and reacted in an engine. The hot exhaust gases from the engine (which can be assumed to be fully oxidised) are then mixed with the second flow of methane and passed into a catalytic reactor that is maintained at a temperature of 700 K, by waste heat from the engine exhaust. The outflow from the reactor is at 700 K and a pressure of 1 bar.

Write down the equation for the reactants and products entering and leaving the reactor: use a basis of 1 kmol of CH_4 entering the reactor, and y kmol of CH_4 leaving the reactor. Express the quantities of products leaving the reactor in terms of y.

For the stoichiometric equation: $- CH_4 - 2H_2O + CO_2 + 4H_2 = 0,$

a) Verify that: $\ln K_p = -5.973$ **at 700 K**

b) Show that if this is the only equilibrium reaction that needs to be considered, and that equilibrium is attained, then the products from the reactor will contain 0.783 kmol of CH_4.

c) Determine the difference in the enthalpy of the reactants and products entering and leaving the reactor, and comment on: how the difference can arise and its significance.

d) State which other (if any) dissociation reaction(s) would be significant.

The reaction in the engine is with the stoichiometric quantity of air, and the question states that the methane is fully oxidised:

$$CH_4 + z(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 3.76zN_2$$

The atomic oxygen balance gives: $2z = 2 + 2 \times 1$, $z = 2$

Thus: $$CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 7.52N_2$$

Entering the catalytic reactor will be these products of combustion, and additional methane:

$$CH_4 + CO_2 + 2H_2O + 7.52N_2 \rightarrow CH_4, CO_2, H_2O, H_2 + 7.52N_2$$

a) We need to verify that: $\ln K_p = -5.973$ at 700 K

For the stoichiometric equation: $- CH_4 - 2H_2O + CO_2 + 4H_2 = 0,$

$\ln K_p = -\Delta G/R_oT$, where: $\Delta G = \Sigma \nu_i G_i$,

so: $\ln K_p = -\Sigma \nu_i G_i/R_oT$, where: ν_i is the stoichiometric coefficient for species i

Using the data for 700 K from Tables A.4 and A.5 with units of MJ gives:

$$\begin{aligned}\ln K_p &= -[(-1 \times -213.275) + (-2 \times -380.73) + (1 \times -551.29) + (4 \times -97.17)]/(8.3143\times10^{-3} \times 700)\\ &= \mathbf{-5.973}\end{aligned}$$

The catalyst will not change the equilibrium, but merely the rate at which it is achieved.

b) Next we need to establish whether 0.783 kmols of methane satisfies the equilibrium conditions, so the first step is to determine the concentration of all the species in terms of y, the number of kmols of methane.

$$CH_4 + CO_2 + 2H_2O + 7.52N_2 \rightarrow yCH_4 + aCO_2 + bH_2O + cH_2 + 7.52N_2$$

Using atomic balances gives:

C: $1 + 1 = y + a$ or $a = 2 - y$

O: $1 \times 2 + 2 \times 1 = 2a + b$ thus $b = 4 - 2a$ or $b = 2y$

H: $1 \times 4 + 2 \times 2 = 4y + 2b + 2c$ thus $8 = 4y + 4y + 2c$ or $c = 4 - 4y$

So:

$$CH_4 + CO_2 + 2H_2O + 7.52N_2 \rightarrow yCH_4 + (2 - y)CO_2 + 2yH_2O + (4 - 4y)H_2 + 7.52N_2$$

For: $-CH_4 - 2H_2O + CO_2 + 4H_2 = 0$, with $y = 0.783$, and a system pressure of 1 bar:

$\text{Ln}\, K_p = \Sigma\nu_i \ln p^*_i$, $p^*_i = Pn_i/\Sigma n_i = 1 \times n_i/(0.783 + [2 - 0.783] + 2\text{x}0.783 + 4[1 - 0.783]) = n_i/11.954$

$$\ln K_p = -\ln(0.783/11.954) + \ln([2\text{-}0.783]/11.954) - 2\ln(2\text{x}0.783/11.954) + 4\ln([4 - 4 \times 0.783]/11.954)$$

$\ln K_p = -5.984$ Compared with -5.973, there is a 1% difference in K_p, which is acceptable.

c) We can now assess the molar enthalpies of the reactants and products.

The molar enthalpy of the reactants (CH_4, CO_2, H_2O, N_2) at 700 K is found from the data in Tables A.4 and A.5:

$$H_R = \Sigma n_i H_i = -55.724 - 375.753 - 2\text{x}227.639 + 7.52\text{x}11.934 = -797.011 \text{ MJ/kmol\_CH}_4$$

The molar enthalpy of the products (CH_4, CO_2, H_2O, H_2, N_2) at 700 K is found from the data in Tables A.4 and A.5:

$$H_P = \Sigma n_i H_i = 0.783\text{x}(-55.724) + (2 - 0.783)\text{x}(-375.753) + 2\text{x}0.783\text{x}(-227.639) + 4(1 - 0.783)\text{x}11.750 + 7.52\text{x}11.934 = -757.463 \text{ MJ/kmol\_CH}_4$$

The molar enthalpy of the products is less negative (by 39.55 MJ) than for the reactants, so this will be provided by a heat input to the reactor. Since the reactants and products are at the same temperature, the increase in enthalpy means that the calorific value of the methane has been increased by the reformation process (by about 5%).

d) The other dissociation reaction that might be important is the water gas reaction (reaction 7 in Table A.6):

$-CO - H_20 + CO_2 + H_2 = 0$ for which $\ln K_p = 2.249$ at 700 K, or $K_p = 9.478$

Since the concentrations of H_20 and CO_2 are approximately equal, then the concentration of CO will be about an order of magnitude lower than the concentration of the H_2.

DISCUSSION:

The significance of other equilibrium reactions can be established by using STANJAN for a more comprehensive equilibrium analysis:

Species	STANJAN	This Problem	
CH_4	0.76428	0.783	
CO	0.06779	-	
CO_2	1.16792	1.217	
H_2	0.87507	0.868	
H_2O	1.59636	1.566	
N_2	7.52000	7.520	
O_2	2.709×10^{-3}	-	
H	-751.86	-757.46	MJ/kmol_CH_4

This confirms the above order of magnitude argument in respect of the likely CO level, and that the equilibrium of $-CO - \frac{1}{2}O_2 + CO_2 = 0$ does not need to be considered. The enthalpy is higher when these additional species are considered (by 5.6 MJ/kmol_CH_4), to form the CO and increase the level of methane dissociation.

This problem is equivalent to saying that an engine is being operated with exhaust gas recirculation (EGR), in which the EGR and the incoming fuel/air mixture are mixed and reacted prior to entering the engine, but by separating the engine from the subsequent catalytic reactor, the question gives more indication of how the answer should be reached. Such a high level of EGR (about 50%) might well be acceptable, because the hydrogen present in the reformed fuel will increase the tolerance to a high level of dilution by additional inert species (the water vapour, and carbon dioxide).

3.18 Octane (C_8H_{18}) is burnt with dry air in a steady-flow constant pressure combustion system at a pressure of 15 bar and an equivalence ratio of 0.666. The fuel enters the combustion chamber as liquid at 25°C, whilst the air enters at a temperature of 600K. The products leaving the combustion chamber are in equilibrium at a temperature of 1800 K, and consist solely of N_2, O_2, H_20, CO_2 and NO.

Write down the stoichiometric and actual combustion equations, and determine the concentration of nitric oxide (NO) in the products of combustion. Calculate the heat transferred from the combustion chamber during combustion per unit mass of fuel.

Why might the concentration of nitric oxide in the exhaust differ from the equilibrium prediction.

$$C_8H_{18} + z(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 3.76zN_2$$

An atomic oxygen balance gives: $2z = 8 \times 2 + 9 = 25$ or $z = 12\frac{1}{2}$

$$C_8H_{18} + 12\tfrac{1}{2}(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 47.02N_2$$

When the equivalence ratio is 0.666 and there is nitric oxide (NO) in the products we need to introduce a temporary variable y.

$$C_8H_{18} + (12\tfrac{1}{2}/0.666)(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 2yNO + (47.02/0.666 - y)N_2$$
$$+ [12\tfrac{1}{2}(1/0.666 - 1) - y]O_2$$

$$C_8H_{18} + 18.77(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 2yNO + (70.57 - y)N_2 + (6.27 - y)O_2$$

For the equilibrium of NO, we need equilibrium reaction 3 from Table A.6:

$N_2 + O_2 - 2NO = 0$, and at 1800 K, $\ln K_p = 9.036$

$\ln K_p = -2\ln(P^*_{NO}) + \ln(P^*_{N2}) + \ln(P^*_{O2})$ (where P^* is a dimensionless quantity, numerically equal to the partial pressure in units of bar)

For species i, the partial pressure $P^*_i = Pn_i/\Sigma n_i$. Let $P/\Sigma n_i = P'$

Thus $\ln K_p = \ln(n_{N2}) - \ln(P') + \ln(n_{O2}) - \ln(P') - 2\ln(n_{NO}) - 2\ln(P')$

or $\ln K_p = \ln(n_{N2}) + \ln(n_{O2}) - 2\ln(n_{NO})$ $9.036 = \ln(70.57 - y) + \ln(6.27 - y) - 2\ln(2y)$

$\exp(9.036) = (70.57 - y)(6.27 - y)/(2y)^2$ $8400.1 = (70.57 - y)(6.27 - y)/(2y)^2$

or $33600.4y^2 = y^2 - (70.57 + 6.27)y + 442.47$ or $33599.4y^2 + 76.84y - 442.47 = 0$

Using the standard method of solving a quadratic equation gives:

$$y = [-76.84 \pm\surd(76.84^2 + 4 \times 33599.4 \times 442.47)]/(2 \times 33599.4)$$

Taking the positive solution, gives: $y = 0.114$

There will thus be $2y$ or 0.228 kmol_NO/kmol_fuel. The concentration of nitric oxide in the exhaust is:

$$0.228/\Sigma n_i = 0.228/(8 + 9 + 2y + 70.57 - y + 6.27 - y) = 0.228/93.84 = 0.00243 \text{ or } \mathbf{0.243\%}$$

In the absence of any work: $\Sigma(n_iH_i)_R = \Sigma(n_iH_i)_P + Q$ where Q is the heat flow leaving the system.

$$\Sigma(n_iH_i)_R = (n_{C8H18}H_{C8H18})_{298.15K} + (n_{O2}H_{O2} + n_{N2}H_{N2})_{600K}$$

Noting that the problem here concerns liquid fuel, we have to subtract the enthalpy of vaporisation (Table A.3) from the 'absolute' molar enthalpy (Table A.5):

$$H_{C8H18} = -224.01 - 35.142 = -259.15 \text{ MJ/kmol\_liquid\_fuel at } 25°C$$

$$\Sigma(n_iH_i)_R = -259.15 + 18.77 \times 9.247 + 70.57 \times 8.893 = 541.995 \text{ MJ/kmol\_fuel}$$

$$\Sigma(n_iH_i)_P = (n_{CO2}H_{CO2} + n_{H2O}H_{H2O} + n_{NO}H_{NO} + n_{O2}H_{O2} + n_{N2}H_{N2})_{1800K}$$

$$= 8\times(-314.151) + 9\times(-179.212) + 0.228 \times 140.808 + 6.16 \times 51.652 + 70.46 \times 48.949$$

$$\Sigma(n_iH_i)_P = -326.89 \text{ MJ/kmol\_fuel}$$

$$Q = \Sigma(n_iH_i)_R - \Sigma(n_iH_i)_P = 541.995 - (-326.89) = 868.89 \text{ MJ/kmol\_fuel}$$

The molar mass (M) of the fuel is 114.23 kg/kmol, so $q = Q/M = 868.89/114.23 =$ **7.61 MJ/kg**

(This amounts to about 17% of the calorific value of the fuel)

The nitric oxide concentration will be lower than its equilibrium concentration, because the reaction rates are for its formation are low, and the residence time in the combustion chamber will be insufficient for equilibrium to be attained.

This question specified a constant pressure combustion system which is applicable to gas turbine combustion. If a reciprocating engine was being considered, then it would be necessary to use internal energies, not enthalpies. Because the formation of the nitric oxide does not change the total number of moles of products, then the NO formation would not affect the pressure in a constant volume combustion system.

3.19 A mixture of air and methane with initially at a temperature of 600K and pressure of 20 bar is burnt at a constant volume.

What is the non-dimensional air fuel ratio (Lambda) ?

By considering the equilibrium of the 6 species in the following table, determine the combustion temperature by considering the water gas equilibrium, and verify that both equilibrium and the 1st Law of Thermodynamics are satisfied.

species	**mols**
CO	**3.15222E-01**
CO_2	**6.84778E-01**
H_2O	**1.87628E+00**
H_2	**1.23718E-01**
O_2	**1.94700E-02**
N_2	**6.76800E+00**

The combustion equation with methane is:

$$y\mathrm{CH_4} + \mathrm{Air} \rightarrow 0.315222\mathrm{CO} + 0.684778\mathrm{CO_2} + 1.87628\mathrm{H_2O} + 0.123718\mathrm{H_2} + 0.01947\mathrm{O_2} + 6.768\mathrm{N_2}$$

An atomic hydrogen balance gives: $4y = 1.87628 \times 2 + 0.123718 \times 2 = 4.00$ or $y = 1$

As confirmation an atomic carbon balance gives: $y = 0.315222 + 0.684778 = 1.00$ or $y = 1$

A molecular oxygen balance gives: $\frac{1}{2}(0.315222) + 0.684778 + \frac{1}{2}(1.87628) + 0.01947 = 1.799999$

There are 3.76 moles of nitrogen for every mole of oxygen, so $6.768\mathrm{N_2} \Rightarrow (6.768/3.76 =)$ 1.8 moles of O_2

The stoichiometric combustion equation for methane is:

$$\mathrm{CH_4} + z(\mathrm{O_2} + 3.76\mathrm{N_2}) \rightarrow \mathrm{CO_2} + 2\mathrm{H_2O} + 3.76z\mathrm{N_2}$$

An atomic oxygen balance gives: $2z = 1 \times 2 + 2 = 4$ or $z = 2$

We have 1.8 moles of oxygen, so the non-dimensional air/fuel ratio is (1.8/2 =) **0.9.**

.oOo.

Next we will consider the equilibrium equations.

$\ln K_p = \Sigma \nu_i \ln P^*_i$ (where P^* is a dimensionless quantity, numerically equal to the partial pressure in units of bar)

For species i, the partial pressure $P^*_i = Pn_i/\Sigma n_i$. Let $P/\Sigma n_i = P'$

Table A.6 Reaction 7: $- CO - H_2O + CO_2 + H_2 = 0$

$$\ln K_p = -\ln(P^*_{CO}) - \ln(P^*_{H2O}) + \ln(P^*_{CO2}) + \ln(P^*_{H2}) \qquad \text{and:}$$

$$\ln K_p = -\ln(n_{CO}) - \ln(P') - \ln(n_{H2O}) - \ln(P') + \ln(n_{CO2}) + \ln(P') + \ln(n_{H2}) + \ln(P') \qquad \text{(A}$$

$$\ln K_p = -\ln(n_{CO}) - \ln(n_{H2O}) + \ln(n_{CO2}) + \ln(n_{H2})$$

$$\ln K_p = -\ln(0.31522) - \ln(1.87628) + \ln(0.684778) + \ln(0.123718)$$

$$\ln K_p = -1.9432$$

It is very fortunate that the pressure terms have cancelled out, since at this stage we do not know the final pressure. If the pressure terms had not cancelled, then Eqs A and B (see later) would become a pair of simultaneous equations (with the pressure and temperature being the two unknowns) that would have to be solved iteratively.

Inspection of Table A.6 for Reaction 7, indicates a temperature between 2800 and 2900 K.

T (K):	2800	2900
$\ln K_p$:	-1.918	-1.948

$$T = 2800 + 100\text{x}(1.943 - 1.918)/(1.948 - 1.918) = 2883 \text{ K}$$

We can now determine the final pressure by applying the equation of state:

$$P_P = P_R\,(T_P n_P)/(T_R n_R) \qquad n_R = (1 + 1.8\text{x}[100/21]) = 9.571429 \qquad \text{(B}$$

$$n_P = 0.315222 + 0.684778 + 1.87628 + 0.123718 + 0.01947 + 6.768 = 9.787468$$

$$P_P = 20 \text{ x } (2883 \text{ x } 9.787468)/(600 \text{ x } 9.571429) = 98.27 \text{ bar}$$

To check that equilibrium is satisfied, we also need to consider the equilibrium of: CO, CO_2 and O_2. This is Reaction 6 in Table A.6: $- CO - ½O_2 + CO_2 = 0$

$$\ln K_p = -\ln(P^*_{CO}) - ½\ln(P^*_{O2}) + \ln(P^*_{CO2}) \quad \text{and:}$$

$$\ln K_p = -\ln(n_{CO}) - \ln(P') - ½\ln(n_{O2}) - ½\ln(P') + \ln(n_{CO2}) + \ln(P')$$

$$\ln K_p = -\ln(n_{CO}) - ½\ln(n_{O2}) + \ln(n_{CO2}) - ½\ln(P') \qquad \text{Where } P' = P/\Sigma n_i$$

$$\ln K_p = -\ln(0.31522) - ½\ln(0.01947) + \ln(0.684778) - ½\ln(98.27/9.787468) = 1.592$$

Inspection of Table A.6 for Reaction 6, indicates a temperature between 2800 and 2900 K.

T (K):	2800	2900
$\ln K_p$:	1.891	1.486

$$T = 2800 + 100\text{x}(1.592 - 1.891)/(1.468 - 1.891) = 2871 \text{ K}$$

The determination of the combustion temperature from Reaction 6 will be less accurate than from Reaction 7, since: a) there will be more errors in the determination of the partial pressures, since the concentration of oxygen is only given with 4 significant figures. b) Inspection of Table A.6 shows that ln K_p is less linearly dependant on temperature in the case of Reaction 6.

We now need to compare the internal energy of the reactants and products; taking the reactants first:

i	n_i	U_i	n_iU_i
CH_4	1	-66.220	-66.220
O_2	1.8	4.258	7.6644
N_2	6.768	3.828	25.8704
			========
		$U_R = \Sigma n_iU_i =$	-32.685 MJ/kmol_CH_4

and for the products (interpolating for the temperature of 2883 K):

i	n_i	U_i	n_iU_i
CO	0.31522	-45.291	-14.277
CO_2	0.68478	-271.864	-186.167
H_2O	1.87628	-145.931	-273.808
H_2	0.12372	70.774	8.756
O_2	0.01947	69.485	1.353 0.761
N_2	6.768	64.452	463.210
			========
		$U_P = \Sigma n_iU_i =$	-27.933 MJ/kmol_CH_4

The mean heat capacity of the mixture is about 0.33 MJ/K_kmol_CH_4. Comparing U_P with U_R indicates an overestimate of the temperature by about 13 K. Whilst not good, this result is satisfactory.

An alternative approach would have been to evaluate U_P at both 2800 K and 2900 K, and then to use linear interpolation to find the temperature of the products:

$$T = 2800 + 100(U_R - U_{P,2800})/(U_{P,2900} - U_{P,2800})$$

This is a slightly slower method, but perhaps more informative method, so the reader is encouraged to undertake this for themselves.

3.20 The combustion of a rich mixture of air and methane can be simplified to:

$$CH_4 + 1.8O_2 + 6.77N_2 \rightarrow CO,\ CO_2,\ H_2O,\ H_2,\ N_2$$

Assume a water gas equilibrium constant of 5.2 (the reverse of Reaction 7 in Table A.6) to evaluate the composition of the products of combustion. By considering the energy balance, show that the flame (constant pressure, adiabatic) temperature is close to 2200 K when the reactants are initially at 1 bar and 25°C.

The generalised combustion equation is:

$$CH_4 + 1.8O_2 + 6.77N_2 \rightarrow aCO + bCO_2 + cH_2O + dH_2 + 6.77N_2$$

We have already applied the nitrogen balance, so this leaves 3 atomic balance equations:

C: $1 = a + b$ (A

H: $1 \times 4 = 2c + 2d$ or $2 = c + d$ (B

O: $1.8 \times 2 = a + 2b + c$ or $3.6 = a + 2b + c$ (C

We now have 3 equations but we introduced 4 unknowns (*a, b, c, d*), so the fourth equation comes from equilibrium considerations, namely the water gas reaction:

$ac/bd = 5.2$ or $ac = 5.2bd$ (D

Equations A and B can be used to eliminate *b* and *d* from Eq. D:

$ac = 5.2(1 - a)(2 - c)$ or $ac = 10.4 - 10.4a - 5.2c + 5.2ac$

or $2 = 2a + c - 0.808ac$ (E

We have not yet used Eq. C, and Eq. A can be used to eliminate *b*:

$3.6 = a + 2(1 - a) + c$ or $1.6 = - a + c$ or $c = 1.6 + a$ (F

Equations E and F are now a pair of simultaneous equations with variables *a* and *c*, so we can substitute for *c* into Eq. E, which gives the following quadratic equation:

$2 = 2a + (1.6 + a) - 0.808a(1.6 + a)$ or $0.4 = (3 - 1.2928)a - 0.808a^2$

or $0.808a^2 - 1.7072a - 0.4 = 0$ (G

Using the standard solution for a quadratic equation gives:

$$a = \frac{1.7072 \pm \sqrt{1.7072^2 - 4 \times 0.808 \times 0.4}}{2 \times 0.808}$$

$a = (1.7072 \pm 1.2735)/1.616$ so $a = 0.2684$ or $a = 1.844$

Since *a* and *b* both have to be positive, then $0 < a < 1$, so $a = 0.2684$

Back substitution into Eq. A gives: $b = 1 - 0.2684 = 0.7316$

Back substitution into Eq. C gives: $c = 3.6 - 0.2684 - 2 \times 0.7316 = 1.8684$

Finally, back substitution into Eq.B gives: $d = 2 - 1.8684 = 0.1316$

The combustion equation is thus:

$$CH_4 + 1.8O_2 + 6.77N_2 \rightarrow 0.2684CO + 0.7316CO_2 + 1.868H_2O + 0.1316H_2 + 6.77N_2$$

At 298.15K, the enthalpy of the reactants is: $H_R = \Sigma n_i H_i = -74.52 + 1.8 \times 0.0 + 6.77 \times 0.0$

$H_R = -74.52$ MJ/kmol_CH$_4$

At 2200 K, the enthalpy of the products (CO, CO_2, H_2O, H_2, N_2) is:

$$H_P = \Sigma n_i H_i = 0.2684 \text{x}(-46.527) + 0.7316 \text{x}(-289.981) + 1.868 \text{x}(-158.810) + 0.1316 \text{x}(59.870) + 6.77 \text{x} 63.351$$

$$H_P = -84.53 \text{ MJ/kmol\_CH}_4$$

There is a difference of about 10 MJ/kmol_CH_4, but when this is compared with the calorific value of the methane (802.64 MJ/kmol) it can be seen that the energy balance is satisfactory. An alternative approach is to determine the heat capacity of the combustion products, which is about 0.5 MJ/kmol_CH_4_K. The estimate of the temperature is thus about 20 K low.

DISCUSSION

The results from this question can be compared with those from STANJAN, both for the species considered in the question, and when additional species are considered.

Species	This Question	Case 1	Case 2	Case 3
CO	0.2684	0.2695	0.27324	0.2767
CO_2	0.7316	0.7305	0.72677	0.7233
OH	-	-	-	0.0126
H_2	0.1316	0.1305	0.1332	0.1360
H_2O	1.8685	1.8695	1.8668	1.8544
NO	-	-	-	0.0043
N_2	6.7700	6.7700	6.7700	6.7679
O_2	-	-	0.0032	0.0025
T (K)	2220	2224	2219	2203

Case 1 provides a direct comparison of results from STANJAN with this question, and shows that the simple interpolation gave a reasonable result. Case 2 includes oxygen in the products ($CO_2 \leftrightarrow CO + \frac{1}{2}O_2$), and this lowers the temperature of the products by 5K, but has a negligible effect on the composition of the products. Finally, Case 3 includes: OH, O, H, N and NO. The hydroxyl radical (OH) is the most abundant additional species, and the products temperature is lowered by a further 16 K.

3.21 For the combustion of a stoichiometric mixture of air and methane:

$$CH_4 + 2O_2 + 7.52N_2 \rightarrow CO, CO_2, H_2O, H_2, O_2, N_2$$

If the initial temperature is 25°C, show that the equilibrium adiabatic combustion temperature is 2247 K for a constant pressure combustion process at 1 *atm*, by considering the energy balance, and the equilibrium of the 6 species.

In order to evaluate the energy balance, we will need to know the composition of the products, so our first step must be to apply the atomic balances and equilibrium equations. The generalised combustion equation is:

$$CH_4 + 2O_2 + 7.52N_2 \rightarrow aCO + bCO_2 + cH_2O + dH_2 + eO_2 + 7.52N_2$$

We have already applied the nitrogen balance, so this leaves 3 atomic balance equations:

C: $1 = a + b$ or $b = 1 - a$ (A

H: $1 \times 4 = 2c + 2d$ or $c = 2 - d$ (B

O: $2 \times 2 = a + 2b + c + 2e$ or $4 = a + 2(1 - a) + (2 - d) + 2e$
or $e = \frac{1}{2}a + \frac{1}{2}d$ (C

These 3 equations can be used to eliminate 3 of the variables, leaving a and d as unknowns:

$$CH_4 + 2O_2 + 7.52N_2 \rightarrow aCO + (1-a)CO_2 + (2-d)H_2O + dH_2 + (\tfrac{1}{2}a + \tfrac{1}{2}d)O_2 + 7.52N_2$$

Two independent equilibrium equations are needed; with reference to Table A.6:

For Reaction 6: $- CO - \frac{1}{2}O_2 + CO_2 = 0$

$\ln K_{p,6} = - \nu_i \ln P^*_i = - \ln(P^*_{CO}) - \frac{1}{2}\ln(P^*_{O2}) + \ln(P^*_{CO2})$ where: P^*_i is the partial pressure of species i, and:

$\ln K_{p,6} = - \ln(n_{CO}) - \ln(P') - \frac{1}{2}\ln(n_{O2}) - \frac{1}{2}\ln(P') + \ln(n_{CO2}) + \ln(P')$ Where $P' = P/\Sigma n_i$

$\ln K_{p,6} = - \ln(n_{CO}) - \frac{1}{2}\ln(n_{O2}) + \ln(n_{CO2}) - \frac{1}{2}\ln(P')$

$P = 1$ atm $= 1.01325$ bar, $\Sigma n_i = a + (1-a) + (2-d) + d + (\frac{1}{2}a + \frac{1}{2}d) + 7.52 = 10.52 + \frac{1}{2}(a + d)$

We can remove the log terms by replacing the plus by multiply, the ½ by $\sqrt{\ }$, and the minus by divide:

$K_{p,6} = [(1 - a)/a] \times \sqrt{[(10.52 + \frac{1}{2}a + \frac{1}{2}d)/\{1.01325 \times (\frac{1}{2}a + \frac{1}{2}d)\}]}$

$K_{p,6} = [(1 - a)/a] \times \sqrt{[(21.04 + a + d)/(1.01325a + 1.01325d)]}$ (D

For Reaction 7: $- CO - H_2O + CO_2 + H_2 = 0$

$\ln K_{p,7} = - \ln(P^*_{CO}) - \ln(P^*_{H2O}) + \ln(P^*_{CO2}) + \ln(P^*_{H2})$ and:

$\ln K_{p,7} = - \ln(n_{CO}) - \ln(P') - \ln(n_{H2O}) - \ln(P') + \ln(n_{CO2}) + \ln(P') + \ln(n_{H2}) + \ln(P')$

$\ln K_{p,7} = - \ln(n_{CO}) - \ln(n_{H2O}) + \ln(n_{CO2}) + \ln(n_{H2})$

$K_{p,7} = (1 - a)(d)/[(a)(2 - d)]$ (E

	T (K)	$\ln K_{p,6}$	$\ln K_{p,7}$
	2200	5.117	-1.649
	2300	4.460	-1.707
By linear interpolation for	2247	4.808	-1.676

$K_{p,7} = \exp(-1.676) = 0.1871 = (1 - a)(d)/[(a)(2 - d)]$

thus $0.1871(a)(2 - d) = (1 - a)(d)$ or $0.3742a - 0.1871ad = d - ad$

or $0.3742a = d - 0.8129ad$ and $d = 0.3742a/(1 - 0.8129a)$ (F

We can now return to Reaction 6: $K_{p,6} = \exp(4.808) = 122.486$

Substitution into Eq. E gives

$$122.486 = [(1 - a)/a] \times \sqrt{[(21.04 + a + d)/(1.01325a + 1.01325d)]}$$

Squaring both sides and rearranging gives:

$$(122.486a)^2 (1.01325a + 1.01325d) = (1 - a)^2 \times (21.04 + a + d)$$

Substitution for d from Eq. F, and multiplying both sides by $(1 - 0.8129a)$ gives:

$$15201.6a^3 [(1 - 0.8129a) + 0.3742] = (1 - 2a + a^2) \times [(21.04 + a)(1 - 0.8129a) + 0.3742a)]$$

or

$$-12357.4a^4 + 20890.0a^3 = (1 - 2a + a^2) (-0.8129a^2 - 15.729a + 21.04)$$

or

$$-12357.4a^4 + 20890.0a^3 = -0.8129a^4 - 17.355a^3 + 51.685a^2 - 57.809a + 21.04$$

or

$$f(a) = 12356.6a^4 - 20907.4a^3 + 51.685a^2 - 57.809a + 21.04 = 0$$

or for ease of evaluation with a simple calculator:

$$f(a) = ((((12356.6a - 20907.4)a + 51.685)a - 57.809)a + 21.04 = 0$$

This equation has to be solved iteratively, and we can try linear interpolation which needs two initial guesses. We know that there will be about 1% CO in the products of combustion, and there will be about 10 kmols of products, so our first guess can be $a = 0.1$. This makes $f(a)$ negative, so our second guess for a should be a little less, say 0.09.

For the third and subsequent guesses we can utilise linear interpolation:

$$[a_{n+1} - a_n]/f(a_n) = [a_{n-1} - a_n]/[f(a_{n-1}) - f(a_n)]$$

and

$$a_{n+1} = a_n - f(a_n)[a_{n-1} - a_n]/[f(a_{n-1}) - f(a_n)]$$

guess	a	$f(a)$
1	0.1	-3.896
2	0.09	1.825
3	0.09319	0.1132
4	0.093401	-0.0036

We can thus take $a = 0.0934$. Equation F allows us to find d:

$$d = 0.3742a/(1 - 0.8129a) = 0.3742 \times 0.0934/(1 - 0.8129 \times 0.0934) = 0.0378$$

From Eq. A: $b = 1 - a = 1 - 0.0934 = 0.9066$

From Eq. B: $c = 2 - d = 2 - 0.0378 = 1.9622$

From Eq. E: $e = \frac{1}{2}(a + d) = \frac{1}{2}(0.0934 + 0.0378) = 0.0656$

Thus:

$$CH_4 + 2O_2 + 7.52N_2 \rightarrow 0.0934CO + 0.9066CO_2 + 1.9622H_2O + 0.0378H_2 + 0.0656O_2 + 7.52N_2$$

Now that we know the composition of the products we can find the enthalpy of the mixture, and compare this with the enthalpy of the reactants, to see if the energy balance is satisfied.

At 298.15 K, the enthalpy of the reactants is: $H_R = \Sigma n_i H_i = -74.85 + 2 \times 0.0 + 7.52 \times 0.0$

$$H_R = -74.85 \text{ MJ/kmol\_CH}_4$$

At 2247 K, the enthalpy of the products is: $H_P = \Sigma n_i H_i$ The values of H_i will have to be found by linear interpolation between the data tabulated in Table A.4 at 2200 and 2300 K

species	n_i	$H_{i,2300}$	$H_{i,2200}$	$H_{i,2247}$	$n_i H_{i,2247}$
CO	0.0934	-42.863	-46.527	-44.805	-4.185
CO_2	0.9066	-283.870	-289.981	-287.127	-260.309
H_2	0.0378	63.373	59.870	61.506	2.325
H_2O	1.9622	-153.553	-156.810	-155.289	-304.708
O_2	0.0656	70.630	66.787	68.582	4.499
N_2	7.5200	66.991	63.351	65.051	489.183
					+++++
				$\Sigma n_i H_i =$	-73.195

There is a difference of about 1.7 MJ/kmol_CH$_4$, and if this is compared with the calorific value of the methane (802.64 MJ/kmol) it can be seen that the energy balance is very satisfactory. An alternative approach is to determine the heat capacity of the combustion products, which is about 0.5 MJ/kmol_CH$_4$_K. The estimate of the temperature is thus about 3 K high.

DISCUSSION

The results from this question can be compared with those from STANJAN, both for the species considered in the question, and when additional species are considered.

Species	This Question	Case 1	Case 2	Case 3
CO	0.0934	0.09346	0.09453	-
CO_2	0.9066	0.90654	0.90547	1.00
H	-	-	0.00411	-
OH	-	-	0.03016	-
H_2	0.0378	0.03776	0.03837	-
H_2O	1.9622	1.96220	1.94450	2.00
N	-	-	1.5×10^{-7}	-
NO	-	-	0.02093	-
N_2	7.5200	7.52000	7.50953	7.52
O	-	-	0.00248	-
O_2	0.0656	0.06561	0.04834	-
T (K)	2247	2247	2226	2328

Case 1 provides a direct comparison of results from STANJAN with this question, and shows good agreement in he concentration of all species. The differences will have arisen because of rounding errors, and differences in the thermochemical data. Case 2 includes 5 additional species (and thus 5 additional equilibrium equations).

There is a negligible effect on the composition of the major species apart from the oxygen, but there is a significant lowering of the temperature by about 20 K. Finally, Case 3 assumes complete combustion, and this leads to an over-prediction by 102 K.

3.22 For a fuel of arbitrary composition $C_\alpha H_\beta O_\gamma N_\delta$, show that the brake specific emissions of carbon monoxide in g_CO/kWh can be evaluated from:

$$bsfc \times \frac{M_C}{M_C + (\beta/\alpha)M_H + (\gamma/\alpha)M_O + (\delta/\alpha)M_N} \times \frac{\%CO}{\%CO_2 + \%CO + ppm\,CH_4/10^4} \times \frac{M_{CO}}{M_C}$$

Where bsfc - brake specific fuel consumption (g/kWh)
M - molar masses
and there is no solid carbon present in the exhaust.

Generalise the above equation for any species, and comment on the accuracy of any other atomic balance that might be used to evaluate the brake specific emissions.

For a fuel composition $C_\alpha H_\beta O_\gamma N_\delta$, the brake specific carbon consumption is proportional to the carbon mass fraction in the fuel:

$$bsfc \times \frac{\alpha M_C}{\alpha M_C + \beta M_H + \gamma M_O + \delta M_N} \qquad [g\ Carbon/kWh] \qquad \text{(A}$$

If there is no solid carbon in the exhaust, then the fraction of carbon as carbon monoxide will be:

$$\%CO/(\%CO_2 + \%CO + ppm\ CH_4/10^4) \qquad \text{(B}$$

M_C kg of carbon will form M_{CO} kg of carbon monoxide.

Dividing Eq. A by M_C and combining with Eq. B gives the brake specific emissions of carbon monoxide:

$$bsfc \times \frac{M_C}{M_C + (\beta/\alpha)M_H + (\gamma/\alpha)M_O + (\delta/\alpha)M_N} \times \frac{\%CO}{\%CO_2 + \%CO + ppm\,CH_4/10^4} \times \frac{M_{CO}}{M_C} \qquad \text{(C}$$

Equation C can be rewritten for species *i* by inspection:

$$\frac{\%i \times M_i}{(\%CO_2 + \%CO + ppm\,CH_4/10^4) \times [M_C + (\beta/\alpha)M_H + (\gamma/\alpha)M_O + (\delta/\alpha)M_N]} \times bsfc \quad [g\ species\ i/kWh]$$

The emissions of unburned hydrocarbons need to be expressed here as ppm of C_1. If the analyser had been calibrated with ppm of propane (C_3H_8), then the reading would have to be converted by multiplying with 3, since it is carbon atoms that we are counting. An alternative approach would have been to use a hydrogen balance, and to consider the mass of unburnt hydrocarbons. This would lead to an equation for the brake specific emissions of the unburnt hydrocarbons, that could then be generalised as with the carbon balance method. The hydrogen balance is less satisfactory for a number of reasons:

a) The water vapour is not measured, so instead it is necessary to calculate this via an oxygen balance.

b) There will be some hydrogen in the exhaust of rich mixtures, and it is rare for this to be measured, so an estimate would have to be made by assuming a value for the water gas equilibrium.

c) It will be necessary to establish the average number of hydrogen atoms in the unburnt hydrocarbons (the x in CH_x). The Flame Ionisation Detection (FID) hydrocarbons analyser works by 'counting' the number of carbon atoms.

Finally, the carbon monoxide and carbon dioxide concentrations can both be measured comparatively cheaply and accurately, so the carbon balance should be the more reliable method.

3.23 A test is being conducted on a spark ignition engine which is being operated on iso-octane with an equivalence ratio (ϕ) of 1.1. The combustion products can be assumed to contain no oxygen, and the concentration of the hydrogen is half that of the carbon monoxide. Write down the combustion equation.

The temperature of the exhaust is 1000 K, and the ambient temperature is 25°C. Calculate the enthalpy of the exhaust relative to 25°C, and the calorific value of the partial products of combustion at 25°C, and express these as a proportion of the calorific value of the fuel.

If the mass flowrate of the exhaust is 0.1 kg/s, atmospheric pressure is 1 bar, and the cross-sectional area of the exhaust pipe is 10 cm², calculate the ratio of the exhaust kinetic energy to the fuel calorific value.

We first need to establish the stoichiometric combustion equation for 1 kmol of fuel:

$$C_8H_{18} + z(O_2 + 3.76N_2) \rightarrow aCO_2 + bH_2O + 3.76zN_2$$

We have already applied the nitrogen balance, so this leaves 3 <u>atomic</u> balance equations from which to find a, b and z:

C: $8 = a$

H: $18 = 2b$ or $b = 9$

O: $2z = 2a + b$ or $z = 8 + 9/2 = 12.5$

The stoichiometric combustion equation for 1 kmol of fuel is thus:

$$C_8H_{18} + 12.5(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 47.0N_2$$

When the equivalence ratio is 1.1 there will be 12.5/1.1 (= 11.3636) kmols of O_2, and the generalised combustion equation (noting that we have been told that there is no oxygen in the products) will be:

$$C_8H_{18} + 11.3636(O_2 + 3.76N_2) \rightarrow aCO + bCO_2 + cH_2O + dH_2 + 42.727N_2$$

We have again applied the nitrogen balance, so this leaves 3 <u>atomic</u> balance equations:

C: $8 = a + b$ or $b = 8 - a$ (A

H: $18 = 2c + 2d$ or $9 = c + d$ (B

O: $11.3636 \times 2 = a + 2b + c$ or $22.7272 = a + 2b + c$ (C

We now have 3 equations but 4 unknowns (a, b, c, d), so the fourth equation comes from the statement in the question, that the concentration of the hydrogen is half that of the carbon monoxide:

$a = 2d$ (D

Eliminating d from Eq. C gives:

$9 = c + d = c + a/2$ or $c = 9 - a/2$ (E

We can now use Eqs A and E to eliminate b and c in Eq. C

$$22.7272 = a + 2b + c = a + 2(8 - a) + 9 - a/2 = 25 - 1.5a$$

or $1.5a = 25 - 22.7272$ and $a = 1.5152$ (C

Next we can back-substitute this numerical value of a into Eqs A, D and E, to find the concentrations of the other species:

$$b = 8 - a = 8 - 1.5152 = 6.4848$$

$$d = \tfrac{1}{2}a = 1.5152/2 = 0.7576$$

$$c = 9 - a/2 = 9 - 1.5152/2 = 8.2424$$

The combustion equation for 1 kmol of fuel is thus:

$$C_8H_{18} + 11.3636(O_2 + 3.76N_2) \rightarrow 1.5152CO + 6.4848CO_2 + 8.2424H_2O + 0.7576H_2 + 42.727N_2$$

Using the data in Table A.4 at 1000 K, the enthalpy of the products (CO, CO_2, H_2O, H_2, N_2) is:

$$H_P = \Sigma n_i H_i = 1.5152\text{x}(-88.838) + 6.4848\text{x}(-360.112) + 8.2424(-215.841) + 0.7576\text{x}20.686 + 42.727\text{x}21.459$$

$$H_P = -3316.36 \text{ MJ/kmol\_fuel}$$

At 298.15 K, the enthalpy of the products is:

$$H_P = \Sigma n_i H_i = 1.5152\text{x}(-110.525) + 6.4848\text{x}(-393.512) + 8.2424(-241.824) + 0.7576 \text{ x } 0.0 + 42.727 \text{ x } 0.0$$

$$H_P = -4712.52 \text{ MJ/kmol\_fuel}$$

The relative enthalpy (H_{rel})at 1000K is thus -3316.36 - (-471.52) = **1396.16 MJ/kmol_fuel**

The Calorific Value of the partial products of combustion (CV_{pp}) can be evaluated from:

$$CV_{pp} = n_{CO}CV_{CO} + n_{H2}CV_{H2}$$

Where CV_{CO} and CV_{H2} will correspond to the differences between the 'absolute' enthalpy of the partial products of combustion and their fully oxidised products at 25°C.

$CO + \frac{1}{2}O_2 \rightarrow CO_2$, thus: $CV_{CO} = H_{CO} + \frac{1}{2}H_{O2} - H_{CO2} = -110.525 + \frac{1}{2}x0.0 - (-393.512)$

$CV_{CO} = 282.987$ MJ/kmol_CO

$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$, thus: $CV_{H2} = H_{H2} + \frac{1}{2}H_{O2} - H_{H2O} = 0.0 + \frac{1}{2}x0.0 - (-241.824)$

$CV_{H2} = 234.899$ MJ/kmol_H_2

So: $CV_{pp} = n_{CO}CV_{CO} + n_{H2}CV_{H2} = 1.5152 \text{ x } 282.987 + 0.7576 \text{ x } 234.899 =$ **606.741 MJ/kmol_fuel**

The Calorific Value of iso-octane (Table A.3) is 5100.50 MJ/kmol.

Thus the relative enthalpy of the exhaust gas (H_{rel}) is:

$H_{rel}/CV_{fuel} = 1396.16/5100.50 = 0.2737$ or **27.37%** of the fuel Calorific Value

and the Calorific Value of the partial products of combustion (CV_{pp}) is:

$CV_{pp}/CV_{fuel} = 606.741/5100.50 = 0.1190$ or **11.90%** of the fuel Calorific Value

To find the Kinetic Energy of the exhaust stream, we need to know the volume flow rate (V). The equation of state ($pV = nR_oT$) will enable us to find the volume flow rate if we can determine the molar flow rate (n - kmol/s). Since we are given the mass flow rate, all we need to do is find the mean molar mass (M_m)of the exhaust products.

$M_m = \Sigma(n_iM_i)/\Sigma n_i = (1.5152x28 + 6.4848x44 + 8.2424x18 + 0.7576x2 + 42.727x28)/\Sigma n_i$

$= 1673.99/(1.5152 + 6.4848 + 8.2424 + 0.7576 + 42.7278) = 1673.99/59.7278 = 28.03$ kg/kmol

Thus $V = nR_oT/p = (m/M_m) \text{ x } R_oT/p = (0.1/28.03) \text{ x } 8314.3 \text{ x } 1000/10^5 = 0.2966 \text{ m}^3/\text{s}$

The velocity, $v = V/A = 0.2966/(10x10^{-4}) = 296.6$ m/s

The Kinetic Energy Flux will be $\frac{1}{2}mv^2$, where m is the mass flow rate.

Kinetic Energy Flux $= \frac{1}{2}mv^2 = \frac{1}{2}x0.1 \text{ x } 296.6^2 = 4.40$ kW

We now need to find what the molar flow rate of the fuel is. We have already fond the molar flow rate of the products (m/M_m) to be (0.1/28.03 =) 3.5676 mol/s. We also know that there are Σn_i (= 59.7278) kmols of product per kmol of fuel. The molar flowrate of the fuel is thus:

$3.5676x10^{-3}/59.7278 = 59.7x10^{-6}$ kmol_fuel/s

The fuel energy flux is therefore: $59.7x10^{-6} \text{ x } 5100.50x10^6 = 304.5$ kW
The kinetic energy of the exhaust thus represents (4.4/304.5) about 1.4% of the fuels calorific value.

3.24 The calibration of an air fuel ratio analyser is to be checked by using the following gas mixture, that represents the dry products of combustion from a hydrocarbon fuel:

Constituent	**Volume**
methane, CH_4	**550 ppm**
hydrogen, H_2	**3.23%**
carbon monoxide, CO	**6.20%**
carbon dioxide, CO_2	**12.29%**
nitrogen, N_2	**balance**

Calculate and comment on the values of:

a) the molar hydrogen/carbon ratio of the fuel,

b) the gravimetric air/fuel ratio (AFR) corresponding to these products,

c) the gravimetric, stoichiometric AFR and the equivalence ratio,

d) the water gas constant.

If a fuel of this composition was to be burnt in a spark ignition engine, sketch the response of the emissions (CO, CO_2, O_2, H_2, HC, H_2O, NOx) plotted on a wet basis to variation in the equivalence ratio. (HINT: It may be helpful to utilise the data from the first part of this question.)

a) Assume that the hydrocarbon (C_xH_y), reacts with z kmols of oxygen to produce 100 kmols of dry products of combustion, (there will of course be water present in the exhaust, so that our specified quantity of reactants produces more than 100 kmols of products).

The molar (or volumetric) composition of air can be assumed to be 21% oxygen and 79% nitrogen. Thus for every kmol of oxygen there are (79/21 =) 3.76 kmols of nitrogen. Our reaction is thus:

$$C_xH_y + z(O_2 + 3.76N_2) \rightarrow \text{100 kmols of dry products and water vapour}$$

First we need to find the number of kmols of nitrogen:

species	kmols
methane, CH_4	0.055
hydrogen, H_2	3.23
carbon monoxide, CO	6.20
carbon dioxide, CO_2	12.29
	====
TOTAL	21.78
nitrogen, N_2	78.22 to total 100 kmols

The combustion equation is thus:

$$C_xH_y + z(O_2 + 3.76N_2) \rightarrow 12.29CO_2 + 6.2CO + 3.23H_2 + 0.055CH_4 + 78.22N_2^* + wH_20$$

The four atomic balances are:

N balance $3.76 \text{ x } 2z = 2 \text{ x } 78.22, \ z = 20.793$ (A

C balance $x = 12.29 + 6.2 + 0.055 = 18.545$ (B

O balance $2z = 12.29 \text{ x } 2 + 6.2 + w = 30.78 + w$ (C

Substituting for the value of z from Eqn A:

$2 \text{ x } 20.793 = 30.78 + w, \quad w = 10.806$ (D

H balance $y = 2w + 2 \text{ x } 3.23 + 4 \text{ x } 0.055$ (E

Substituting for the value of w from Eqn D: $y = 28.292$ (F

The molar composition of the fuel is thus: $C_{18.545}H_{28.292}$. However, since the specification of 100 kmol of dry products was arbitrary, it might be better to represent the fuel as $C_xH_{28.292x/18.545}$ or $C_xH_{1.526x}$.

This slightly low H/C ratio would be typical of a fuel with a high level of aromatics, namely benzene - C_6H_6, toluene - $C_6H_5.CH_3$ and xylene - $C_6H_5.2(CH_3)$.

b)

To find the gravimetric air fuel ratio, we need to find the mass of fuel ($C_{18.545}H_{28.292}$), and the mass of air that this reacts with.

Mass of carbon :- $xM_C = 18.545 \text{ x } 12 = 222.54$

Mass of hydrogen :- $yM_{H2} = 28.292 \text{ x } 1 = 28.292$ Total Mass $= 250.83$ (G

There are 20.793 kmols of oxygen, so there are (20.793 x 4.76 =) 98.975 kmols of air. The molar mass of air is 29 kg/kmol, so we have (98.975 x 29 =) 2870.3 kg. Division by the mass of fuel (232.44 kg) gives us the air fuel ratio:

The **gravimetric AFR** = 2870.3/250.83 = **11.44** - as expected, a rich mixture.

c) The stoichiometric gravimetric air fuel ratio is found by determining the quantity of air required for stoichiometric combustion:

Define z_s as the quantity of oxygen required for stoichiometric combustion:

$$C_{18.545}H_{28.292} + z_s(O_2 + 3.76N_2) \rightarrow aCO_2 + bH_2O + cN_2$$

The atomic balances are:

C balance $18.545 = a$

H balance $28.292 = 2b$

Thus, $C_{18.545}H_{28.292} + z_s(O_2 + 3.76N_2) \rightarrow 18.545CO_2 + 14.146H_2O + cN_2$

(H

O balance $2z_s = 2 \text{ x } 18.545 + 14.146, \ z_s = 25.618$

The stoichiometric air/fuel ratio can be found from the mass of fuel (Eq G), and the mass of the stoichiometric quantity of air (z_s).

Mass of Air $z_s(O_2 + 3.76N_2)$ is: $z_s(M_{O2} + 3.76M_{N2}) = 25.618(32 + 3.76 \text{ x } 28.15) = 3531.3$ kg

AFR$_s$ = 3531.1/250.8 = **14.08**

The equivalence ratio is AFR$_s$/AFR = 14.08/11.44 = **1.23**

A quicker method would have been to have found the equivalence ratio from $z_s/z = 25.618/20.793 =$ **1.23**, which has been done here to provide a check.

d) The water gas constant = $(\%CO \text{ x } \%H_2O)/(\%CO_2 \text{ x } \%H_2) = (n_{CO} \text{ x } n_{H2O})/(n_{CO2} \text{ x } n_{H2})$

$$= (6.2 \text{ x } 10.806)/(12.29 \text{ x } 3.23) = 1.688$$

The equilibrium constant (K_p) for reaction number 7 (Table A.6) is the reciprocal of the water gas reaction, so:

$$\ln(K_p) = \ln(1/1.688) = -0.524$$

Inspection of Table A.6 indicates a temperature just below 1300 K. Usually the composition of the exhaust products is assumed to freeze close to 1800 K, with a water gas equilibrium constant of about 3.5.

We need to construct a table (see below), to show the data to be plotted. Starting with the data from the question, we can use this to represent the products of combustion from a rich mixture. We assumed 100 kmols of dry products of combustion (which excludes the 10.806 kmols of water vapour determined from Eq. D). There will thus be 110.806 kmols of wet products of combustion, and we divide by this to determine the wet percentages of the constituents.

For the stoichiometric condition we can utilise Eq. H:

$$C_{18.545}H_{28.292} + 25.618(O_2 + 3.76N_2) \rightarrow 18.545CO_2 + 14.146H_2O + cN_2$$

$$c = 25.618 \text{ x } 3.76 = 96.32$$

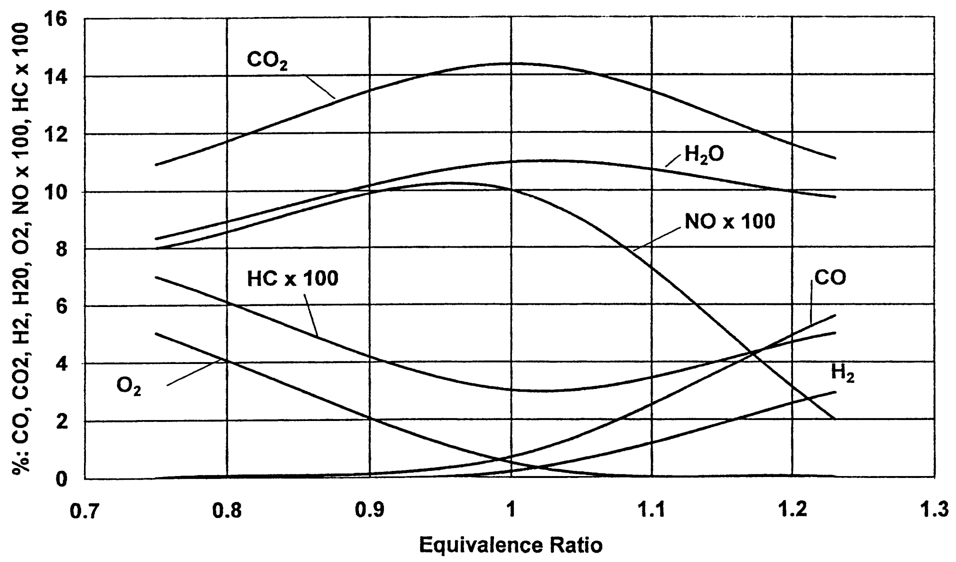
Finally, we need to consider a weak mixture, with say an equivalence ratio of 0.75, for which we will assume there is neither carbon monoxide or hydrogen in the exhaust. Thus:

$$C_{18.545}H_{28.292} + (25.618/0.75)(O_2 + 3.76N_2) \rightarrow 18.545CO_2 + 14.146H_2O + qO_2 + cN_2$$

N_2 balance: $(25.618/0.75) \text{ x } 3.76 = c = 128.43$

O_2 balance: $25.618/0.75 = 18.545 + \frac{1}{2} \text{ x } 14.146 + q$ $q = 8.54$

Species:	CO	CO_2	O_2	H_2	HC	H_2O	N_2	Σ
rich	6.20	12.29	0.0	3.23	0.055	10.806	78.23	110.806 kmols
ϕ = 1.23	5.60	11.09	0.0	2.92	0.050	9.75	70.60	100% wet basis
stoichiometric	-	18.55	-	-	-	14.15	96.32	129.02 kmols
ϕ = 1.00	-	14.37	-	-	-	10.97	74.66	100% wet basis
weak	-	18.55	8.54	-	-	14.15	128.43	169.67 kmols
ϕ = 0.75	-	10.93	5.03	-	-	8.34	75.69	100% wet basis



The emissions of NOx will all need to be estimated, as will the hydrocarbon emissions for the weak and stoichiometric mixtures. For the stoichiometric mixture, it is probably more reasonable to assume 1% CO and ½% O_2; the CO_2 has thus been reduced by 1% - the slight change that this makes to the total number of kmols has been ignored.

3.25 The results of a dry gas analysis of an engine exhaust are as follows:

Carbon dioxide, CO_2	**10.7 per cent**
Carbon monoxide, CO	**5.8 per cent**
Atmospheric nitrogen, N_2^*	**83.5 per cent**

Stating any assumptions, calculate:

(i) the gravimetric air/fuel ratio.
(ii) the gravimetric composition of the fuel
(iii) the stoichiometric gravimetric air fuel ratio.

The level of carbon monoxide suggests that this is a spark ignition engine. The quoted emissions add up to 98%, and with this level of carbon monoxide, the balance of 2% is probably hydrogen. There could be some oxygen in the exhaust, but there is no reference to any equilibria, or 'freezing' temperature for the exhaust gases.

Assume that the hydrocarbon (C_xH_y), reacts with z kmols of oxygen to produce 100 kmols of dry products of combustion, (there will of course be water present in the exhaust, so that our specified quantity of reactants produces more than 100 kmols of products).

The molar (or volumetric) composition of air can be assumed to be 21% oxygen and 79% nitrogen. Thus for every kmol of oxygen there are (79/21=) 3.76 kmols of nitrogen. Our reaction is thus:

$$C_xH_y + z(O_2 + 3.76N_2) \rightarrow 100 \text{ kmols of dry products and water vapour}$$

$$C_xH_y + z(O_2 + 3.76N_2) \rightarrow 10.7CO_2 + 5.8CO + 2H_2 + 81.5N_2^* + wH_20$$

The four atomic balances are:

N balance $3.76 \times 2z = 2 \times 81.5,$ $z = 21.68$ (A

C balance $x = 10.7 + 5.8 = 16.5$ (B

O balance $2z = 10.7 \times 2 + 5.8 + w = 27.2 + w$ (C

Substituting for the value of z from Eqn A:

$2 \times 21.68 = 27.2 + w,$ $w = 16.15$ (D

H balance $y = 2(w + 2)$ (E

Substituting for the value of w from Eqn D: $y = 36.30$ (F

The molar composition of the fuel is thus: $C_{16.5}H_{36.3}$.

i)

To find the gravimetric air fuel ratio, we need to find the mass of fuel ($C_{16.5}H_{36.3}$), and the mass of air that this reacts with.

Mass of carbon - $xM_C = 16.5 \times 12 = 198.0$

Mass of hydrogen - $yM_{H2} = 36.3 \times 1 = 36.3$ Total Mass = 234.3 (G

There are 21.68 kmols of oxygen, so there are (21.68 x 4.76 =) 103.2 kmols of air. The molar mass of air is 29 kg/kmol, so we have (103.2 x 29 =) 2992.7 kg. Division by the mass of fuel (234.3 kg) gives us the air fuel ratio:

The **gravimetric AFR** = 2992.7/234.3 = **12.77**

(ii) To find the gravimetric composition of the fuel, we need to rearrange equation G:

Mass fraction of carbon 198.0/234.3 = **0.845**

Mass fraction of hydrogen 36.3/234.3 = **0.155**

or (0.845/0.155 =) **5.45** kg_C per kg_H

(iii) The stoichiometric gravimetric air fuel ratio is found by determining the quantity of air required for stoichiometric combustion:

Define z_s as the quantity of oxygen required for stoichiometric combustion:

$$C_{16.5}H_{36.3} + z_s(O_2 + 3.76N_2) \rightarrow aCO_2 + bH_2O + cN_2$$

The <u>atomic</u> balances are:

C balance $16.5 = a$

H balance $36.3 = 2b$

Thus, $C_{16.5}H_{36.3} + z_s(O_2 + 3.76N_2) \rightarrow 16.5CO_2 + 18.15H_2O + cN_2$

O balance $2z_s = 2 \times 16.5 + 18.15, \qquad z_s = 25.575$

The stoichiometric air/fuel ratio can be found from the mass of fuel (Eq G), and the mass of the stoichiometric quantity of air (z_s).

Mass of Air $z_s(O_2 + 3.76N_2)$:- $z_s(M_{O2} + 3.76M_{N2}) = 25.575(32 + 3.76 \times 28.15) = 3525.36$

AFR$_s$ = 3525.36/234.3 = **15.05**

3.26 A mixture of propane (C_3H_8) and air are burnt in a constant pressure adiabatic system at a pressure of 1 bar. The composition of the exhaust gases includes:

3.87 kmols H_2O
0.13 kmols H_2
2.49 kmols CO_2
0.51 kmols CO
0.82 kmols O_2

Assuming that there is no nitric oxide present, and stating clearly any additional assumptions:

a) What is the equivalence ratio of the reactants,

b) What is the temperature of the products of combustion, and

c) What is the temperature of the reactants?

Assuming that nitrogen is the only other species present in the products, then the combustion equation can be written as:

$$yC_3H_8 + z(O_2 + 3.76)N_2 \rightarrow 3.87H_2O + 0.13H_2 + 2.49CO_2 + 0.51CO + 0.82O_2 + 3.76zN_2$$

We have already applied a nitrogen balance, and the carbon and hydrogen balances can be used to determine the quantity of propane reacted, and check on the likelihood of any other species being present:

C balance: $3y = 2.49 + 0.51 = 3$ $\quad y = 1$

H balance: $8y = 3.87 \times 2 + 0.13 \times 2 = 8$ $\quad y = 1$

With the exception of unburnt propane (which cannot be deduced form these hydrogen and carbon balance equations), there is not likely to be any other significant hydrogen or carbon containing species present.

The oxygen balance will enable us to determine the equivalence ratio:

O balance: $2z = 3.87 + 2.49 \times 2 + 0.51 + 2 \times 0.82 = 11.00$

The combustion equation is thus:

$$C_3H_8 + 5.5(O_2 + 3.76)N_2 \rightarrow 3.87H_2O + 0.13H_2 + 2.49CO_2 + 0.51CO + 0.82O_2 + 20.68N_2$$

For stoichiometric combustion:

$$C_3H_8 + z_s(O_2 + 3.76)N_2 \rightarrow 4H_2O + 3CO_2 + 3.76z_sN_2$$

$$z_s = 4/2 + 3 = 5.0$$

The equivalence ratio (ϕ) is given by: $\phi = z_s/z = 5.0/5.5 = \mathbf{0.91}$

b) The temperature of the products of combustion can be determined by assuming that the products are in equilibrium, and by considering either of the following two equilibria:

Reaction 6 $\quad -CO - \frac{1}{2}O_2 + CO_2 = 0$
Reaction 7 $\quad -CO - H_2O + CO_2 + H_2 = 0$

Using the equation numbers of the equilibrium data in Table A.6 in the Appendix:

For the generalised reaction: $\Sigma \nu i A i = 0$, ν_i is the stoichiometric coefficient of species A_i, and the equilibrium constant K_p is defined by:

$$\ln K_p = \Sigma \nu_i \ln p^*_i \qquad (6$$

where p^*_i is numerically equal to the partial pressure of substance A_i, with pressure units of bar.

$$p^*_i = Pn_i/\Sigma n_i$$

For Reaction 6:

$\ln K_p = - \ln(P^*_{CO}) - \frac{1}{2}\ln(P^*_{O2}) + \ln(P^*_{CO2})$ and:

$$\ln K_p = - \ln(n_{CO}) - \ln(P') - \frac{1}{2}\ln(n_{O2}) - \frac{1}{2}\ln(P') + \ln(n_{CO2}) + \ln(P')$$

$$\ln K_p = - \ln(n_{CO}) - \frac{1}{2}\ln(n_{O2}) + \ln(n_{CO2}) - \frac{1}{2}\ln(P')$$

Where $P' = P/\Sigma n_i = 1/(3.87 + 0.13 + 2.49 + 0.51 + 0.82 + 20.68) = 0.0351$ bar

$\ln K_p = -\ln(0.51) - ½\ln(0.82) + \ln(2.49) - ½\ln(0.0351) = 3.360$

Inspection of Table A.6 for Reaction 6, indicates a temperature between 2400 and 2500 K.

T (K):	2400	2500
$\ln K_p$:	3.858	3.306

And by linear interpolation:

$$T = 2400 + 100 \text{ x } (3.360 - 3.858)/(3.306 - 3.858) = 2490 \text{ K}$$

Alternatively, for Reaction 7: $-CO - H_2O + CO_2 + H_2 = 0$

$\ln K_p = -\ln(P^*_{CO}) - \ln(P^*_{H2O}) + \ln(P^*_{CO2}) + \ln(P^*_{H2})$ and:

$$\ln K_p = -\ln(n_{CO}) - \ln(P') - \ln(n_{H2O}) - \ln(P') + \ln(n_{CO2}) + \ln(P') + \ln(n_{H2}) + \ln(P')$$

$$\ln K_p = -\ln(n_{CO}) - \ln(n_{H2O}) + \ln(n_{CO2}) + \ln(n_{H2})$$

$$\ln K_p = -\ln(0.51) - \ln(3.87) + \ln(2.49) + \ln(0.13) = -1.808$$

Inspection of Table A.6 for Reaction 7 indicates a temperature between 2500 and 2600 K.

T (K):	2500	2600
$\ln K_p$:	-1.805	-1.847

And by linear interpolation:

$$T = 2500 + 100(-1.808 - [-1.805])/(-1.847 - [-1.805]) = 2507 \text{ K}$$

This is likely to be less accurate than from the consideration of Reaction 6, because of the low resolution with the measurement of the hydrogen (0.13 kmols). None the less, an average of the two equilibrium combustion temperatures will be used, to give:

Combustion Temperature 2499 K

c) The temperature of the reactants can be found by evaluating the enthalpy of the products of combustion, and then finding what temperature the reactants have to be at fro the same enthalpy.

We thus have to start by determining the enthalpy of the products of combustion. Using Table A.4, and evaluating the enthalpy at 2500 K (since this rounding introduces a negligible error compared with the uncertainty in the combustion temperature) gives:

i	n_i	H_i	n_iH_i
CO	0.51	-35.504	-18.107
CO_2	2.49	-271.587	-676.252
H_2O	3.87	-142.883	-552.957
H_2	0.13	70.474	9.162
O_2	0.82	78.381	64.272
N_2	20.69	74.308	1537.433
			========
		$H_P = \Sigma n_iH_i =$	363.551 MJ/kmol_C_3H_8

We now have to estimate the temperature of the reactants ($C_3H_8 + 5.5O_2 + 20.69N_2$). The nitrogen and oxygen can be represented as (5.5 + 20.69 =) 26.19 kmols of air, and for the first guess we can ignore the fuel.

The molar enthalpy of the air is approximately: 359.451/26.19 = 13.7 MJ/kmol. This is closest to the value at 800K (15.164 MJ/kmol_air), and ignoring the fuel will have led to an underestimate of the temperature. The next step is to calculate the enthalpy of the reactants at 800K, and then at either 700 K or 900 K in the light of the evaluation at 800K. The fuel data comes from Table A.5:

800K: i	n_i	H_i	n_iH_i
C_3H_8	1	-44.836	-44.836
O_2	5.5	15.837	87.104
N_2	20.69	15.042	311.219
			========
		$H_R = \Sigma n_iH_i =$	353.487 MJ/kmol_C_3H_8

The enthalpy of the reactants (353.487 MJ/kmol_C_3H_8) is slightly lower than the enthalpy of the products (359.451 MJ/kmol_C_3H_8), so the temperature of the reactants is too low, and we will need to find the enthalpy of the reactants at 900 K:

900 K: i	n_i	H_i	n_iH_i
C_3H_8	1	-28.713	-28.713
O_2	5.5	19.244	105.842
N_2	20.69	18.219	376.951
			========
		$H_R = \Sigma n_iH_i =$	454.080 MJ/kmol_C_3H_8

And by linear interpolation:

$$T = 800 + 100(363.551 - 353.487)/(454.080 - 353.487) = 810 \text{ K}$$

The estimate of the reactant temperature is thus **810 K**

DISCUSSION

The question was in fact constructed the opposite way round, starting with reactants at a temperature of 800K, and STANJAN predicting a temperature of 2490.7 K, and the composition quoted in this question. Allowing for rounding errors, and the sensitivity of the equilibrium combustion equations to the few significant figures quoted in the question, then the result is very reasonable. Especially compared with the temperature when additional species (NO and OH) are considered which falls to 2441 K.

Species Temperature (K):	kmols 2491	 2441
H_2O	3.87	3.76
H_2	0.13	0.11
CO_2	2.49	2.54
CO	0.51	0.46
O_2	0.82	0.62
NO	-	0.19
OH	-	0.22

The additional 2 dissociation reactions lead to a 50 K lower temperature, which in turn leads to a lower level of carbon dioxide dissociation. The equilibrium levels of: oxygen, carbon monoxide and hydrogen are lower. The inclusion of the hydroxyl radical lowers the water vapour level, and the inclusion of nitric oxide lowers the nitrogen level.

3.27 **An adiabatic constant volume combustion chamber is filled with a mixture of air and methane; lambda (AFR/AFRs) of 1.3. The initial temperature of the mixture is 25°C, and its pressure is 1 bar. After laminar combustion from a single ignition source (and ignoring dissociation) the pressure would rise to 7.27 bar. Any heat transfer within the gas may also be ignored. Assuming the following values of the ratio of heat capacities:**

unburnt gas 1.377 burnt gas 1.237

Calculate:

a) the temperature of the gas to burn first, immediately after the start of combustion,
b) the temperature of the gas to burn first, after the end of combustion,
c) the temperature of the gas to burn last, immediately before the end of combustion, and
d) the temperature of the gas to burn last, after the end of combustion.

Comment on whether dissociation is likely to be significant, and how it might affect the final pressure, the first burnt gas temperatures immediately after the start and end of combustion, and the last burnt gas temperature immediately after the end of combustion.

The equation for the stoichiometric combustion of methane in teh absence of dissociation is:

$$CH_4 + 2O_2 + 7.52N_2 \rightarrow CO_2 + 2H_2O + 7.52N_2$$

With a lambda of 1.3, the combustion equation is:

$$CH_4 + 1.3(2O_2 + 7.52N_2) \rightarrow CO_2 + 2H_2O + (1.3 - 1)2O_2 + 1.3 \times 7.52N_2$$

$$\rightarrow CO_2 + 2H_2O + 0.6O_2 + 9.78N_2$$

a) The temperature of the first burnt gas is found by considering isenthalpic combustion, since the first burnt gas makes a negligible change to the system pressure.

The enthalpy of the reactants at the initial temperature of 25°C is solely that of the methane (since the other species are in their standard state).

From Table A.6 H_R = -74.52 MJ/kmol_methane

Since we know the composition of the products we can find the enthalpy of the mixture at an estimated temperature, and then compare this with the enthalpy of the reactants, until the energy balance is satisfied.

Using 2000 K as the first guess, the enthalpy of the products is: $H_P = \Sigma n_i H_i$

species	n_i	$H_{i,2000}$	$n_i H_{i,2000}$	$H_{i,1900}$	$n_i H_{i,1900}$
CO_2	1.0	-302.128	-302.128	-308.158	-308.158
H_2O	2.0	-169.146	-338.292	-174.215	-348.430
O_2	0.6	59.171	35.503	55.399	33.239
N_2	9.78	56.114	548.794	52.522	513.665
			++++		++++
		$\Sigma n_i H_i$ =	-56.122		-109.684

At 2000 K the enthalpy of the products is greater than that of the reactants (it is less negative), so we need a slightly lower estimate, say 1900 K. This has been included in the above table.

Linear interpolation gives: $T = 1900 + 100(109.684 - 74.52)/(109.684 - 56.122) = 1966$ K

The temperature of the gas to burn first, immediately after the start of combustion is 1966 K

b) The temperature of the gas to burn first, after the end of combustion ($T_{b,f,e}$), is found by compressing the first burnt gas ($T_{b,f,i}$) isentropically:

$$T_{b,f,e} = T_{b,f,i}\,(P_e/P_i)^{(\gamma - 1)/\gamma} = 1966 \times 7.27^{(1.237 - 1)/1.237} = 2875 \text{ K}$$

The temperature of the gas to burn first, immediately after the end of combustion is 2923 K

c) The temperature of the gas to burn last, immediately before the end of combustion ($T_{l,u,e}$), is found by compressing the unburnt gas (25°C) isentropically:

$$T_{l,u,e} = T_o\,(P_e/P_i)^{(\gamma - 1)/\gamma} = 298 \times 7.27^{(1.377 - 1)/1.377} = 513 \text{ K}$$

The temperature of the gas to burn last, immediately before the end of combustion is 513 K.

d) The temperature of the gas to burn last, after the end of combustion is found by considering the isenthalpic combustion of mixture at an initial temperature of 513 K, since the last infinitesimal amount of mixture burnt will occur at constant pressure.

The enthalpy of the reactants at the initial temperature of 513 K is found by interpolation of data from Tables A.4 and A.5.

species	n_i	$H_{i,500}$	$H_{i,600}$	$\mathrm{H}_{i,513}$	$n_iH_{i,513}$
CH_4	1.0	-66.197	-61.231	-65.551	-65.551
O_2	2.6	6.089	9.247	6.500	16.90
N_2	9.78	5.909	8.893	6.297	61.584
					++++
			H_R =	Σn_iH_i =	12.933

Since we know the composition of the products we can find the enthalpy of the mixture at an estimated temperature, and then compare this with the enthalpy of the reactants, until the energy balance is satisfied. Using 2200 K as the first guess, the enthalpy of the products is: $H_P = \Sigma n_iH_i$

species	n_i	$H_{i,2200}$	$n_iH_{i,2200}$	$\mathrm{H}_{i,2100}$	$n_iH_{i,1900}$
CO_2	1.0	-289.981	-289.981	-296.068	-296.068
H_2O	2.0	-158.810	-317.620	-164.009	-328.018
O_2	0.6	66.787	40.072	62.967	37.780
N_2	9.78	63.351	619.573	59.725	584.111
			++++		++++
		Σn_iH_i =	52.044		-2.196

At 2200 K the enthalpy of the products is greater than that of the reactants, so we need a slightly lower estimate, say 2100 K. This has been included in the previous table.

Linear interpolation gives: $T = 2100 + 100(12.933 + 2.196)/(52.044 + 2.196) = 2128$ K

The temperature of the gas to burn last, immediately after combustion is 2128 K

Discussion

The effect of dissociation will be to lower the temperature, and thus the pressure. The first burnt gas temperature will be slightly lower immediately after combustion ($T_{f,b,i}$) because of dissociation. But the first burnt gas temperature will be significantly lower after the end ($T_{f,b,e}$) of combustion because:

a) dissociation will be more significant at this higher temperature, and
b) the final pressure will be lower, so the isentropic temperature ratio will be lower.

The temperature of the gas to burn last, immediately before the end of combustion ($T_{l,u,i}$) will be slightly lower (because of the lower pressure ratio and isentropic temperature ratio). The temperature of the gas to burn last, after the end of combustion ($T_{l,b,e}$) will be reduced more because of the effects of dissociation. The final temperature difference between the first and last burnt gas will be reduced, because the temperature of the first burnt gas will be lowered more by dissociation.

This question was constructed with the aid of a multizone combustion model, using 25 zones of equal mass, and this model can also be used to quantify the effects of dissociation (see the tabulation below). STANJAN can be used to check these results, but only by using the multizone model prediction of the pressure rise. This is because STANJAN would treat the problem as a single zone, and thus predict a higher pressure rise (this value is shown in the tabulation below in brackets).

	Multi-Zone Model		Single Zone Model
	No Dissociation	With Dissociation	STANJAN (with dissociation)
$T_{f,b,i}$ (K)	1965	1948	1949
$T_{f,b,e}$ (K)	2875	2657	2690
$T_{l,u,i}$ (K)	513	510	510
$T_{l,b,e}$ (K)	2133	2105	2103
P_e (bar)	7.27	7.06	(7.97)

	Composition (%)					
	N_2	O_2	H_2	CO_2	H_2O	CO
f,b,i	72.89	4.32	0.14	7.44	14.86	0.30
f,b,e	71.48	4.07	0.36	6.29	13.74	1.09
l,b,e	72.80	4.23	0.17	7.43	14.84	0.40
No Dissociation	73.09	4.49	0.00	7.48	14.95	0.00

3.28 The Rice and Herzfeld mechanisms for thermal decomposition of hydrocarbons (in which R refers to any radical and M any molecule) are:

(1) dissociation	$M_1 \rightarrow R_1 + R_1'$	k_1
(2) propagation	$R_1 + M_1 \rightarrow R_1H + R_2$	k_2
(3) dissociation	$R_2 \rightarrow R_1 + M_2$	k_3
(4) termination	$R_1 + R_2 \rightarrow M_3$	k_4
(5) termination	$2R_1 \rightarrow M_4$	k_5
(6) termination	$2R_2 \rightarrow M_5$	k_6

where only one of the three termination or chain-termination steps (4), (5), and (6) would be expected to be important in a given reaction.

a) **If reaction (5) is the chain termination reaction, then shown that the overall rate of decomposition of M_1 is to the power of three-halves:**

$$-\frac{d\,[M_1]}{dt} \approx k_2 \left(\frac{k_1}{2k_5}\right)^{\frac{1}{2}} [M_1]^{\frac{3}{2}}$$

b) **If reaction (6) is the chain termination reaction, then shown that the overall rate of decomposition of M_1 is to the power of a half:**

$$-\frac{d\,[M_1]}{dt} \approx k_3 \sqrt{\frac{k_2}{2k_6}}\,[M_1]^{\frac{1}{2}}$$

a) When reaction (5) is the chain termination reaction:

$$\frac{d\,[R_1]}{dt} = k_1[M_1] - k_2\,[R_1]\,[M_1] + k_3\,[R_2] - 2k_5\,[R_1]^2 = 0 \qquad \text{(A}$$

$$\frac{d\,[R_2]}{dt} = k_2\,[R_1]\,[M_1] - k_3\,[R_2] = 0 \qquad \text{(B}$$

re-arranging equation B gives:

$$k_3\,[R_2] = k_2\,[R_1]\,[M_1] \qquad \text{(C}$$

and this can be substituted into equation A:

$$k_1[M_1] - k_2\,[R_1]\,[M_1] + k_2\,[R_1]\,[M_1] - 2k_5\,[R_1]^2 = 0$$

or

The overall rate for the decomposition of M_1 is given by:

$$\left[R_1\right] = \left(\frac{k_1}{2k_5}\left[M_1\right]\right)^{\frac{1}{2}} \qquad \text{(D}$$

$$-\frac{d\left[M_1\right]}{dt} \approx k_1\left[M_1\right] + k_2\left[R_1\right]\left[M_1\right] \qquad \text{(E}$$

Substituting for $[R_1]$ from equation D gives

$$-\frac{d\left[M_1\right]}{dt} \approx k_1\left[M_1\right] + k_2\left(\frac{k_1}{2k_5}\right)^{\frac{1}{2}}\left[M_1\right]^{\frac{3}{2}} \qquad \text{(F}$$

Remembering that k_1 is small in comparison to k_2 and k_5 (since this reaction depends on the rupture of a C-C bond), then equation F can be further approximated as:

$$-\frac{d\left[M_1\right]}{dt} \approx k_2\left(\frac{k_1}{2k_5}\right)^{1/2}\left[M_1\right]^{3/2} \qquad \text{(G}$$

b) When reaction (6) is the chain termination reaction:

$$\frac{d\left[R_1\right]}{dt} = k_1\left[M_1\right] - k_2\left[R_1\right]\left[M_1\right] + k_3\left[R_2\right] = 0 \qquad \text{(A}$$

$$\frac{d\left[R_2\right]}{dt} = k_2\left[R_1\right]\left[M_1\right] - k_3\left[R_2\right] - 2k_6\left[R_2\right]^2 = 0 \qquad \text{(B}$$

Re-arranging equation A gives:

$$k_3\left[R_2\right] = k_2\left[M_1\right]\left[R_1\right] - k_1\left[M_1\right] \qquad \text{(C}$$

Equation C can be used to eliminate $\left[R_2\right]$ from equation B:

$$k_2\left[R_1\right]\left[M_1\right] - k_2\left[M_1\right]\left[R_1\right] + k_1 M_1 - \frac{2k_6}{k_3^2}\left(k_2\left[R_1\right] - k_1\right)^2\left[M_1\right]^2 = 0 \qquad \text{(D}$$

Multiplying through by $\left[k_3\right]^2 \,/\, 2k_5\left[M_1\right]$ and expanding, gives:

$$\frac{k_3^2\, k_1}{2k_6} - \left(k_2^2\, [R_1]^2 + k_1^2 - 2\, k_1 k_2\, [R_1]\right) [M_1] = 0$$

or

$$[M_1]\, k_2^2\, [R_1]^2 - 2k_1 k_2\, [M_1]\, [R_1] + \left(k_1^2\, [M_1] - \frac{k_3^2\, k_1}{2k_6}\right) = 0 \qquad \text{(E}$$

The solutions to this quadratic equation are:

$$[R_1] = \frac{2\, k_1 k_2 [M_1]}{2\, [M_1]\, k_2^2} \pm \sqrt{\frac{4k_1^2 k_2^2\, [M_1]^2}{4[M_1]^2\, k_2^4} + \frac{k_3^2\, k_1 - 2k_6 k_1^2\, [M_1]}{2k_6\, [M_1]\, k_2^2}} \qquad \text{(F}$$

or

$$[R_1] = \frac{k_1}{k_2} \pm \sqrt{\frac{k_1^2}{k_2^2} + \frac{k_3^2 k_1}{2k_6 k_2^2\, [M_1]} - \frac{k_1^2}{k_2^2}} \qquad \text{(G}$$

Since only the positive solution is valid:

$$[R_1] = \frac{k_1}{k_2} + \frac{k_3}{k_2}\sqrt{\frac{k_1}{2k_6\, [M_1]}} \qquad \text{(H}$$

As argued before, k_1 is small compared to k_2 , so:

$$[R_1] \approx \frac{k_3}{k_2}\sqrt{\frac{k_2}{2k_6\, [M_1]}} \qquad \text{(I}$$

The overall rate for the decomposition of $[M_1]$ is:

$$-\frac{d\,[M_1]}{dt} = k_1\, [M_1] + k_2\, [R_1]\, [M_1] \qquad \text{(J}$$

Substitution of $[R_1]$ from equation I gives:

$$-\frac{d\,[M_1]}{dt} = k_1\,[M_1] + k_2\,\frac{k_3}{k_2}\sqrt{\frac{k_2}{2k_6\,[M_1]}}\;[M_1] \qquad \text{(K}$$

Since k_1 is small:

$$-\frac{d\,[M_1]}{dt} \approx k_3\sqrt{\frac{k_2}{2k_6}}\;[M_1]^{\frac{1}{2}} \qquad \text{(L}$$

4 Spark Ignition Engines

4.1* Why does the optimum ignition timing change with engine-operating conditions. What are the advantages of electronic ignition with an electronic control system.

First we need to describe the characteristics of spark ignition engine combustion, an then we can remind ourselves of what the optimum ignition timing is. The flame kernel is created as a result of energy from the spark initiating chain reactions that lead to self-sustaining combustion. The initial size of the flame kernel will be little larger than the spark plug gap, so it will be of the order 1 mm in diameter. The spark will have created radicals that are important in the propagation of combustion, and it will have raised the temperature in the spark channel to 1000s of Kelvin. This initial flame kernel (say 1mm in diameter) is very small compared to the turbulent length scales (which might be typically an order of magnitude larger). Thus the initial growth of the flame front will be determined by the laminar burning velocity. The transition to fully turbulent combustion will not be complete until about 10% of the fuel has been burnt; this period is also known as the early burn period or (less correctly) the ignition delay period since there will be negligible pressure rise due to combustion. The main part of combustion (say when 10-90% of the fuel is burnt), is dominated by turbulence so is often called the turbulent combustion phase. The final burn phase (90-100% burn) is much slower, since by now the flame front area will be progressively reducing because of contact with the combustion chamber surfaces. Combustion in the final burn period is also affected by the desorption of fuel from the oil films and crevices.

In the present question, we will take optimum ignition timing to be the MBT (Minimum ignition advance for Best Torque) value. Under some circumstances MBT ignition timing would not be used, for example to avoid ***knock***, or to reduce ***nitric oxide*** (or NOx) emissions. If we had adiabatic and instantaneous combustion, then the optimum ignition timing would be at top dead centre (tdc). However, as we have described above, combustion occupies a finite period. Figure 4.a shows the trade-offs between igniting the mixture too early or too late:

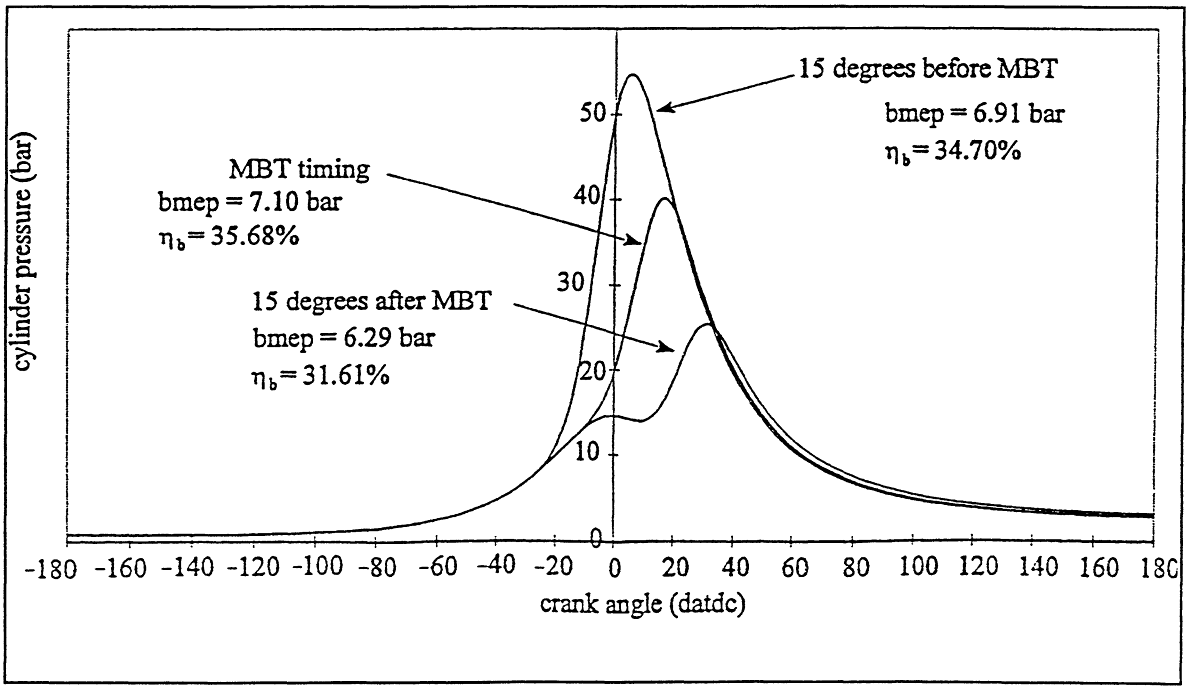


Figure 4.a The effect of ignition timing on the pressure history

i) ignite too early and the increased pressure rise before tdc leads to a greater increase in compression work than the increase in expansion work, whilst

ii) ignite too late and the reduced pressure rise after tdc leads to a greater reduction in expansion work than the decrease in compression work.

In many cases the dependence of either the efficiency or output on the ignition timing has a broad maxima, as shown in Figure 4.b. The MBT ignition timing is selected on the basis of minimum advance, since this reduces the peak pressures in the cylinder, and will minimise the risk of knock.

We are now in a position to answer the question, since we can discuss the effect of the engine operating conditions on each phase of combustion. We will consider the effects of: a) air fuel ratio, b) load, and c) speed.

a) The fastest burning velocities occur with air fuel ratios that are about 10% rich of stoichiometric; these being the mixtures that give the highest flame temperatures. Thus when the air fuel ratio is either richened or weakened from this value, then the ignition timing will have to be advanced if the MBT value is to be maintained.

b) As the load on the engine is reduced (at constant speed) the throttle will be closed, and the in-cylinder pressures will be reduced, and during the gas exchange processes the reduced inlet manifold pressure will lead to higher levels of exhaust residuals in the cylinder. The lower cylinder pressure will tend to increase the burning velocities, but this is outweighed by: the presence of the residuals, and the lower in-cylinder temperatures, both tending to reduce the burning velocity. The overall result, is thus a need to advance the ignition timing as the load is reduced.

c) When the engine speed is increased the turbulence intensity increases almost linearly with speed. Thus to a first approximation the main burn period occupies an almost constant crank angle period. However, the early burn crank angle period will increase, since the early stages of combustion are dominated by the laminar burning velocity which will be unaffected by the turbulence. Thus, as the

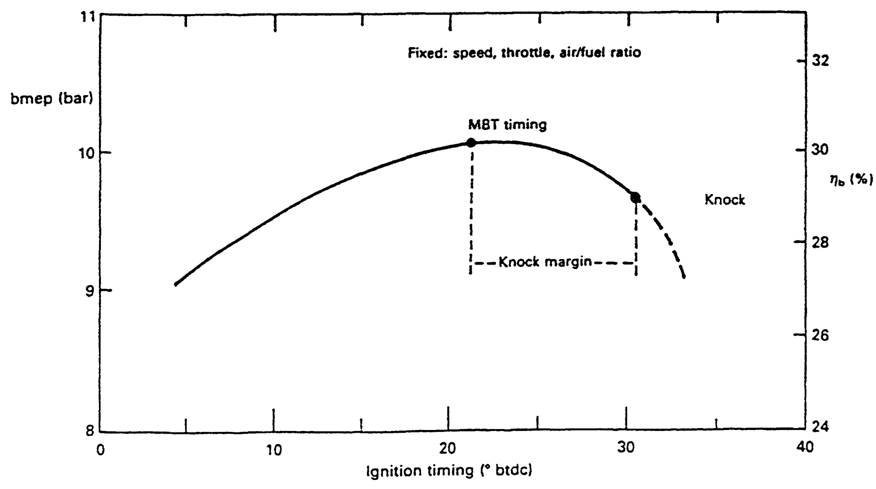


Figure 4.b The effect of ignition timing on the engine performance

engine speed is increased, the MBT ignition timing becomes more advanced.

Electronic Ignition and Control

Electronic ignition has a cost penalty, but the following advantages:

1) Elimination of the contact breaker which is subject to wear, and thus detrimental changes in the ignition timing and the coil on period (referred to as the dwell time or dwell angle).

2) The energy stored in the coil (E_s) is given by Eq. 4.11

$$E_s = 0.5\, L_1 I^2_p \qquad (4.3$$

Where: L_1 is the primary inductance of the coil, and
I_p is the current flowing in the coil when the primary circuit is opened

The rate at which the current rises in the primary (or LT) winding is given by Eq. 4.9:

$$I = \frac{V_s}{R}\,[1 - \exp\frac{Rt}{L_1}] \qquad (4.9$$

The energy stored in the coil is thus controlled by I_p, and an electronic ignition system is able to control this by means of regulating the voltage applied to the base of the switching transistor. In a contact breaker based ignition system I_p is determined by the battery voltage (which might be low) and the coil resistance. Eq. 4.9 shows that the coil resistance (R) also limits the rate at which the current in the coil grows. Thus an electronic ignition system can operate with a lower resistance coil, so a to always ensure that the chosen value of I_p is attainable in the available time. It is also possible to control the instant that the coil is switched on, so that I_p is attained at the exact time the coil primary circuit is to be opened - this reduces the resistive losses (RI^2) in the coil.

The use of lower resistance coils is particularly important for multi-cylinder engines (especially 8 cylinders and above) operating at high speeds, for which there is a very short interval between successive cylinders firing.

Electronic ignition timing control has the advantage of more accurate and comprehensive control. A conventional contact breaker ignition system, can only respond to engine speed and manifold pressure (this being a proxy for the torque or load); see Fig 4.35. These responses are invariably linear and can only be added, that is to say, that at a particular speed the speed determined ignition advance is independent of the load, and *vice versa*. In contrast an engine management system (see Fig 4.36) can provide ignition timing control that has speed, load, air fuel ratio, coolant temperature etc as independent variables. Additional features can be provided, such as ignition cut-off above a certain speed (to prevent over-speeding of the engine), and automatic switching-off of the ignition if the engine is stationary (so as to prevent overheating of the coil).

4.2* Explain the principal differences between fixed jet and variable jet carburettors. Why does the mixture strength become richer with increasing flowrate in a simple carburettor?

By answering the second part of this question first, it will make it easier to understand the design requirements of the fixed jet and variable jet carburettors.

In a simple fixed jet carburettor there is a venturi (the reduction in flow area) that causes an increase in the velocity of the air, and thus a reduction in the static pressure. The float chamber provides a constant level of fuel, and if the simplest case this might coincide with the level of the fuel exit into the venturi. If both flows were incompressible, steady and frictionless, then we would be able to apply Bernoulli's equation (in our case, for a fixed value of height):

$$p_o = p + \tfrac{1}{2}\rho v^2$$

where: p_o is the ambient pressure
p is the static pressure where the velocity is v, and
ρ is the density of the fluid.

Emphasising that we are considering both flows to be incompressible, then we can say that the mass flowrate of each (m_a for air, m_f for fuel) will be proportional to the local velocity. Thus for the air flow:

pressure drop in the venturi ($\Delta p = p_o - p$) $\propto v_a^2 \propto m_a^2$

For the fuel flow:

$m_f \propto v \propto \surd$[pressure drop in the fuel system ($\Delta p = p_o - p$)], or

$m_f^2 \propto v_f^2 \propto \Delta p$

Thus combining the results of applying Bernoulli's equation to both the air and fuel flows gives:

$m_f^2 \propto v_f^2 \propto \Delta p \propto v_a^2 \propto m_a^2$ or, $m_f \propto m_a$

Thus this simple incompressible model tells us that the air fuel ratio would remain constant. However, air is of course compressible, so that as the pressure reduces, then the density also reduces. The engine will require a certain mass flow rate of air, so if the density of the air is less in the venturi, then there will be a higher air velocity than was predicted by our simple incompressible model. The fuel is incompressible for these small changes in pressure, so the larger pressure drop will cause a higher fuel flow rate, so the air fuel ratio will be richer than predicted by our simple incompressible model. There is infact a self-feeding effect so that the faster the air flow, the larger the pressure drop, the greater the reduction in the density (and for our specified mass flow rate of air) the higher the necessary velocity and the larger the pressure drop and so on. Thus the air fuel ratio will richen at an increasing rate as the air mass flow rate is increased. (In the limiting case the velocity would equal the speed of sound in the venturi, and this places a limit on the possible air flow rate. However, in the case of a carburettor, the maximum air velocity would never be this high, since there would be unacceptably high frictional pressure drops.)

A fixed jet carburettor will thus have to be designed so that as the air flowrate increases, there is a means to prevent the air fuel ratio richening. This is achieved by having parallel paths for the fuel flow. There is a main jet, which behaves like a simple fixed jet carburettor, and a compensating jet which provides a decreasing fuel flow as the air flow increases. The compensating jet works by using an air bleed into the emulsion tube shown in Figure 4.43.

At very low air flow rates the fuel level surrounding the emulsion tube would be the same as in the float chamber, as the air flow is increased, two things happen:

1) Air will flow through the air bleed orifice and through the emulsion tube, so that mixture of air and fuel flows into the venturi. This air flow also means that

2) The pressure difference across the compensating jet will be reduced (as the air bleed will make the pressure surrounding the emulsion tube lie between atmospheric pressure and the venturi pressure), and

there will be a reduced fuel flow.

There is thus a weakening of the air fuel ratio, and by selecting the size and disposition of the holes in the emulsion tube, it is possible to achieve the desired variation of fuel flow through the compensating jet. The way the main jet flows and secondary flows combine is illustrated in Fig 4.44.

The variable jet carburettor (such as Fig 4.40) incorporates a device that responds to the air flow rate through the carburettor. As the air flow is increased, then the area of the fuel jet (the jet is the orifice through which the fuel flows) is increased, so as to maintain the intended air fuel ratio. In the case of Figure 4.40 the piston responds to the downstream pressure, and rises as the air flow rate increases so as to maintain a constant pressure drop in the region of the fuel jet. The tapered needle rises in the fuel jet, thereby increasing the orifice area, so that as the air flow increases, then the fuel flow will also increase.

4.3* What are the air/fuel requirements for a spark ignition engine at different operating conditions? How are these needs met by a fixed jet carburettor?

(This question was formulated with carburetted engines in mind, but passing reference will be made to engines equipped with catalysts).

Non-Catalyst equipped spark ignition engines require:

1) A mixture up to about 10% rich of stoichiometric at full throttle, in order to obtain the maximum bmep

2) A mixture weak of stoichiometric at part load so as to give the maximum efficiency, until at very light loads

3) the mixture has to be richened so as to compensate for the high levels of exhaust gas residuals left in the cylinder after the exhaust stroke

At full throttle, the maximum economy will occur with mixtures that are about 10% weak of stoichiometric. However, as the load required is reduced further the maximum economy will occur with somewhat weaker mixtures. At a fixed load and speed the frictional losses are essentially constant, so that by further weakening of the mixture the efficiency is improved for two reasons:

a) the throttle is more open, so the inlet manifold pressure will be higher, and the pumping work will be reduced, and secondly

b) the weaker the air fuel ratio, the closer the behaviour of the reactants and products to air, so the higher the fuel-air cycle efficiency.

There will be a limit, since as the mixture is weakened the combustion stability will deteriorate (especially at lower loads when there are more residuals present), so that the increase in hydrocarbon missions and the cycle-by-cycle variations in combustion overwhelm any efficiency gains.

Catalyst equipped engines that are intended to run at stoichiometric often operate with rich mixtures at full throttle and high speed (if the legislation does not preclude this), since this leads to lower exhaust and catalyst temperatures. Also, following a cold start different strategies are used so as to minimise the engine-out emissions, and or accelerate the catalyst warm-up.

A fixed jet carburettor (Figure 4.47) requires a number of systems to provide the necessary air fuel ratio variation. A more detailed discussion of the main jet performance can be found in the answer to the previous question, but the main details will be repeated here.

A simple incompressible model tells us that the air fuel ratio would remain constant. As the air flow increases the pressure drop is proportional to the square of the flow rate, and a similar relation governs the fuel flow.

However, air is of course compressible, so that as the pressure reduces, then the density also reduces. The engine will require a certain mass flow rate of air, so if the density of the air is less in the venturi, then there will be a higher air velocity than was predicted by our simple incompressible model. The fuel is incompressible for these small changes in pressure, so the larger pressure drop will cause a higher fuel flow rate, so the air fuel ratio will be richer than predicted by our simple incompressible model. There is infact a self-feeding effect so that the faster the air flow, the larger the pressure drop, the greater the reduction in the density (and for our specified mass flow rate of air) the higher the necessary velocity and the larger the pressure drop and so on. Thus the air fuel ratio will richen at an increasing rate as the air mass flow rate is increased. (In the limiting case the velocity would equal the speed of sound in the venturi, and this places a limit on the possible air flow rate. However, in the case of a carburettor, the maximum air velocity would never be this high, since there would be unacceptably high frictional pressure drops.)

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At very low air flow rates the fuel level surrounding the emulsion tube would be the same as in the float chamber, as the air flow is increased, two things happen:

1) Air will flow through the air bleed orifice and through the emulsion tube, so that mixture of air and fuel flows into the venturi. This air flow also means that

2) The pressure difference across the compensating jet will be reduced (as the air bleed will make the pressure surrounding the emulsion tube lie between atmospheric pressure and the venturi pressure), and there will be a reduced fuel flow.

There is thus a weakening of the air fuel ratio, and by selecting the size and disposition of the holes in the emulsion tube, it is possible to achieve the desired variation of fuel flow through the compensating jet. The way the main jet flows and secondary flows combine is illustrated in Fig 4.44.

This leaves two requirements, firstly to richen the mixture at full throttle, and secondly to enrich the mixture at very low load conditions (and compensate for the fuel exit in the venturi being above the liquid level in the float chamber).

1) The mixture is richened at full load, by making the mixture richer than needed at all operating points, and using a spring loaded valve that admits air at all conditions other than wide open throttle.

2) At low air flowrates the pressure drop across the venturi is very small, so instead the pressure drop is generated across the throttle plat is employed. Figure 4.45 shows a progression of holes in the region of the throttle plate, which it can be seen will only have any influence when the throttle plate is almost closed.

4.4* List the advantages and disadvantages of electronic fuel injection.

Electronic fuel injection is interpreted here as referring to both single point injection and multi-point injection, but not direct injection of any form.

The over-riding advantage of electronic fuel injection is its ability to satisfy emissions legislation, since air/fuel ratio can now be controlled. In steady-state operation a lambda sensor in the exhaust system can be used to maintain stoichiometric or any other desired air/fuel ratio. In the case of engines fitted with 3-way catalyst systems, then the air fuel ratio has to be kept within 1% of stoichiometric, or otherwise the catalyst efficiency falls.

During load change transients, the engine speed, inlet manifold pressure, and throttle position can be monitored by the electronic control unit (ECU), and control strategies can be developed that minimise excursions from the target air/fuel ratio. These excursions occur because of changes in the extent of the liquid fuel film in the inlet manifold. When the throttle is closed, the fall in the inlet manifold pressure causes part of the liquid fuel film to evaporate, and this leads to a rich air/fuel ratio excursion. When the throttle is opened, the pressure in the inlet manifold rises, and this causes fuel that has already been vaporised to condense. Some of the fuel will condense on to droplets which move more slowly than the air, and some of the fuel will condense onto the liquid fuel film that moves even more slowly. Without any correction, this leads to a weak air/fuel ratio excursion at a time when the requirement is perhaps for a slightly rich mixture to give the maximum torque. Electronically controlled fuel injection can achieve smaller deviations from the desired air/fuel ratio than is the case with a carburetted engine. This is especially the case with multi-point fuel injection, since the injectors are very close to the inlet manifold, and this will minimise the extent of the liquid fuel film, and the amount of fuel in transit as droplets.

During engine warm-up, electronic fuel injection can maintain closer control of the air/fuel ratio. Prior to the lambda sensor being operational, the electronic fuel injection will be determined by look-up tables that refer to parameters such as engine speed, inlet manifold pressure, and throttle position. The fuelling strategy will then be modified in response to the air and coolant temperatures. There is also scope for the ignition timing to be modified, so as to improve drivability or speed engine warm-up (by retarding the ignition timing). Cold start air/fuel ratio control is particularly important for meeting emissions legislation, since before the catalyst has reached its light-off temperature, it is essential to minimise the engine out emissions. With carburettors that are fitted with some form of automatic cold start enrichment (known as the 'choke' or 'strangler'), the operation can only be controlled comparatively crudely, by devices such as bi-metallic trips that respond to the coolant temperature.

An additional advantage of multi-point fuel injection is that the inlet manifold can be designed for optimum air flow, since the liquid fuel films and droplets are confined to a region close to the injector. There is thus no need to have sharp cornered junctions to disrupt the fuel film, but also reduce the volumetric efficiency. It is also possible to have much longer inlet tracts that are part of a tuned-induction system. Indeed it is also possible to have variable geometry induction system, in which resonating pipes and chambers are used in different combinations, so as to raise the volumetric efficiency (and thus the torque output) across a wide range of engine speeds.

The main disadvantage of electronic fuel injection is the cost and complexity, but when this is required to meet emissions legislation, then there is no choice. Perhaps surprisingly, multi-point fuel injection can lead to greater inter-cylinder air/fuel ratio variations at light load. With a carburettor or single point injector, then most of the fuel will be entering the engine as vapour or very fine droplets, and this will ensure a uniform air/fuel ratio. Multi-point injectors control the quantity of fuel injected by the duration for which they are opened. The opening time is about 1 ms, and at full load they might be open for 20 ms every cycle. At light loads, the injector may only be open for say 2 ms, so any variation in the opening delay will have a much more significant effect on the quantity of fuel that is injected. However, a fast response lambda sensor, which is close to the exhaust manifold junction, gives the possibility of resolving the air/fuel ratio on a cylinder basis.

4.5* Contrast high-turbulence, high compression ratio combustion chambers with those designed for lower compression ratios.

The highest useful compression ratio (HUCR) in spark ignition engines is usually defined by the onset of 'knock' - when the unburnt mixture is self-ignited the ensuing rapid pressure rise can cause structural oscillations that are audible as 'knock'. Self-ignition occurs when the unburnt mixture has been at a high enough temperature for sufficient time, and clearly increasing the compression ratio will increase the unburnt mixture temperatures. Knock is undesirable, since the pressure waves in the combustion chamber disrupt the thermal boundary layers, and this can lead to overheating of components. However, if the combustion is sufficiently rapid, then there will be insufficient time for self-ignition to occur, and instead the whole of the unburnt mixture will be consumed by the steady propagation of the turbulent flame front. Figure 4.9 (redrawn here in problem 4.11) shows that for a stoichiometric mixture, then the turbulent combustion system allows the compression ratio to be increased from about 8:1 to 10:1.

Figure 4.9 also shows that knock is most likely to occur with mixtures that are slightly rich of stoichiometric. The more turbulent combustion means that combustion is centred more closely around top centre, when the unburnt mixture temperature is highest, and this extends the weak and rich mixture flammability limits. Thus, when a lean burn strategy is possible, the compression ratio can be further increased.

4.6* Two spark ignition petrol engines having the same swept volume and compression ratio are running at the same speed with wide open throttles. One engine operates on the two-stroke cycle and the other on the four-stroke cycle. State with reasons:

(i) which has the greater power output
(ii) which has the higher efficiency

The two-stroke engine will have the higher power output, because there are twice as many firing strokes per second. However, the power output will not be double, because: the two-stroke engine will have a lower efficiency (see below), and the quantity of charge trapped in the cylinder will be lower (there will be more exhaust residuals (since the two-stroke engine does not have a separate exhaust stroke, and the transfer port in the two-stroke engine is likely to be closed later than the inlet valve in the four-stroke engine.

The two-stroke engine will have a lower efficiency because of: short-circuiting, in which fuel flows directly from the transfer passage to the exhaust port, and the actual compression ratio will be lower because of the later trapping of the in-cylinder charge.

4.7* The Rover M16 spark ignition engine has a swept volume of 2.0 litres, and operates on the four-stroke cycle. When installed in the Rover 800, the operating point for a vehicle speed of 120km/h corresponds to 3669 rpm, and a torque of 71.85 Nm, for which the specific fuel consumption is 298 g/kWh.

Calculate the bmep at this operating point, the arbitrary overall efficiency and the fuel consumption (litres/100km). If the gravimetric air fuel ratio is 20:1, calculate the volumetric efficiency of the engine, and comment on the value.

The calorific value of the fuel is 43 MJ/kg, and its density is 795 kg/m^3. Ambient conditions are 27°C and 1.05 bar.

Explain how both lean-burn engines and engines fitted with three-way catalysts obtain low exhaust emissions. What are the advantages and disadvantages of lean-burn operation?

bmep $= 4\pi T/V_s = 4\pi 71.85/2.0\text{x}10^{-3} =$ **4.51 bar** (5.5

$\eta_o = W_b/Q$ when W_b = 1 kWh = 3.6 MJ, this uses 298 g fuel, of Calorific Value (CV) 43 MJ/kg, thus Q = 0.298x43 = 12.814 MJ

$\eta_b = W_b/Q = 3.6/12.814 =$ **0.281**

To determine the volumetric fuel consumption, we need to find the fuel flow rate into the engine.

$m_f = W$ x bsfc $= (T \text{ x } 2\pi N/60)$ x bsfc $= (71.85 \text{ x } 2\pi \text{ x } 3669/60)\text{x}10^{-3}$ x 0.298 = **8.227 kg/h**

This needs to be converted to a volume flowrate V_f: $V_f = m_f/\rho = 8.23/0.795 = 10.35$ L/hr

In 1 hour the vehicle travels 120 km and uses 10.35 litres of fuel, the volumetric fuel consumption is thus:

(10.35/120) x 100 = 8.62 **L/100km**

The volumetric efficiency is found from the air flow rate into the engine. We can do this by using the fuel flowrate, and using the stated AFR.

$m_a = m_f$ x AFR = 8.23 x 20 = 164.6 kg/hour

The volume flowrate (V_a) is found by applying an equation of state:

$V_a = m_a \text{ x } RT/p = 164.6/60^2 \text{ x } 287 \text{ x } 300/(1.05\text{x}10^5) = 37.5$ L/s

The volumetric efficiency is: $\eta_{vol} = V_a/(V_s \text{ x } N') = 37.5/(2 \text{ x } [3669/120]) =$ **0.613**

A volumetric efficiency of 61.3% is reasonable, since the engine is operating at part load, in other words it is throttled. The maximum bmep of this engine is over 10 bar (using of course a slightly rich mixture); the maximum speed of the vehicle is over 200 km/h.

Engines equipped with three way catalysts operate with significant levels of engine out emissions (say 2000 ppm NOx, 1000 ppm Hc and 1% CO) and rely on the engine operating within about 1% of stoichiometric, so that the catalyst can both oxidise the partial products of combustion (CO and HC) and reduce the nitric oxides. Compared with lean burn operation, there is about a 10% fuel economy penalty, most of which is attributable to having to operate at stoichiometric, as opposed to the mixture for maximum fuel economy (see Fig 4.1).

The lean burn engine has to operate sufficiently weak of stoichiometric, such that the NOx emissions in particular are very low (this might require an equivalence ratio of 0.6 or even weaker), see Figs 4.16 and 14.6. When operating weak of stoichiometric the CO emissions should be low, and if the hydrocarbon emissions are unacceptable, then a simple oxidation catalyst can be used. There is also now scope for considering the use of lean-burn NOx reducing catalysts, although they have a comparatively low efficiency and limited durability.

The advantage of employing lean burn is of course the improved fuel economy. The disadvantages are that lean burn can only be used at low loads, and that at higher torques and speeds it is necessary to switch to stoichiometric operation (see Fig 4.14). As with three way catalysts, at high speeds and loads the mixture is rich of stoichiometric to give an increased power output, and to limit the temperature in the catalyst.

4.8* **A spark ignition engine is to be fuelled by methanol (CH_3OH). Write down the equation for stoichiometric combustion with air, and calculate the stoichiometric gravimetric air fuel ratio.**

Compare the charge cooling effects of fuel evaporation in the following two cases:

(i) A stoichiometric air/methanol mixture in which 25 per cent of the methanol evaporates,

(ii) 60 per cent of a 14.5:1 gravimetric air/petrol mixture evaporates.

The enthalpy of evaporation for methanol is 1170 kJ/kg,and that of petrol is 310 kJ/kg. State clearly any assumptions that are made.

If in a lean-burn engine the gravimetric air/fuel ratio is 8:1, rewrite the combustion equation, and determine the volumetric composition of the products that should be found from a dry gas analysis. What is then equivalence ratio for the air/fuel ratio? Why might methanol be used as a fuel for spark ignition engines?

The generalised stoichiometric combustion equation for methanol is:

$$CH_3OH + a(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + a3.76N_2$$

From the atomic oxygen balance:

$$1 + 2a = 2 + (2x1), \quad \text{and} \quad a = 1.5$$

The stoichiometric combustion equation for methanol is thus:

$$CH_3OH + 1.5(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 4.64N_2$$

The gravimetric stoichiometric air/fuel ratio is thus:

$$1.5(M_{O2} + 3.76M_{N2}) : (M_C + 4M_H + M_O)$$

$$1.5(32 + 3.76 \text{ x } 28) : (12 + 4 \text{ x } 1 + 16)$$

$$205.92 : 32$$

$$6.44 : 1$$

Ignoring the heat capacity of the fuel vapour and assuming the fuel and air were initially at the same temperature, then for 1 kg of air, an energy balance gives:

$$c_{p,air}\Delta T = y \text{ x } h_{fg}/\text{AFR},$$

or:

$$\Delta T = y\ x\ h_{fg}/(\text{AFR}\ c_{p,air}),$$

where: y is the fraction of the fuel that is vaporised

For methanol: $\Delta T_{methanol} = 0.25 \text{ x } 1170/(6.44 \text{ x } 1.01) = 45.0$

For petrol: $\Delta T_{petrol} = 0.25 \text{ x } 1170/(14.5 \text{ x } 1.01) = 12.7$

The 8:1 air/fuel ratio is stated as being lean, so this must refer to a methanol/air mixture.

The equivalence ratio (ϕ) is defined as ϕ = AFRs/AFR,

so $\phi = 6.44/8 = 0.805$

The lean combustion equation for methanol is thus:

$$CH_3OH + (1.5/\phi)(O_2+3.76N_2) \rightarrow CO_2 + 2H_2O + (1/\phi - 1)O_2 + (4.64/\phi)N_2$$

substituting for $\phi = 0.805$, gives:

$$CH_3OH + (1.5/0.805)(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + (1/0.805 - 1)O_2 + (4.64/0.805)N_2$$

$$CH_3OH + 1.863(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 0.242O_2 + 7.006N_2$$

To find the composition of the exhaust gases on a dry gas basis, we have to determine the mole fraction of each species having assumed that all the water vapour will have condensed:

$$\%CO_2:\ n_{CO2}/(n_{CO2} + n_{O2} + n_{N2}) = 1/(1 + 0.242 + 7.006) = 1/8.248 = 12.1\%$$

$$\%O_2:\ n_{O2}/(n_{CO2} + n_{O2} + n_{N2}) = 0.242/8.248 = 2.9\%$$

$$\%N_2:\ n_{N2}/(n_{CO2} + n_{O2} + n_{N2}) = 7.006/8.248 = 84.9\%$$

Methanol is likely to be used under two quite different circumstances. Firstly, methanol can be produced from renewable sources, and it can be readily produced from methane. Although there is an 'energy cost' associated with the production of methanol from methane, it results in a fuel which can be much more readily stored in a vehicle.

Secondly, methanol is used in certain high performance applications. The substantial evaporative cooling effect leads to an improvement in the volumetric efficiency, and thus also the power output. The high octane rating (RON of 106) permits higher compression ratios, or more significantly for high performance applications, a higher boost pressure when supercharging. However, the susceptibility of methanol to surface ignition can make pre-ignition a problem. The other high performance advantage of methanol is that the air/fuel ratio for maximum power output is richer than with gasoline, (because of the increased evaporative cooling effect with a richer mixture), and this more than compensates for the slightly lower calorific value on the MJ/kg_stoichiometric_mixture basis (2.68 compared with about 2.7 for gasoline). The lower combustion temperatures associated with methanol (the adiabatic flame temperature for a stoichiometric mixture will be about 100 K lower with methanol, and the initial mixture temperature will be lower because of the evaporative cooling) will reduce the heat transfer from the combustion chamber, and this means that the brake efficiency of the methanol fuelled engine should be higher.

4.9* **The Rover K16 engine is a four-stroke spark ignition engine with a swept volume of 1.397 litres and a compression ratio of 9.5. The maximum torque occurs at a speed of 4000 rpm, at which point the power output is 52 kW; the maximum power output of the engine is 70 kW at 6250 rpm. Suppose the brake specific fuel consumption is 261.7 g/kWh using 95 RON lead-free fuel with a calorific value of 43 MJ/kg.**

Calculate the corresponding Otto cycle efficiency, the maximum brake efficiency, and the maximum brake mean effective pressure. Give reasons why the brake efficiency is less than the

Otto cycle efficiency. Show the Otto cycle on the p-V state diagram, and contrast this with an engine indicator diagram - identify the principal features.

Explain why, when the load is reduced, the part-load efficiency of a diesel engine falls less rapidly than the part-load efficiency of a spark ignition engine.

$\eta_{\text{Otto}} = 1- 1/r_v^{\gamma-1} = 1- 1/(9.5^{1.4-1}) = 0.594$ (2.8

$\eta_b = W_b/Q$ when $W_b = 1$ kWh $= 3.6$ MJ, this uses 267.1g fuel, of Calorific Value (CV) 43 MJ/kg, thus $Q = 0.2671 \times 43 = 11.485$ MJ

$\eta_b = W_b/Q = 3.6/11.485 = 0.313$

bmep $= W_b/(V_s N^*)$, where $N^* =$ rpm/120 for a 4-stroke engine (2.17

bmep $= 52\text{x}10^3/(1.397\text{x}10^{-3} \text{ x } 4000/120) = 11.17$ bar or

bmep $= 70\text{x}10^3/(1.397\text{x}10^{-3} \text{ x } 6250/120) = 9.62$ bar

The maximum bmep is thus 11.17 bar at 4000 rpm.

$\eta_{\text{Otto}} < \eta_b$ because:

a) No account is taken of mechanical losses,

b) There is heat transfer, especially during combustion and the early stages of expansion,

c) The air/fuel mixture and combustion products do not behave as perfect gases,

d) $\gamma < 1.4$; a value of 1.3 would be more realistic, thus reducing η_{Otto} to 0.491,

e) combustion is not instantaneous,

f) combustion is not complete - there are unburnt hydrocarbons,

g) the exhaust valve opens before the piston reached bottom dead centre,

h) work is dissipated in the gas exchange processes.

The fall in part load efficiency with a diesel engine is less severe than in a petrol engine because (see Fig 5.1:

a) There is no throttling - at part load a conventional spark ignition engine requires an air fuel ratio that is always close to stoichiometric, and thus the air flow has to be reduced, as well as reducing the fuel flow. In a diesel engine, only the fuel flow is reduced.

b) A diesel engine operates with increasingly weak air fuel ratios, so the ratio of the specific heat capacities rise towards 1.4.

c) As the load is reduced in a diesel engine the combustion duration becomes shorter, whilst combustion in a spark ignition engine becomes slower.

The Otto cycle is shown in Fig 2.1; an indicator diagram is shown in Fig 2.6.

4.10* Since the primary winding of an ignition coil has a finite resistance, energy is dissipated while the magnetic field is being established after switching on the coil. If the primary winding has an inductance of 5.5 mH, and a resistance of 1.9 Ohms, and the supply voltage is 11.6 V, show that::

(i) the energy stored after 2 ms would be 26 mJ, increasing to 79 mJ after 6 ms,

(ii) the theoretical efficiency of energy storage is about 65 per cent for a 2 ms coil-on-time, falling to 32 per cent for a 6 ms coil-on-time.

What are the other sources of loss in an ignition coil?

Define MBT ignition timing, and describe how it varies with engine speed and load. Under what circumstances are ignition timings other than MBT used?

The variation of current with time is given by Eq 4.9:

$$i = (V_s/R)(1 - \exp(-Rt/L))$$

where: V_s is the supply voltage (V)
R is the resistance (Ohms)
t is the time the coil has been switched on (s)
L is the inductance of the primary winding (H).

Substitution of the fixed numerical values gives:

$$\begin{aligned} i &= (11.6/1.9)(1 - \exp(-1.9t/5.5\text{x}10^{-3})) \\ &= 6.11(1 - \exp(-345.5t)) \end{aligned}$$

Letting I_2 be the current after 2 ms, and I_6 be the current after 6 ms gives:

$$I_2 = 6.11(1 - \exp(-345.5 \text{ x } 0.002)) = 3.05 \qquad \text{A}$$

$$I_6 = 6.11(1 - \exp(-345.5 \text{ x } 0.006)) = 5.34 \qquad \text{A}$$

The energy stored in the primary winding (E_s) is given by Eqn 4.11:

$$E_s = 0.5LI_p^2$$

where I_p is the current flowing in the primary winding.

Letting E_2 be the energy stored after 2 ms, and E_6 be the energy stored after 6 ms, gives:

$$E_2 = 0.5 \text{ x } 5.5\text{x}10^{-3} \text{ x } 3.05^2 = 25.6 \text{ mJ}$$

$$E_6 = 0.5 \text{ x } 5.5\text{x}10^{-3} \text{ x } 5.34^2 = 78.5 \text{ mJ}$$

The energy input to the (E_p) coil is found by integration of the supply voltage multiplied by the instantaneous current, which can be found from Eqn 4.9:

$$\begin{aligned} E_p &= \int_0^{t'} V_s i \,\mathrm{d}t = (V_s^2/R) \int_0^{t'} 1 - \exp(-Rt/L)\mathrm{d}t \\ &= (V_s^2/R)\ \Big[(t + L/R\exp(-Rt/L))\Big]^{t'} \end{aligned}$$

where t' is the duration of the current flow.

$$E_p = (V_s^2/R)\ [(t' - 0 + L/R(\exp(-Rt'/L) - 1))]$$

$$= (11.6^2/1.9)\ [(t' + 5.5\text{x}10^{-3}/1.9(\exp(-1.9t'/5.5\text{x}10^{-3}) - 1))]$$

$$= 70.82[(t' + 2.89\text{x}10^{-3}(\exp(-345.5t') - 1))]$$

Letting E_{p2} be the energy input after 2 ms, and E_{p6} be the energy input after 6 ms, gives:

$$E_{p2} = 70.82[(0.002 + 2.89\text{x}10^{-3}(\exp(-345.5 \text{ x } 0.002) - 1))] = 39.5 \text{ mJ}$$

$$E_{p6} = 70.82[(0.006 + 2.89\text{x}10^{-3}(\exp(-345.5 \text{ x } 0.006) - 1))] = 246.0 \text{ mJ}$$

The storage efficiency of the primary winding is thus the ratio of the stored energy divided by energy the energy supplied:

$25.6/39.5 = 65\%$ after 2 ms, and

$78.5/246 = 32\%$ after 6 ms.

Because of hysteresis losses in the magnetisation of the iron core (there is a loop formed on a plot of (B) against (H)), then not all of the energy stored is recovered electrically.
Secondly, because of the resistance of the HT windings, there are resistive losses in the HT windings.

MBT ignition timing is the Minimum ignition advance for Best Torque. Fig 4.3 shows the response of the engine torque or bmep to ignition timing at an otherwise fixed operating point. Clearly there is a fairly broad maximum, and the MBT ignition timing is the least advanced ignition timing that gives the maximum torque, since this then ensures the maximum knock margin. When the ignition timing is advanced, then the pressures in the unburnt gas will become higher, and this in turn leads to higher temperatures in the unburnt gas. If the temperature is high enough for sufficient time, then self-ignition can occur. This causes very rapid combustion of any remaining unburnt gas, and the ensuing rapid pressure rise can lead to structural vibrations that are heard audibly as knock. Knock is undesirable since the rapid pressure rise can destroy thermal boundary layers in the combustion chamber, leading to failure of components such as the piston.

Since combustion does not occur instantaneously at top dead centre, then the best compromise is to ensure about half of the charge is burnt before top dead centre. Advancing the ignition timing increases the compression work and the expansion work since the pressure at top dead centre will be raised. However, there is a point at which the increase in compression work is greater than the increase in the expansion work, hence the maxima seen in Fig 4.3. The MBT ignition timing varies with engine speed and load, because the burn rate of the mixture varies, even if the air/fuel ratio is fixed.

The combustion duration is largely dependent on two phases of combustion:

Early burn period -	this might account for the first 10% of the fuel being burnt, and its duration is influenced by the laminar burning velocity of the mixture. Initially the flame front will be laminar, since the turbulence length scales are large compared to the size of the flame kernel.
Main burn period -	this is typically when 10 to 90% of the fuel is burnt and it is governed by the turbulent propagation of the flame front.

When engine speed is increased, the main burn period will occupy an approximately constant crankangle duration, since the turbulence intensity increases with engine speed, and there is a more or less corresponding increase in the turbulent burning velocity. However, the early burn period will occupy only a slightly shorter time period (and thus an increased crank angle duration), since the initial laminar flame growth will be unaffected by the change in engine speed. The ignition timing thus has to be advanced as the engine speed is increased.

When engine load is reduced, the ignition timing has to be advanced, because the exhaust residuals level in the charge will have increased. The exhaust residuals are essentially inert, and will increase the duration of both phases of the combustion process. The exhaust residuals increased as the load is reduced, since when the engine is throttled the inlet manifold pressure is reduced, and during the valve overlap period exhaust gases will flow into the inlet manifold and not the exhaust port. The exhaust gases are then re-admitted to the cylinder during the induction stroke.

As the ignition timing is advanced the in-cylinder temperatures and pressures are reduced. The lower pressure is associated with a faster laminar burning velocity, while the lower temperature is associated with a slower laminar burning velocity. The effect of the temperature change is usually stronger, so that as the ignition timing is advanced the laminar burning velocity is reduced. This reduces the gains associated with advancing the ignition timing.

Ignition timings retarded from MBT are used for avoiding knock (as discussed above in the selection of the MBT ignition timing) and for reducing NOx. A retarded ignition timing also increases the exhaust gas temperatures (because less work has been extracted by the piston and there has been less time for in-cylinder heat transfer), and this can be useful following a cold start to warm-up a catalyst more quickly. The retarded ignition timing will also be used for reducing the engine-out NOx emissions. The retarded ignition timing will lead to lower pressures during combustion, and this in turn leads to lower burnt gas temperatures. The formation of NOx is very temperature dependent, and a reduction in the maximum cycle temperature will lead to a halving of the NOx emissions.

4.11 Redraw figure 4.9 using a scale of lambda (the relative air fuel ratio, the reciprocal of equivalence ratio), and comment under what circumstances that this is a more appropriate form for presenting the data.

Figure 4.9 (plotted against equivalence ratio) shows the effect of the non-dimensional fuel air ratio on engine operation. It is thus most relevant to full throttle operation, in which the air flow rate will be approximately constant and the fuelling level is being varied. Figure 4.9 shows that at a high compression ratio, then control with weak mixtures is more difficult than control with rich mixtures.

In contrast, when the same data are plotted here against lambda, a non-dimensional air fuel ratio, then this is representative of part throttle operation. At part throttle the fuelling level will be almost fixed, and the air flow rate will be varied to give the maximum economy (or power output, since the fuelling level is fixed). The plot against lambda shows that at part load operation there is a comparatively wide operating envelope at high compression ratios. The differences in the plots is a consequence of taking reciprocals of numbers either side of unity.

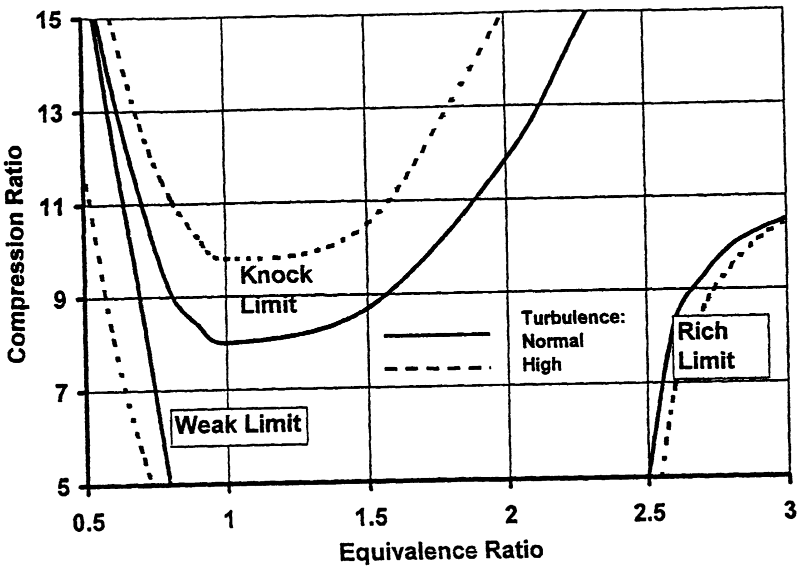
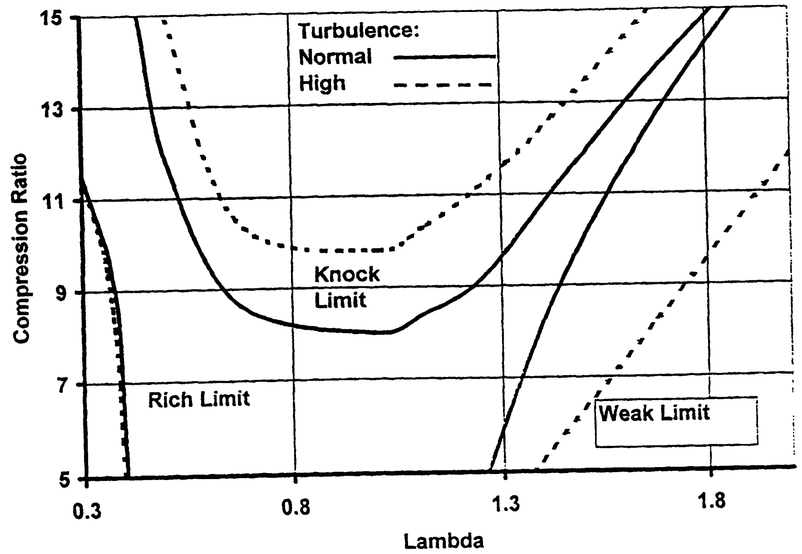


Figure 4.9 Effect of turbulence on increasing the engine operating envelope of spark ignition engines - plotted against equivalence ratio.



The same data as in Figure 4.9 (effect of turbulence on increasing the engine operating envelope of spark ignition engines), but plotted against lambda.

5 Compression Ignition Engines

5.1* Contrast the advantages and disadvantages of indirect and direct compression ignition engines.

The advantages of the indirect injection (IDI) engine are its quieter combustion and a combustion system that is more amenable to high speed operation. The disadvantage of the IDI engine, is that the direct injection (DI) engine has a 10-15% lower fuel consumption.

The use of a separate pre-chamber for fuel injection ensures that there is very active air flow (with a high turbulence intensity, and in the case of the swirl chamber, a high mean flow velocity). The pre-chamber is usually thermally isolated from the cylinder head in some way. Since the fuel is injected into the pre-chamber, the high temperature of the pre-chamber helps to minimise the ignition delay. This leads to quieter combustion, since there is less time for the flammable air/fuel mixture to form during the ignition delay period. The high activity of the flow into which the fuel is injected, means that good mixing of the air and fuel occurs with modest (say 350 bar) fuel injection pressures. This also facilitates high speed operation: 5000 rpm and higher.

The fuel consumption of IDI engines is higher than that of direct injection (DI) engines, because of heat transfer (and less significantly pressure drop) caused by the high velocity flow in and out of the pre-chamber.

5.2* Discuss the problems in starting compression ignition engines, and describe the different starting aids.

In a cold compression ignition engine there will be increased levels of heat transfer, and this can mean that the compression temperatures are only just sufficient to ignite the fuel. This is particularly so for indirect injection (IDI) diesel engines in which the fuel is injected into a prechamber. The IDI prechamber has intense air motion that is generated by restrictions in the flow passage from the main chamber, this in turn means that there will be high levels of heat transfer in the pre-chamber, and the passageways leading to it. The compression ratio for IDI engines is invariably dictated by the starting requirement, and the compression ratio is likely to be higher than is optimum for normal operation. In both direct injection (DI) and IDI diesel engines a cold engine is likely to suffer more from blow-by, since the lubricant will not yet have reached the piston rings and oil control ring. In DI engines, some of the fuel injected while the engine is being cranked over will contact the cylinder walls, and this will help to seal the piston rings. Some fuel injection pumps over-fuel the engine during cranking to facilitate this effect. If the fuel has a low cetane rating, then this too will make starting more difficult (or even impossible).

There are many different approaches to assisting the starting of diesel engines, and the order adopted here will be: in-cylinder, external to the cylinders and engine design features.

Heater Plugs are electrically heated devices, about 6 mm diameter and protruding about 20 mm into the combustion chamber. They are switched on prior to starting the engine, so that once the engine is cranked over, when the fuel is injected some of it will strike a hot surface, thereby facilitating evaporation and ignition. Heater plugs are invariably used in IDI engines, and are frequently used on smaller (say 0.5 L/cylinder) DI engines. The heater plugs can remain switched on (perhaps at a reduced power level) during the early stages of warm-up, since they will shorten the ignition delay period, and result in quieter combustion.

Manifold Heaters are used in DI engines, and they can be either electrical or burners using diesel fuel (but ignited electrically). The high levels of heat transfer associated with the pre-chamber throat in IDI engines means that heating the air in the inlet manifold is of limited benefit.

Ether Injection is very effective, since diethyl ether is very volatile (a boiling point of 35°C), it burns over a very wide range of air/fuel ratios, and it has a very low self-ignition temperature.

Decompression Levers (Valve Lifters) act on the valves (usually the inlet), so that the valve remains partially open. These are usually found on hand started engines, since it enables the engine to be accelerated to a reasonable speed, without work being dissipated on compression. Since it is the speed of the compression stroke that is important, then it is usual to also fit a large flywheel, so as to ensure high compression temperatures once the decompression lever is released.

Variable Compression Ratio (VCR) Devices enable a higher compression ratio to be adopted for starting. VCR pistons have been developed, in which there is a hydraulic chamber between a two part piston - the outer part forming the piston crown and skirt, and the inner part being connected to the piston pin; see Fig 5.A. The oil feed is through the connecting rod, and the VCR piston valves control the peak cylinder pressures. Thus during cold starting the VCR piston would provide a high compression ratio. VCR pistons have had limited use, mostly with high bmep engines for military applications. Another (simpler) approach with IDI engines is to vary the volume of the pre-chamber. This has most frequently been done with engines that use an air-cell. Figure 5.B shows how the air cell is connected to the pre-chamber by a throat. During normal operation, unburnt mixture will initially flow into the air cell during compression, after immediately after ignition burning mixture will flow into the air cell, but as the pressure in the pre-chamber falls below that of the air cell the flow reverses. The flow in and out of the air-cell adds to the turbulence level in the pre-chamber. By sealing the air cell from the pre-chamber, then the compression ratio can be increased to assist cold starting.

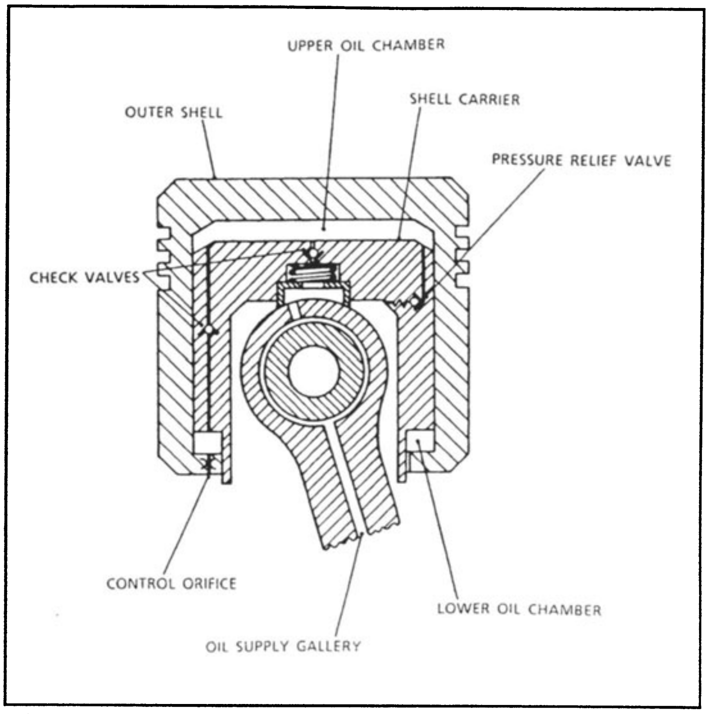


Fig 5.a A Variable Compression Ratio Piston

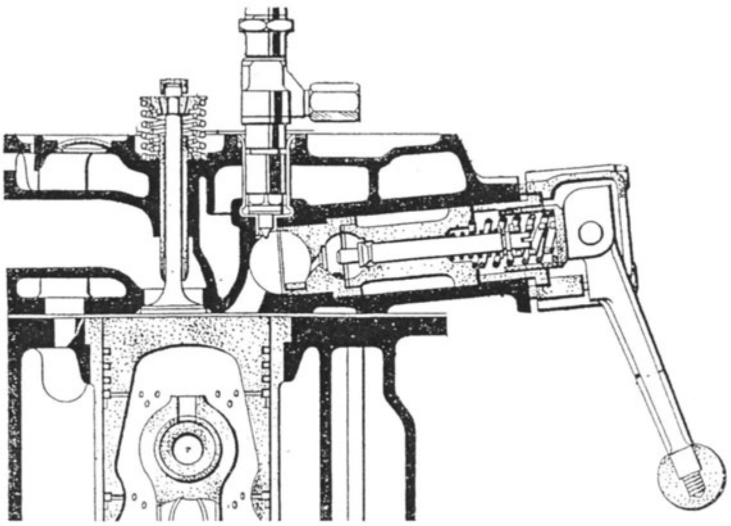


Fig 5.B A high compression system for cold starting

5.3* Comment on the differences between in-line and rotary fuel injection pumps.

In-line fuel injection pumps have a plunger pumping element for each fuel injector. In contrast, rotary or distributor injection pumps have a single pumping unit, and the high pressure fuel is directed to the appropriate injector via a radial passage in the rotating element.

Until the mid 1980s, the maximum injection pressure with rotary pumps was limited to about 350 bar whilst in-line pumps were capable of 700 bar and higher. However, with the development of small high speed direct injection engines, rotary pumps were developed with the ability to develop pressures of 700 bar. Both types of injection pump are now capable of injection pressures of 1000 bar and higher.

Rotary injection pumps automatically deliver the same quantity of fuel to each injector. In comparison, each pumping element in an in-line pump has to be calibrated to deliver the same quantity of fuel to each injector.

5.4* Describe the different ways of producing controlled air motion in compression ignition engines.

In Direct Injection (DI) engines an ordered air motion is required, so as to ensure intimate mixing of the fuel and air. This is known as swirl, and the air flow forms a vortex rotating about an axis that is parallel to the cylinder axis. The swirl is generated by the geometry of the inlet port, or (rarely) by means of a shroud on the inlet valve. The air tends to enter from a tangential direction, and this leads to swirl in the cylinder. The kinetic energy associated with the swirling flow comes from an increased pressure drop in the inlet system (and thus a lower volumetric efficiency). The swirl also tends to increase the heat transfer, so there is a trend to reduce the levels of swirl. This in turn requires a greater dispersion of the diesel fuel, by means of a larger number of smaller holes in the nozzle; this in turn requires higher injection pressures.

With Indirect Injection (IDI) the air motion is generated in the pre-chamber. Since the pressure difference is generated by the piston motion, then high velocity flows can be produced with no volumetric efficiency penalty. Consequently, in IDI diesel engines the fuel injection requirements are less demanding.

5.5* An engine manufacturer has decided to change one of his engines from a spark ignition type to a compression ignition type. If the swept volume is unchanged, what effect will the change have on:

(i) maximum torque?
(ii) maximum power?
(iii) the speed at which maximum power occurs?
(iv) economy of operation?

i) The maximum torque will be reduced because the bmep is lower. Diesel engines can only operate smoke-free with air/fuel ratios weak of stoichiometric, say $\phi < 0.8$. The volumetric efficiency of the diesel engine will be lower than the spark ignition engine, because there is no evaporative cooling caused by fuel vaporisation. There will thus be less fuel trapped in each cylinder, and although the efficiency of fuel conversion is greater in a diesel engine (say 40% instead of 30%) the maximum bmep in a diesel engine will be lower (say 7.5 bar, compared with a bmep of 10 bar for a spark ignition engine).

ii) The maximum power will be lower because the torque is lower, and the maximum speed is lower, and the power is the product of speed and torque.

iii) The speed at which maximum power occurs is lower in the diesel engine than the spark ignition engine, because of the nature of diesel engine combustion. With spark ignition engines a flammable air fuel mixture is formed prior to ignition, whilst with diesel engines, the fuel has to be injected, then ignited, with the major part of combustion being diffusion controlled.

iv) The diesel engine will have a higher maximum efficiency than the spark ignition engine because: a) it will have a higher compression ratio, b) during the main part of compression, only air will be present, and c) it will always operate with a weak air/fuel mixture, so the products of combustion behave more like a perfect gas.

5.6. Show that the efficiency of the Air Standard Diesel Cycle is:

$$\eta_{Diesel} = 1 - \frac{1}{r_v^{\gamma-1}}\left[\frac{\alpha^{\gamma} - 1}{\gamma(\alpha-1)}\right]$$

where r_v = volumetric compression ratio

α = volumetric expansion ratio during constant-pressure heat addition

(i) By considering the combustion process to be equivalent to the heat input of the Diesel cycle, derive an expression that relates the load ratio (α), to the gravimetric air/fuel ratio (F). Assume that the calorific value of the fuel is 44 MJ/kg, the compression ratio is 15:1, the air inlet temperature is 13°C, and for the temperature range involved, c_p = 1.25 kJ/kgK and γ = 1.33. State clearly any assumptions.

(ii) Calculate the Diesel cycle efficiencies that correspond to gravimetric air/fuel ratios of 60:1 and 20:1, and comment on the significance of the result.

With reference to Figure 2.3:

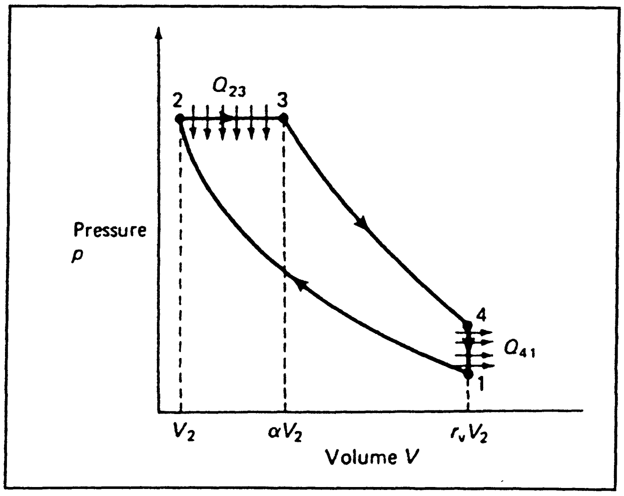


Figure 2.3 Ideal Air Standard Diesel Cycle

$$\alpha = V_3/V_2 \qquad \text{(A}$$

$$V_4 = V_1 = r_v V_2 \qquad \text{(B}$$

and $$V_3 = \alpha V_1/r_v \qquad \text{(C}$$

For any cycle, the First Law of Thermodynamics can be applied:

$$\eta_{Diesel} = 1 - Q_{out}/Q_{in} = 1 - Q_{41}/Q_{23} \qquad \text{(D}$$

Next we can evaluate the heat flows in terms of the temperatures around the cycle, but to do so we need to invoke the assumption of having a Perfect Gas (with constant specific heat capacities), and a fixed mass (m):

$$Q_{41} = m \times c_v\,(T_4 - T_1) \qquad \text{(E}$$

$$Q_{23} = m \times c_v\,(T_3 - T_2) \qquad \text{(F}$$

Substitution of equations E and F into equation D gives:

$$\eta_{Diesel} = 1 - \left[\frac{T_4 - T_1}{c_p / c_v (T_3 - T_2)} \right] \qquad \text{(G}$$

or

$$\eta_{Diesel} = 1 - \left[\frac{T_4 - T_1}{\gamma (T_3 - T_2)} \right] \qquad \text{(H}$$

We now need to work around the cycle, so as to evaluate all the temperatures in terms of a single temperature. We will start with T_1 and proceed in a clockwise direction. It would of course be possible to start at any temperature, and proceed in either direction. Sometimes it is expedient to work clockwise and anti-clockwise from the initial temperature, when it is not possible to complete the cycle in any other way.

1 → 2 assumed to be reversible and adiabatic, and thus isentropic: $T_2 = T_1 r_v^{\gamma-1}$ (I

2 → 3 heat addition at constant pressure, so application of the equation of state ($pV = mRT$) gives

$$T_3 = T_2 V_3 / V_2$$

substitution for T_2 from Equation (I) and for V_4/V_3 from Equation (B) gives:

$$T_3 = T_1 r_v^{\gamma-1} \alpha \qquad \text{(J}$$

3 → 4 is assumed to be reversible and adiabatic, and thus isentropic: $T_4 = T_3 (V_3/V_4)^{\gamma-1}$

substitution for T_3 from Equation (L) and for V_3/V_4 from Equation (C) gives:

$$T_4 = T_1 r_v^{\gamma-1} \alpha (\alpha / r_v)^{\gamma-1} = T_1 \alpha^{\gamma} \qquad \text{(K}$$

Substitution for T_2, T_3 and T_4 in terms of T_1 (using equations I, J and K), into equation (H) gives:

$$\eta_{Diesel} = 1 - \left[\frac{\alpha^{\gamma} - 1}{\gamma r_v^{\gamma - 1} (\alpha - 1)} \right]$$

or

$$\eta_{Diesel} = 1 - \frac{1}{r_v^{\gamma-1}} \left[\frac{\alpha^{\gamma} - 1}{\gamma (\alpha - 1)} \right] \qquad \text{(L}$$

(i) For mass m trapped in the cylinder, an energy balance gives:

$$m c_p (T_3 - T_2) = m_f \mathrm{CV} \qquad \text{(M}$$

where: m_f is the mass of fuel, and CV is its calorific value

$$(m - m_f)/m_f = F \quad \text{or,} \quad m_f = m/(F + 1) \qquad \text{(N}$$

where: F is the air/fuel ratio.

Substitution of Eq (N) into Eq (M) and rearranging gives:

$$T_3 = T_2 + CV/(F + 1)c_p \qquad \text{(O}$$

The load ratio (α) is:

$$\alpha = T_3/T_2 = 1 + CV/T_2(F + 1)c_p \qquad \text{(P}$$

(ii) We can now use these cattiness to find the numerical values in cases 1 and 2.

Equation I yields T_2: $T_2 = T_1 r_v^{\gamma-1} = 286 \text{ x } 15^{1.33-1} = 699 \text{ K}$

So now we can use Eq. (P) to determine α_1 and α_2 for the first and second cases respectively:

$$\alpha_1 = 1 + 44\text{x}10^6/(699 \text{ x } [60 + 1] \text{ x } 1.25\text{x}10^3) = 1.826$$

$$\alpha_2 = 1 + 44\text{x}10^6/(699 \text{ x } [20 + 1] \text{ x } 1.25\text{x}10^3) = 3.398$$

$$\eta_{Diesel} = 1 - \frac{1}{r_v^{\gamma-1}\gamma}\left[\frac{\alpha^\gamma - 1}{(\alpha-1)}\right] = 1 - \frac{1}{15^{1.33-1}\ x\ 1.33}\left[\frac{\alpha^\gamma - 1}{(\alpha - 1)}\right] = 1 - 0.308\left[\frac{\alpha^\gamma - 1}{(\alpha - 1)}\right]$$

Substitution of the numerical values for the load ratio gives:

$$\eta_{Diesel,1} = 1 - 0.308\left[\frac{\alpha_1^\gamma - 1}{(\alpha_1 - 1)}\right] = 1 - 0.308\left[\frac{1.826^{1.33} - 1}{(1.826 - 1)}\right] = 0.542$$

$$\eta_{Diesel,2} = 1 - 0.308\left[\frac{\alpha_2^\gamma - 1}{(\alpha_2 - 1)}\right] = 1 - 0.308\left[\frac{3.398^{1.33} - 1}{(3.398 - 1)}\right] = 0.475$$

the results demonstrate that as the load on the Diesel engine is reduced (and the air/fuel ratio becomes higher), then the indicated efficiency should rise, as $\alpha \rightarrow 1$.

5.7* Some generalised full load design data for naturally aspirated 4-stroke DI diesel engines is tabulated below:

Mean piston speed, v_p	**4**	**6**	**8**	**10**	**12**
Brake specific fuel consumption, bsfc (kg/MJ)	**0.068**	**0.063**	**0.061**	**0.064**	**0.076**
Brake mean effective pressure, p_b (bar)	**7.24**	**8.00**	**8.08**	**7.70**	**6.93**
Volumetric efficiency, η_{vol}, (per cent)	**89.8**	**88.3**	**82.1**	**77.7**	**76.2**

Ambient conditions: p = 105 kN/m2, T = 17°C

Complete the table by calculating : the brake specific power, bsp (MW/m²), the air/fuel ratio, and the brake specific air consumption, bsac (kg/MJ). State briefly what is the significance of squish and swirl in DI combustion. Why does the air/fuel ratio fall as the piston speed increases, what is the significance of the brake specific air consumption, and why is it a minimum at intermediate piston speeds? (It may be helpful to plot the data.)

To find the brake specific power (w), we need to use Eq 2.38:

$$\text{Power, } W = p_b LAN' \qquad (2.17$$

where:
p_b is the bmep (N/m²)
L is the stroke (m)
A is the piston area (m²)
N' is the number of firing strokes/s (s^{-1})

In a four-stroke engine the piston will travel a distance of 4L every cycle, so:

$$N' = v_p/4L \qquad (A$$

Combining these two equations gives the specific power

$$w = W/A = p_b LAN'/A = p_b L v_p/4L = p_b v_p/4 \qquad (B$$

The air/fuel ratio, AFR is defined as:

$$\text{AFR} = m_a/m_f$$

The air mass flow rate (m_a) can be found from the volumetric efficiency:

$$\eta_v = V_a/(V_s N'),\text{ where } V_s = LA \qquad (2.17$$

$$m_a = \rho V_a = \rho\eta_v V_s N' = \eta_v LAN'$$

Substituting for N' from Eq. A $\qquad N' = v_p/4L \qquad$ (A

Gives: $\qquad m_a = \eta_v LAv_p/4L = \eta_v Av_p/4 \qquad$ or $\qquad m_a/A = \eta_v v_p/4 \qquad$ (C

The mass flow rate of the fuel (m_f) can be found per unit piston area from the product of the specific power (w) and the brake specific fuel consumption (bsfc):

$$m_f/A = (W/A) \text{ x bsfc} = (p_b v_p/4) \text{ x bsfc} \qquad (D$$

Dividing Eq. (C) by Eq. (D) yields:

$$\text{AFR} = m_a/m_f = [\eta_v v_p/4]/[(p_b v_p/4) \text{ x bsfc}] = \eta_v/[p_b \text{ x bsfc}] \qquad (E$$

The brake specific air consumption (bsac) is defined by equation 2.27:

$$\text{bsac} = \text{bsfc x AFR} \qquad (F$$

Equations (B), (E) and (F) can now be used to complete the table, once we have calculated the density of the air from the equation of state:

$$\rho = p/RT = 105\text{x}10^3/(287 \text{ x } 290) = 1.262 \text{ kg/m}^3$$

Mean piston speed, v_p	4	6	8	10	12
bsfc (kg/MJ)	0.068	0.063	0.061	0.064	0.076
bmep, p_b (bar)	7.24	8.00	8.08	7.70	6.93
η_{vol}, (per cent)	89.8	88.3	82.1	77.7	76.2
bsp, w (MW/m^2)	0.724	1.200	1.616	1.925	2.079
AFR	23	20	19	18	16.5
bsac (kg_air/MJ)	1.564	1.260	1.160	1.15	1.25

Squish is important in ensuring rapid combustion; it is turbulence generated by the inward radial flow into the piston bowl, that is a result of the small clearance between the piston and cylinder head.

Swirl is important in ensuring good mixing of the fuel and air for complete combustion; it is a bulk air flow about an axis parallel to the cylinder axis, and it is generated by the direction of the air flow into the cylinder.

The falling AFR indicates a richening of the mixture. Up to about a mean piston speed of 9 m/s there is an improvement in combustion since the brake specific air consumption is falling (the better the control of combustion, then the less air that is needed to burn a given quantity of fuel). However, above this speed (9m/s), the volumetric efficiency is falling and the fuelling rate has not been reduced as much, presumably in an attempt to maintain the bmep. However, with a mixture that is so close to stoichiometric there will be a significant quantity of smoke in the exhaust and an increase in the level of unburnt hydrocarbons. This accounts in part for the rapidly increasing bsfc above 10 m/s. The other reason for the increase in the bsfc is that frictional losses will be rising.

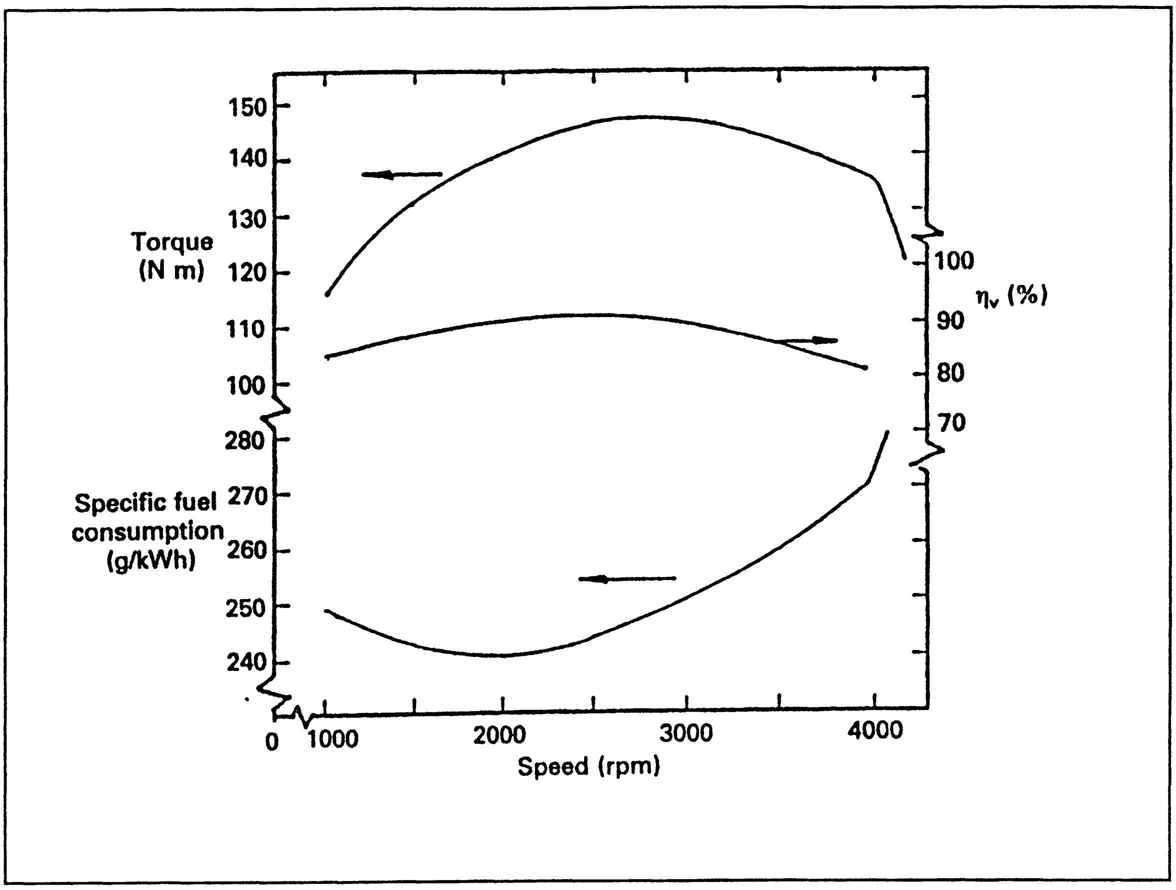
5.8* **A direct injection Diesel engine with a swept volume of 2.5 litres has the full load performance shown in figure 5.44. What is the maximum power output of the engine, and the corresponding air/fuel ratio?**

For both the maximum power and maximum torque, calculate the brake mean effective pressure. What is the maximum brake efficiency?

The fuel has a calorific value of 44 MJ/kg, and the ambient conditions are a temperature of 17°C and a pressure of 1.02 bar.

Identify the differences between direct (DI) and indirect injection (IDI) Diesel engines, and explain why the efficiency of the DI engine is higher. Why is IDI still used for the smallest high speed diesel engines?

The maximum power is when the product of the speed and torque is greatest. With the torque curve in Fig. 5.4, there is a sharp reduction in torque at speeds above 4000 rpm. This suggests that the engine has been governed to give its maximum power at 4000 rpm, when the torque is 135 Nm. Remembering that the speed has to be in radians/second:



$$W = T \times \omega = 135 \times 4000 \times (2\pi/60) = 56.5 \text{ kW}$$

This constant power hyperbola has been sketched onto Fig 5.44, and it can indeed be seen that the maximum power is 56.5 kW. When the maximum power speed is not so obvious, then it is necessary to evaluate the power for a number of speeds that are separated by small increments, and to then plot a graph of power against speed.

The air/fuel ratio, AFR is defined as:

$$\text{AFR} = m_a/m_f$$

The fuel mass flow rate (m_f) can be found from the product of the bsfc and the power:

$$m_f = \text{bsfc} \times W = 0.270 \times 56.5 = 15.26 \text{ kg/hr} \quad \text{or} \quad 4.24 \text{ g/s}$$

The air mass flow rate (m_a) can be found from the volumetric efficiency:

$$\eta_v = V_a/(V_s N^*)$$

$$m_a = \rho V_a = \eta_v V_s N^* \qquad \text{with } N^* \text{ being the number of cycles/s}$$

We can calculate the density of the air from the equation of state:

$$\rho = p/RT = 1.02\text{x}10^5/(287 \times 290) = 1.226 \text{ kg/m}^3$$

so

$$m_a = 1.226 \text{ x } 2.5\text{x}10^{-3} \text{ x } 0.80 \text{ x } 4000/120 = 81.7 \text{ g/s}$$

Thus AFR = m_a/m_f = 81.7/4.24 = **19.3**
To find the brake specific power (w), we need to use Eq 2.38:

$$\text{Power, } W = p_b V_s N^* \qquad (2.15$$

where: V_s is the swept volume (m^3)
N^* is the number of firing cycles/s (s^{-1})

Rearranging gives:

$$p_b = W/V^s N^*$$

At maximum power: $p_b = 56.5\text{x}10^3/(2.5\text{x}10^{-3} \text{ x } 4000/120)$ = **6.78 bar**

The bmep is proportional to torque, so

at maximum torque: $p_b = 6.78 \text{ x } 146/135$ = **7.33 bar**

The maximum efficiency occurs when the brake specific fuel consumption (bsfc) is a minimum; this is 240 g/kWh at 2000 rpm:

Remembering that 1 kWh is equivalent to 3.6 MJ, then a bsfc of 240 g/kWh is equivalent to 66.7 g/MJ

$$\eta_b = 1/(\text{bsfc x CV}) = 1/(66.7\text{x}10^{-3} \text{ x } 44\text{x}10^6) = \mathbf{0.341}$$

With indirect injection (IDI) engines, fuel is injected into a pre-chamber, for example, the Ricardo Comet Mk V swirl chamber. During compression, the air forced into the pre-chamber gains a lot of kinetic energy, that ensures good mixing and rapid combustion once the fuel is injected and ignited. After combustion has started, the burning gases are forced out of the pre-chamber, to generate yet more turbulence when mixed with the air in the main chamber.

In direct injection (DI) engines, fuel is injected directly into the main combustion chamber. Satisfactory mixing with the air and subsequent combustion is ensured by generating swirl, and by high pressure injection (700 bar and higher) through multi-hole nozzles (IDI engines use a single hole injector with a lower injection pressure, about 350 bar).

The IDI engine has a lower efficiency because of the pumping losses through the pre-chamber throat, but more significantly, the high heat transfer through the throat. IDI engines have very high compression ratios (eg 22:1), and the higher compression ratio lead to higher compression pressures and frictional losses that more than offset any thermodynamic gains. The high compression ratios are to ensure adequate starting performance, despite the high heat transfer coefficient associated with the pre-chamber. DI engines have a fuel consumption that is about 10-15% lower than IDI engines.

The combustion speed in DI engines is still limited, and the maximum speed for any DI engine is about 4500 rpm. With displacements of more than 500 cm^3/cylinder this is not significant, since the engine speed is then limited by the maximum permissible piston speed.

5.9 A proposal is being considered to convert a 2 litre automotive spark ignition engine to operation as a diesel engine. In spark ignition form the engine has a maximum bmep (with optimised air fuel ratio and ignition timing) of 10.5 bar. A decision has to be made as to whether the diesel engine will use a direct (DI) or indirect (IDI) combustion system. List concisely the advantages and disadvantages of each type of combustion system, and state the bmep that might be expected in each case.

The indirect injection engine would have less demanding fuel injection requirements, slightly lower combustion noise, but a significant (of order 10-15%) fuel consumption penalty. The emissions characteristics are quite different (see Fig 5.39)

The DI engine will have lower NOx (because of the lower compression ratio), but higher HC emissions (because of dilution at the fringes of the spray). The HC emissions will reduce with increasing load for both engines, but more significantly for the DI (over-dilution becomes less significant). At maximum bmep (about 6 or 7 bar for both engines if naturally aspirated) there is negligible difference between the HC emissions from each sort of engine.

The NOx emissions increase with load for both DI and IDI engines, but with both types retarding the injection timing is an effective way of reducing the NOx emissions. Both engine types are suited to turbocharging, and a bmep of 10.5 bar would be readily obtainable. However, the maximum speed of diesel engines is lower than SI engines, so the diesel engines will still be less powerful than the equivalent displacement SI engine. The DI engine might have a speed limit of 5000 rpm, while the IDI engine might operate at up to 5500 rpm. Higher levels of bmep are possible to compensate for a maximum speed that might be 25% below that of the SI engine. Such a turbocharged diesel engine would require intercooling, and possibly a variable geometry turbocharger and common rail injectors or unit injectors.

6 Induction and Exhaust Processes

6.1* Two possible overhead valve combustion chambers are being considered, the first has two valves, and the second design has four valves per cylinder. The diameter of the inlet valve is 23 mm for the first design and 18.5 mm for the second design. If the second design is adopted, show that the total valve perimeter is increased by 60.8 per cent. If the valve lift is restricted to the same fraction of valve diameter, calculate the increase in flow area. What are the additional benefits in using four valves per cylinder?

In the first case with 2 valves (one inlet and one exhaust), the perimeter (P_2) is:

$$P_2 = \pi d = \pi 23 = 72.26 \text{ mm}$$

In the second case with 4 valves (two inlet and two exhaust), the perimeter (P_4) is:

$$P_4 = 2\pi d = 2\pi 18.5 = 116.24 \text{ mm}$$

The percentage increase in valve perimeter is: $100 \times (P_4 - P_2)/P_2 = 100 \times (116.24 - 72.26)/72.26 = 60.86\%$

Using the valve curtain area (A_c)to define the flow area:

$$A_c = P \times L = \pi k d^2, \qquad \text{where the valve lift } (L) \text{ is: } L = kd$$

Thus:

$$A_{c,2} = \pi k d^2 = \pi k 23^2 = 1662k \text{ mm}^2$$

and:

$$A_{c,4} = 2\pi k d^2 = 2\pi k 18.5^2 = 2150k \text{ mm}^2$$

The increase in valve curtain area is: $(A_{c,4} - A_{c,2})/A_{c,2} = (2150 - 1662)/1662 = 0.29$, or 29%

The other advantages of four valves/cylinder are:

1) There will be a lower camshaft loading. The mass of the valves will scale with length cubed, while the contact length on the cam will scale approximately linearly. The force on the cams that arises from accelerating the valves is proportional to the mass multiplied by the acceleration: the acceleration is proportional to the lift squared. Thus the loading on the cam is proportional to the fifth power of the valve size.

2) Two inlet valves gives greater flexibility for controlling the combustion process. The use of two valves facilitates the generation of tumble (also known as barrel swirl), and this is important of generating homogeneous turbulence just prior to combustion. If one of the two inlet valves is disabled at part load operation, then the air velocity will be increased (leading to more tumble) and the asymmetry will add swirl about an axis parallel to the cylinder axis. The higher levels of swirl will enhance the combustion rate, and compensate for the tendency of the combustion to become slower at part load operation. Clearly the pressure drop across the inlet valve(s) will be increased (in order to give the flow more kinetic energy), but this will not matter, since the same mass of air has to be admitted, and there will be a corresponding reduction in the pressure drop across the inlet valve.

6.2* Describe the differences in valve timing on a naturally aspirated Diesel engine, a turbocharged Diesel engine, and a high performance petrol engine?

The naturally aspirated Diesel engine is likely to have valve timings something like:

Inlet valve opens (ivo)	10° before tdc (btdc)
Exhaust valve closes (evc)	10° after tdc (atdc)
Inlet valve closes (ivc)	40° after bdc (abdc)
Exhaust valve opens (evo)	40° before bdc (bbdc)

This gives a valve overlap period (when both the inlet and exhaust valves are open) of 20 degrees centred on top dead centre (tdc). The valve overlap period might be slightly less, so as to avoid valve clash - that is, the piston hitting the valves at top dead centre. The opening of the exhaust valve is a compromise between:

a) reducing the (positive) expansion work with earlier opening, and

b) reducing the (negative) pumping work, because the pressure in the cylinder will be lower as more of the exhaust gases will have been expelled before the start of the exhaust stroke.

Fortunately the engine performance is fairly insensitive to the exhaust valve opening; a ten degree change would not have much effect.

The inlet valve is closed after bottom dead centre. If there was no fluid friction, and the inlet valve could be closed instantaneously, then the highest volumetric efficiency would be obtained by having the inlet valve close at bottom dead centre (bdc). However, the inlet valve takes a finite time to close, and because of fluid friction, then the pressure in the cylinder will be below the manifold pressure at bdc. The volumetric efficiency is maximised by delaying the inlet valve closure. The greater the speed of the engine, then the later the optimum inlet valve closure. The delayed inlet valve closure reduces the compression ratio slightly - at 40°abdc the piston will have moved about 12% of its stroke, but because the inlet valve closes slowly, the compression process will have started before the inlet valve is closed. In any case, the expansion ratio is a more important determinant of the cycle efficiency than the compression ratio.

The highly turbocharged Diesel engine (with a pressure ratio of say 3) is likely to have the following valve timings:

Inlet valve opens (ivo)	60° before tdc (btdc)
Exhaust valve closes (evc)	60° after tdc (atdc)
Inlet valve closes (ivc)	40° after bdc (abdc)
Exhaust valve opens (evo)	40° before bdc (bbdc)

This gives a valve overlap period of 120 degrees centred on top dead centre (tdc). When the engine is at medium to high loads, then the boost pressure from the compressor will be greater than the back pressure from the turbine, and during the valve overlap period air will flow from the inlet manifold into the exhaust system. This air flow reduces the residuals level in the cylinder, and helps to cool the exhaust valves and piston. Since fuel is only injected during the compression stroke, then there is no los of fuel. Because the maximum speed of the engine will not have changed from the naturally aspirated case, then the exhaust valve opening and the inlet valve closing events are not likely to have been changed.

The high performance spark ignition engine is likely to have the following valve timings:

Inlet valve opens (ivo)	40° before tdc (btdc)
Exhaust valve closes (evc)	40° after tdc (atdc)
Inlet valve closes (ivc)	55° after bdc (abdc)
Exhaust valve opens (evo)	55° before bdc (bbdc)

This gives a valve overlap period of 80 degrees centred on top dead centre (tdc). Such an engine is likely to have induction and exhaust systems that have been tuned to so as to improve the engine performance at the rated speed for maximum power. The exhaust system will have been tuned so that a rarefaction (low pressure) wave arrives at the exhaust valve just prior to the exhaust valve closure; this will help remove the products of combustion, and draw in the new charge of air and fuel. The advantage of opening the inlet valve early, is that when the induction stroke commences, then the inlet valve will well on its way to being fully open. he disadvantages of a large valve overlap with a spark ignition engine are twofold:

> Firstly, at wide open throttle during the valve overlap period, fuel and air will flow directly into the exhaust system. This loss of fuel economy can be tolerated in a high performance engine.
>
> Secondly, at low loads the pressure in the inlet manifold will be sub-atmospheric, so that during the valve overlap period, the exhaust gases will flow into the inlet manifold. These exhaust gases will subsequently be drawn into the cylinder, thereby leading to a high level of exhaust gas residuals. This will lead to significant cycle-by-cycle variations in combustion, that will lead to poor driveability.

The maximum power output of a high performance spark ignition engine, will occur at a very high speed - perhaps double the maximum mean piston speed of a Diesel engine. Thus the inlet valve will be closed later, and the exhaust valve will be opened earlier than in lower performance engines.

6.3* **Devise an induction and exhaust system for an in-line, six-cylinder, four stroke engine with a firing order of 1-5-3-6-2-4, using: (i) twin carburettors, (ii) triple carburettors.**

When designing the inlet manifolds for these engines, the aims should be:

a) to obtain inlet tracts of approximately equal length, and

b) equally spaced induction events within each manifold.

The requirement for the exhaust system will be to have equally spaced exhaust pulses entering each manifold, with no more than three cylinders connected to a single pipe. (The exhaust events can be taken to occupy almost 240°crankangle).

For the exhaust system, cylinders 1, 2 and 3 would have primary their primary pipes connected together, and cylinders 4, 5 and 6 would be similarly connected together. The primary pipes would be about 0.5 m long, and the secondary pipes might each be about 0.7 m long before being joined together.
With the two carburettor system, a similar arrangement can be used to the exhaust system, with cylinders 1, 2 and 3 being connected to one carburettor, and cylinders 4, 5 and 6 being connected to the second carburettor. Each carburettor would be subject to induction pulses every 240°ca. The runner lengths, from the carburettor to the inlet ports, are unlikely to be longer than 0.2 m, so as to avoid excessive fuel hold-up in the inlet manifold.

With the three carburettor system, if equal phasing of the induction pulses is to be attained, then:

cylinders 1 and 6 would be connected to the first carburettor,
cylinders 2 and 5 would be connected to the second carburettor, and
cylinders 3 and 4 would be connected to the third carburettor.

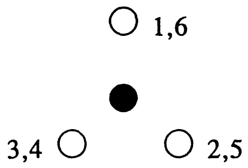
This is clearly going to lead to very complicated pipework, with many pipes having to cross over in a very short length. Furthermore, fuel would tend to accumulate in an undesirable way. The pipework for cylinders 3 and 4 is convenient, and the obvious simplification is:

cylinders 1 and 2 connected to the first carburettor, and
cylinders 5 and 6 connected to the second carburettor.

The first and second carburettors would each see the following pattern of periods between the induction pulses:

240°ca, 480°ca, 240°ca, and 480°ca. This is clearly not ideal, but it is better than trying to tie knots in the inlet manifold pipes. The outer carburettors will see a more unsteady flow than the inner carburettor, and the outer carburettors will thus tend to run richer than the middle carburettor.

It is also worthwhile checking if any other firing order might give a better performance. The following figure shows an end-on view of the crankshaft, with the crankpins numbered, for clockwise rotation:



After cylinder 1 has fired, then either cylinder 2 or 5 must fire, followed by either 3 or 4. This gives rise to three other possible firing sequences:

123654, 124653, or 154623

The first alternative (123654) has cylinders 1&2 and 5&6 firing consecutively, and this is very undesirable. The second alternative (124653) has cylinders 1&2 firing consecutively, so this is undesirable. Finally, the third alternative is no better than the original design:

Cylinders 1&2 fire with 480°ca, 240°ca, 480°ca, and 240°ca intervals,
Cylinders 3&4 fire with 360°ca intervals, and
Cylinders 5&6 fire with 240°ca, 480°ca, 240°ca, and 480°ca intervals.

Rotating the crankshaft anti-clockwise (or swopping the orientations of pins 3&4 with 2&5) would yield another four possible timing sequences, but these would have the same drawbacks as the arrangements considered above.

6.4 During the exhaust blowdown process, sketch on a temperature entropy diagram:

a) the expansion of the first element of gas to leave the cylinder
b) the in-cylinder expansion
c) the expansion of an element of gas to leave the cylinder at pressure p.

Write down in differential form, and equation for the energy associated with the expansion of an element of gas to leave the cylinder at pressure p. The by integrating this equation confirm that the temperature of the fully mixed gas at the end of blowdown is given by:

$$T_{2''} = (m_1 T_1 - m_2 T_2)/\gamma(m_1 - m_2)$$

where states 1 and 2 refer to before and after blowdown

Blowdown is assumed to occur at constant volume,and at the instant when there is mass m in the cylinder the instantaneous pressure is p and the temperature is T. If mass dm leaves the cylinder, since the expansion process is isenthalpic, then the enthalpy that leaves with it is:

$$\mathrm{d}h = c_p T \mathrm{d}m \qquad \text{(A}$$

At the end of blowdown, the mass of gas that will have entered the manifold is $(m_1 - m_2)$, and if its temperature is T_2'', then its enthalpy is:

$$H = c_p T_2''(m_1 - m_2) \qquad \text{(B}$$

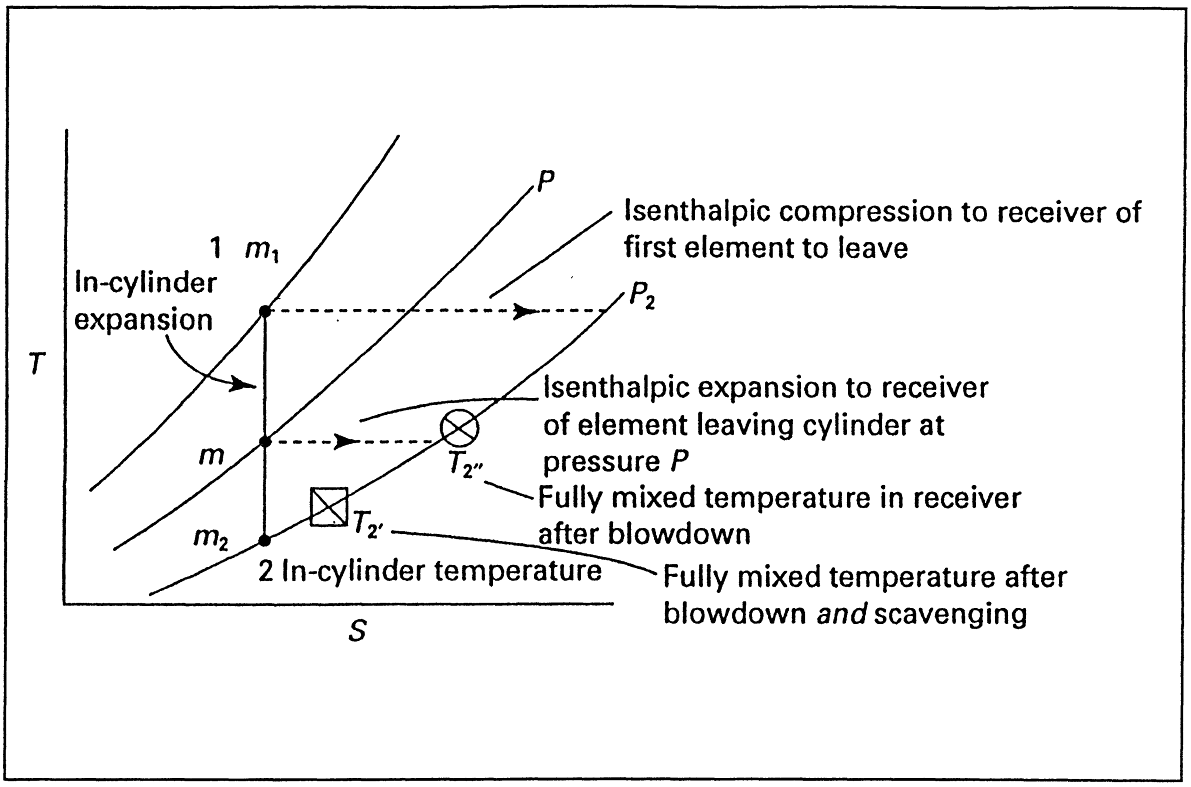


Fig 6.15

and this must correspond to the integration of Eq. A. In order to integrate Eq. A the integration needs to be in terms of mass. Since the in-cylinder expansion is isentropic at constant volume, we can make use of the following isentropic relation:

$$Tv^{\gamma-1} = \text{const.}$$

or

$$T(V/m)^{\gamma-1} = \text{const.} \qquad \text{or as } V \text{ is constant,} \qquad T = \text{const}'m^{\gamma-1} \qquad \text{(C}$$

Equation A can be integrated (by using Eq. C to eliminate T) and equated to Eq. B:

$$H = c_pT_2''(m_1 - m_2) = {}_2\int^1 c_p \,\text{const}'m^{\gamma-1}\,\mathrm{d}m = c_p\,\text{const}'{}^1\int_2 m^{\gamma-1}\,\mathrm{d}m = c_p\,\text{const}'\,[m^\gamma]^1_2/\gamma \qquad \text{(D}$$

Equation C can be used to eliminate const'$m^{\gamma-1}$, and the limits can be introduced

$$c_pT_2''(m_1 - m_2) = c_p\,[Tm]^1_2/\gamma = c_p(\mathrm{T}_1m_1 - T_2m_2) \qquad \text{(E}$$

or: $$T_{2''} = (m_1T_1 - m_2T_2)/\gamma(m_1 - m_2) \qquad \text{QED}$$

This result was obtained as Eq. 6.44, by considering only the start and end states.

6.5 **A four cylinder four-stroke engine is operating at a bmep of 2 bar. The pressure at inlet valve closure is 0.37 bar, and the fmep is 0.8 bar. Assuming that the engine gross indicated efficiency is unchanged, verify that: disablement of the valves on two cylinders would reduce the fuel consumption by about 13%, compared with about an 8% fuel saving if the fuel was not supplied**

to 2 cylinders. Assume that the gross imep is proportional to the pressure at inlet valve closure, and that the gross indicated efficiency is constant. State any additional assumptions that you make. By means of pV diagram sketches, explain why disabling only the inlet valves would have a fuel economy benefit comparable to fuel disablement to 2 cylinders.

With 4 cylinders operating the mep breakdown is as follows:

	mep (bar)
pmep	0.63
fmep	0.8
bmep	2.0
	=====
gross imep	3.43

As p_{ivc} is 0.37 bar, and the in cylinder pressure can be assumed to attain the p_{ivc} immediately after inlet valve opening (ivo)

With two cylinders disabled and no change to the fuel flowrate, then the gross imep would become (2 x 3.42). But since the fuel consumption is reduced by 13%, and the gross imep is assumed to be proportional to fuel flowrate, then the gross imep with 2 cylinders is (2 x 3.43 x 0.87 = 5.97).

For a pair of cylinders (with only one firing):

	mep (bar)	
gross imep	5.97	
bmep	-4.00	
fmep	-1.60	
pmep	-0.36	
	0.01	QED

if the gross imep is proportional to p_{ivc} , then p_{ivc} becomes 0.37 x 5.97/3.43 = 0.64 bar. So the pmep (for one cylinder) is 0.36 bar.

With fuel disablement to two cylinders, then the pumping work is still done in the disabled cylinders. With no change to the fuel flowrate, then the gross imep would become (2 x 3.42). But since the fuel consumption is reduced by 8%, and the gross imep is assumed to be proportional to fuel flowrate, then the gross imep with 2 cylinders firing is (2 x 3.43 x 0.92 = 6.31).

For a pair of cylinders (with only one firing):

	mep (bar)	
gross imep	6.31	
bmep	-4.00	
fmep	-1.60	
pmep	-0.64	
	0.07	QED

if the gross imep is proportional to p_{ivc} , then p_{ivc} becomes 0.37 x 6.31/3.43 = 0.68 bar. So the pmep (for two cylinder) is 0.32 x 2 bar.

If the fuel consumption saving had not been given, then it would have been necessary to make a series of guesses for the pressure at inlet valve closure until the mean effective pressures summed to zero.

The following pV diagrams have been plotted on a logarithmic basis, so that the compression and expansion processes appear as straight lines. It should also be remembered that any loop enclosed by an anti-clockwise path represents negative work.

Fuel Disablement

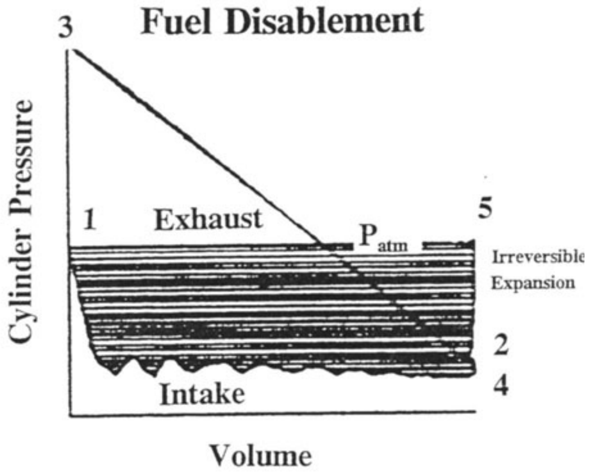
The inlet manifold pressure is assumed to be at atmospheric, and because of a small volume downstream of the throttle plate, the in-cylinder pressure falls rapidly (see Fig 6.24) during induction, 1→2. Compression starts at inlet valve closure (ivc) and the pressure at exhaust valve opening (evo, 4) is lower than at ivc because of in-cylinder heat transfer away from the gas. At evo there is irreversible expansion with the reverse flow of gases from the exhaust manifold, so the in-cylinder pressure rises 4→5. During the exhaust stroke (5→1) work is done in expelling these gases from the cylinder. The work dissipated by pumping approximates to the rectangular area shown.

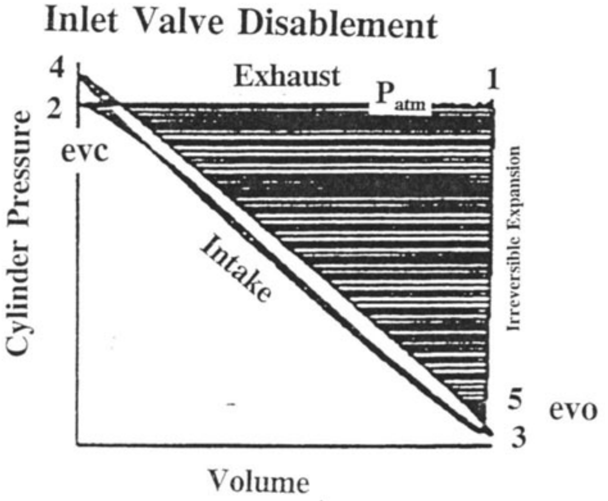
Inlet Valve Disablement

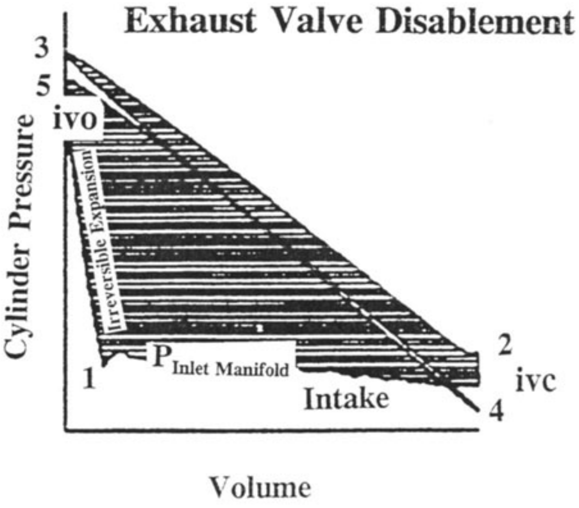
During the exhaust stroke (1→2) the in-cylinder pressure is approximately atmospheric, and after exhaust valve closure (evc) the pressure falls during the 'induction' stroke, 2→3. The compression and expansion processes (3→4→5) follow approximately the same paths, and at the end of the expansion stroke with exhaust valve opening (evo) there is irreversible expansion, with the reverse flow of gases from the exhaust manifold raising the in-cylinder pressure, 5→1. During the exhaust stroke work is done in expelling these gases from the cylinder. The work dissipated by pumping approximates to the triangular area shown.

Exhaust Valve Disablement

During the inlet stroke (1→2) the in-cylinder pressure is approximately equal to the inlet manifold pressure. The compression and expansion processes (2→3→4) follow approximately the same paths, and at the end of the expansion the in-cylinder pressure is slightly below the pressure at the start of compression. During the 'exhaust' stroke (4→5) the charge is again compressed, and at inlet valve opening the there is irreversible expansion (5→1) back to the inlet manifold pressure. The work dissipated by pumping approximates to the triangular area shown.


Fuel Disablement


Inlet Valve Disablement


Exhaust Valve Disablement

Adapted From: Sandford, M H, Allen, J and Tudor, R, (1998),'Reduced Fuel Consumption and Emissions Through Cylinder Deactivation', IMechE Seminar Publication 'Future Engine and System Technologies', Professional Engineering Publications, London.

7 Two-Stroke Engines

7.1 **The Ford 2-stroke engine has a swept volume of 1.2 litres. At a speed of 5500 rpm the full load torque is 108 Nm and the brake specific fuel consumption is 294 g/kWh. Calculate the brake mean effective pressure, and the brake efficiency (assume a Calorific Value of 43 MJ/kg). Give 5 reasons why the brake efficiency is lower than the value predicted by the Otto cycle analysis?**

If the torque is reduced to 27 Nm (at the same speed) suppose that the brake specific fuel consumption rises to 325 g/kWh. Calculate the brake efficiency and explain why it is lower than at full load. What is the key attribute of the Ford/Orbital 2-stroke engine?

Firstly, Power, $W_b = T \text{ x } \omega = 108 \text{ x } (5500/60) \text{ x } 2\pi =$ **62.2 kW**

Next we can calculate the bmep by rearrangement of equation 2.38:

$$\text{bmep} = \text{brake power}/(V_s \text{x} N^*)$$

where: V_s = swept volume, and
N^* = number of times the swept volume is exchanged per second, remembering that this is a two-stroke engine, in which the volume is swept every revolution

$$\text{bmep} = 62.2\text{x}10^3/(1.2\text{x}10^{-3} \text{ x } [5500/60]) = 5.65\text{x}10^5 \qquad \text{or } \mathbf{5.65 \text{ bar}}$$

Equation 2.14 can be rearranged to calculate the brake efficiency (η_b)

$$\eta_b = 1/(\text{bsfc x CV})$$

where: bsfc is the brake specific fuel consumption (kg/MJ), and
CV is the calorific value of the fuel, or

$$\eta_b = 3.6/(\text{bsfc x CV})$$

when: bsfc is the brake specific fuel consumption (kg/kWh), since 1 kWh ≡ 3.6 MJ.

$$\eta_b = 3.6/(0.294 \text{ x } 43) = 0.285 \quad \text{or } \mathbf{28.5\ \%}$$

The brake efficiency is lower than that predicted by the Otto cycle, because:

a) mechanical losses,
b) heat transfer during expansion and compression,
c) non-instantaneous combustion
d) real thermodynamic behaviour of the gases (the increase of the specific heat capacities with increasing temperature),
e) dissociation means that the full calorific value of the fuel is not converted to thermal energy,
f) exhaust port (or valve) opens before the end of the expansion stroke
g) full power implies a rich mixture, and thus partially burnt fuel in the exhaust
h) leakage past the piston (and any valves),
i) cycle-by-cycle variations in combustion.

At part load the bsfc is 325 g/kWh, so the brake efficiency becomes:

$$\eta_b = 3.6/(0.325 \text{ x } 43) = 0.258 \quad \text{or } \mathbf{25.8\ \%}$$

The brake efficiency has fallen at part load, because:

a) mechanical losses have become more significant,
b) the pressure drop associated with throttling dissipates work,
c) the lower inlet system pressure during the gas exchange process means that more exhaust residuals will remain in the cylinder, and this will increase the level of the cycle-by-cycle variations in combustion.

(although the mixture will be weaker than at full load, this is not enough to offset the above losses).

The Ford two-stroke engine uses in-cylinder fuel injection, with air-blast atomisation. Fuel is only injected once the piston covers the inlet/outlet ports, so there are no 'short-circuiting' losses in which fuel passes directly into the exhaust system. The air blast provides a very fine (say 1-5 μm) fuel spray, that can vaporize readily in the short time available ($\approx 60°$ca, corresponding to less than 2 ms at the maximum engine speed).

7.2 The perfect mixing scavenging model assumes:

i) instantaneous homogeneous mixing occurs within the cylinder.

ii) the process occurs at a constant cylinder pressure and volume.

iii) the system is isothermal, with no heat transfer from the cylinder walls.

iv) the incoming air (or mixture) and the burned gases have equal and constant ambient densities.

Show that the scavenging efficiency (η_{sc}) is given by

$$\eta_{sc} = 1 - \exp\left(-\gamma_d\right) \text{ where } \gamma_d \text{ is the delivery ratio}$$

Sketch the variation in the scavenge efficiency with the delivery ratio, and for comparison include the results from the perfect displacement scavenging model.

Assumptions (ii), (iii) and (iv) mean that the total mass in the cylinder (*M*) is constant. The mass of air in the cylinder (m_a) is defined in terms of the instantaneous composition, *x*:

$$x = \frac{\textit{mass of air inside the cylinder}}{\textit{total mass inside the cylinder}} = \frac{m_a}{M} \qquad (1$$

Consider a time interval (dt) at time *t*, during which time a mass (dm) will both enter and leave the system. The composition of the mixture leaving the cylinder will be the same as the cylinder contents, namely a composition of *x*.

Differentiation of Eq. 1 gives: $\mathrm{d}m_a = M\mathrm{d}x$ (2

but the change in the mass of air trapped in the cylinder ($\mathrm{d}m_a$) can also be determined from the difference in the mass of air entering ($\mathrm{d}m_e$) and the mass of air in the gas mixture leaving the cylinder ($x\mathrm{d}m_l$):

$$\mathrm{d}m_a = \mathrm{d}m_e - x\mathrm{d}m_l \quad (3$$

Since the density of all the gases is the same, then:

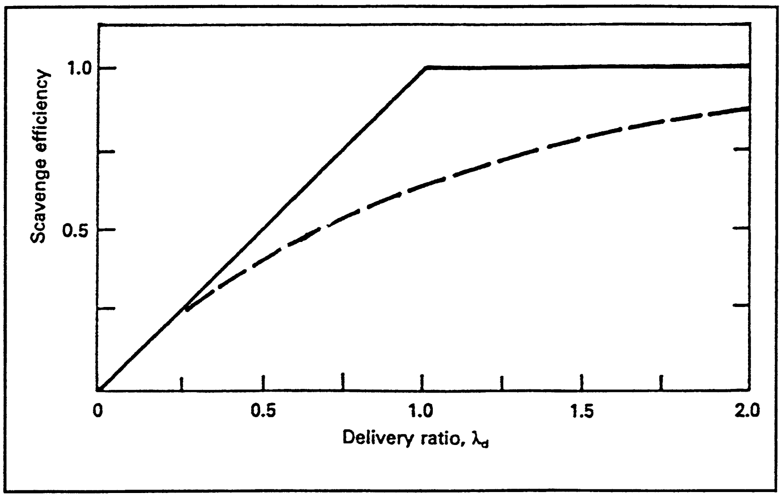
$$\mathrm{d}m_e = \mathrm{d}m_l \quad (4$$

Combining Eqs 2,3 and 4 gives:

$$M\mathrm{d}x = \mathrm{d}m_e(1 - x) \quad (5$$

or

$$\frac{dx}{1 - x} = \frac{dm_e}{M}$$



At time $t = 0$, no mass will have entered the cylinder, so $m_e = 0$, and there will be no air (only residual gases), so $x = 0$. After the end of scavenging, the mass that will have entered the cylinder, is the product of the mass in the cylinder (M) and the delivery ratio (λ_d), so $m_e = M\lambda_d$, and the air mass fraction will correspond to the scavenge efficiency, so $x = \eta_{sc}$. Using these as integration limits gives:

$$\int_0^{\eta_{sc}} \frac{dx}{1 - x} = \int_0^{\lambda_d M} \frac{dm_e}{M}$$

$$-[\ln(1 - \eta_{sc}) - \ln(1 - 0)] = M\lambda_d/M - 0$$

and

$$-\ln(1 - \eta_{sc}) = \lambda_d \qquad \text{or} \qquad \eta_{sc} = 1 - \exp(-\lambda_d)$$

8 In-Cylinder Motion and Turbulent Combustion

8.1 Verify from figure 8.7 that $l^2_m = -2/(\partial^2 R_x/\partial x^2)_{x=0}$, noting that the parabola is symmetric about the y axis.

The parabola is denoted by the broken line in figure 8.7, and we can represent it by the equation:

$$y = ax^2 + bx + c$$

Differentiating twice gives: $\mathrm{d}y/\mathrm{d}x = 2ax + b$ and $\mathrm{d}^2y/\mathrm{d}x^2 = 2a$

At $x = 0$, $y = 1$ and by symmetry $\mathrm{d}y/\mathrm{d}x = 0$, so: $1 = c$ and $0 = b$

At $y = 0$, $x = l_m$, so substitution into the parabola equation gives:

$$0 = al_m^2 + 1, \quad \text{or} \quad a = -1/l_m^2,$$

The curvature in cartesian co-ordinates, $\mathcal{C} = \dfrac{\mathrm{d}^2y/\mathrm{d}x^2}{\{1 + (\mathrm{d}y/\mathrm{d}x)^2\}^{3/2}}$

At the y axis the first derivative is zero, so $(\mathcal{C})_{x=0} = (\mathrm{d}^2y/\mathrm{d}x^2)_{x=0} = 2a = -2/l_m^2$,

The curvature of the parabola matches that of the correlation coefficient at the y axis, and noting that the correlation coefficient has a time dependency (so that partial derivatives need to be used), then finally:

$$l_m^2 = -2/(\partial^2 R_x/\partial x^2)_{x=0}$$

8.2 Evaluate the laminar burning velocity for methanol, propane, iso-octane and gasoline at:

a) 300 K and 1 bar, b) 500 K and 1 bar, and

c) 500K and 5 bar,

for the equivalence ratio range 0.7 to 1.2, using the data from Table 8.2

see over

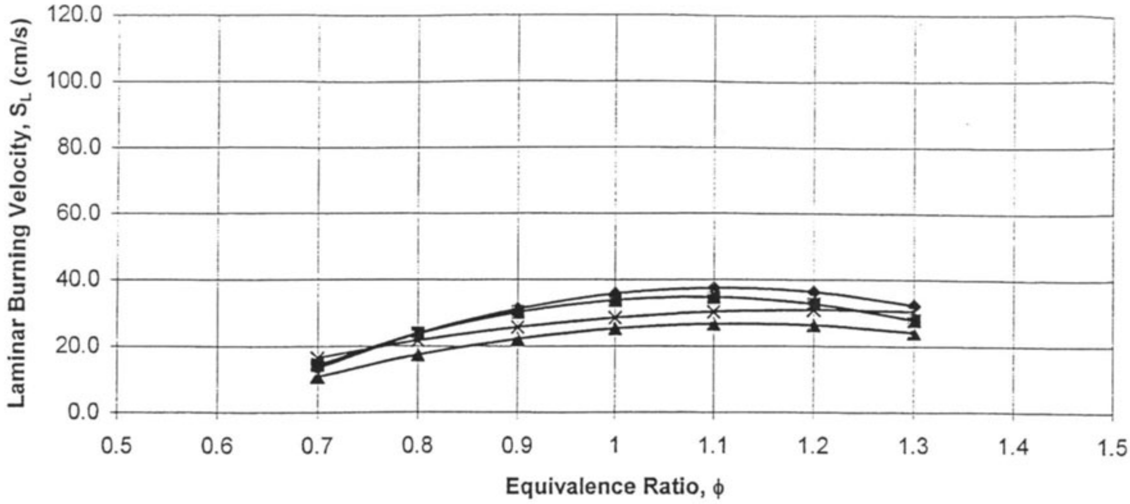


Figure 8.2b Laminar Burning Velocities at 500K and 1 bar

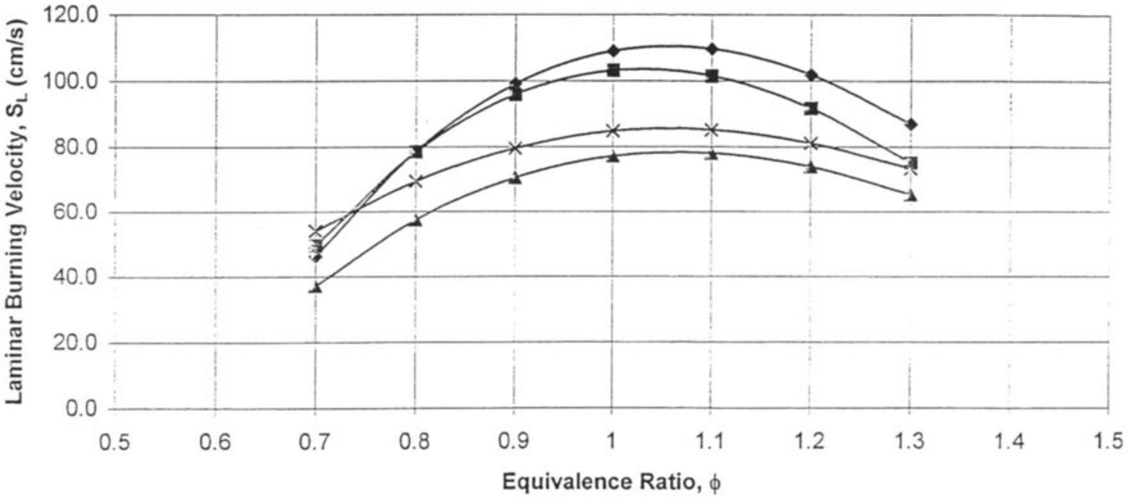
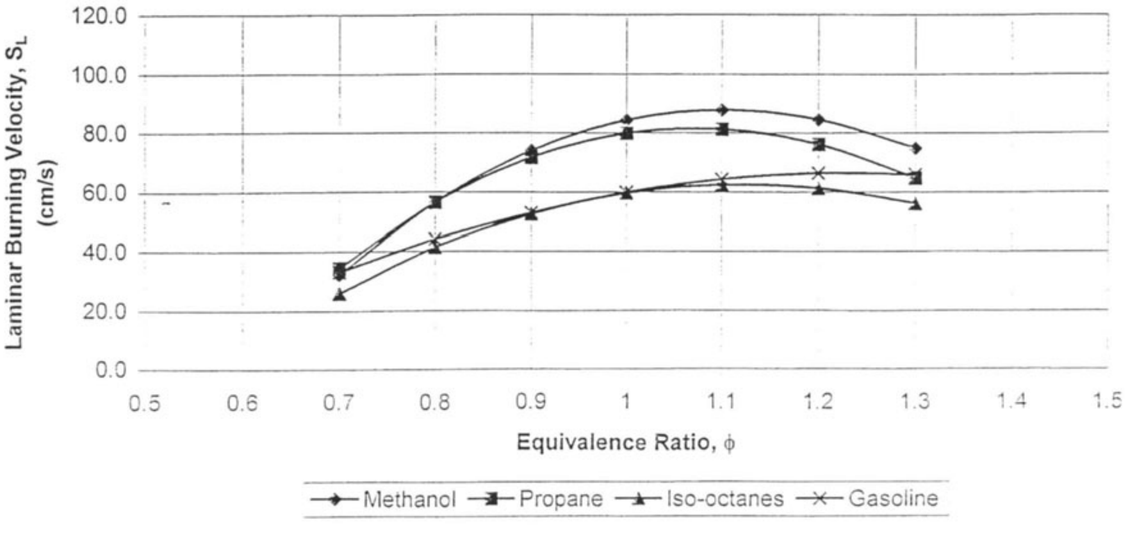


Figure 8.2c Laminar Burning Velocities at 500K and 5 bar



9 Turbocharging

9.1* A spark ignition engine is fitted with a turbocharger that comprises a radial flow compressor driven by a radial flow exhaust gas turbine. The gravimetric air/fuel ratio is 12:1, with the fuel being injected between the compressor and the engine. The air is drawn into the compressor at a pressure of 1 bar and at a temperature of 15°C. The compressor delivery pressure is 1.4 bar. The exhaust gases from the engine enter the turbine at a pressure of 1.3 bar and a temperature of 710°; the gases leave the turbine at a pressure of 1.1 bar. The isentropic efficiencies of the compressor and turbine are 75 per cent and 85 per cent, respectively.

Treating the exhaust gases as a perfect gas with the same properties as air, calculate:

(i) the temperature of the gases leaving the compressor and turbine

(ii) the mechanical efficiency of the turbocharger.

Figure 9.29 has been repeated here, so as to define the stations around the compressor, and to show a comparison between the reversible processes (continuous lines) and the real processes which are irreversible (broken lines).

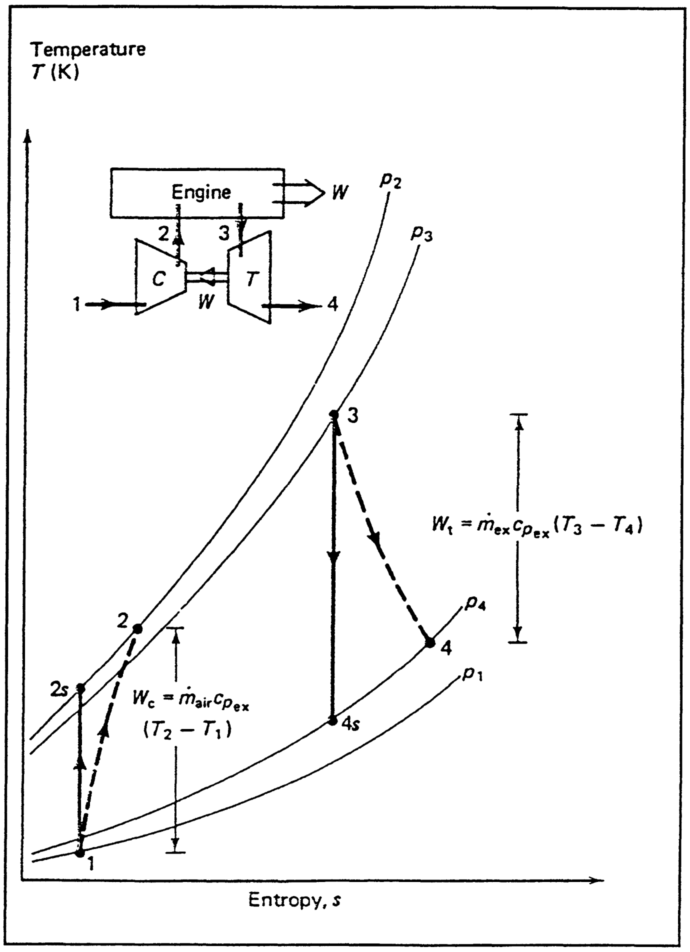


Figure 9.29 Temperature/entropy diagram for a turbocharger

We will assume that for the ratio of specific heat capacities, $\gamma = 1.4$, and the specific heat capacity at constant pressure (c_p)

First we will analyse the compressor. Remembering to use both absolute pressures, and absolute temperatures. For an isentropic process:

$$T_{2S} = T_1\ (p_2/p_1)^{(\gamma-1/\gamma)}$$

$$T_{2S} = 288(1.4/1)^{(1.4-1/1.4)}$$
$$= 317.1 \text{ K}$$

The isentropic compressor efficiency (η_c) is:

$$\eta_c = (T_{2S} - T_1)/(T_2 - T_1)$$

or

$$T_2 = T_1 + (T_{2S} - T_1)/\eta_c$$
$$= 288 + (317.1 - 288)/0.75$$
$$= \mathbf{326.8\ K\ \ or\ \ 54°C}$$

Next we will analyse the turbine. For an isentropic process:

$$T_{4s} = T_3\ (p_4/p_3)^{(\gamma-1/\gamma)}$$

$$T_{4S} = 983\ (1.1/1.3)^{(1.4-1/1.4)}$$
$$= 937.2 \text{ K}$$

The isentropic turbine efficiency (η_t) is:

$$\eta_t = (T_3 - T_4)/(T_3 - T_{4s})$$

or

$$T_4 = T_3 - \eta_t(T_3 - T_{4s})$$
$$= 983 - 0.85(983 - 937.2) = \mathbf{944.1\ K\ \ or\ \ 671°C}$$

To find the mechanical efficiency of the turbocharger, we need to find the power output of the turbine, and the power absorbed by the compressor.

By assuming the compressor and turbine to both be adiabatic, and neglecting changes in the kinetic energy and potential energy, the Steady Flow Energy Equation reduces to:

$h_1 = h_2 + w$ and, for Perfect Gas behaviour we can write: $c_pT_1 = c_pT_2 + w$ or $w = c_p(T_1 - T_2)$

Thus on the T-s plot the vertical distances are proportional to work or heat flow, and an inspection of Fig. 9.20 provides a useful reminder of the definitions of isentropic efficiencies. (An irreversible adiabatic process will lead to an increase in entropy, so the path will always slope to the right. Thus, because the isobars diverge on the T-s plot, the compressor work input is increased, and the turbine work output is reduced.

The work balance equation for the turbocharger is: $W_c = \eta_{mech}W_t$

The compressor work <u>input</u> (W_c) is: $W_c = m_ac_p(T_2 - T_1)$

where: m_a is the mass of air flowing through the compressor

The turbine work <u>output</u> (W_t) is: $W_t = m_{ex}c_p(T_3 - T_4)$

where: m_{ex} is the mass of exhaust flowing through the turbocharger.

The mass flows through the turbocharger are related by the air/fuel ratio (AFR):

$$m_{ex} = m_a + m_f = m_a(1 + m_f/m_a) = m_a(1 + 1/\text{AFR})$$

Combining these four equations leads to:

$$m_ac_p(T_2 - T_1) = \eta_{mech}m_{ex}c_p(T_3 - T_4) = \eta_{mech}m_a(1 + 1/\text{AFR})c_p(T_3 - T_4)$$

or: $T_2 - T_1 = \eta_{mech}(1 + 1/\text{AFR})(T_3 - T_4)$ and $\eta_{mech} = (1 + 1/\text{AFR})^{-1}(T_2 - T_1)/(T_3 - T_4)$

Finally, substitution of the numerical values gives: $\eta_{mech} = (1 + 1/12)^{-1}(54 - 15)/(710 - 671) = \mathbf{0.923}$

9.2* Why is it more difficult to turbocharge spark ignition engines than compression ignition engines? Under what circumstances might supercharger be more appropriate?

The speed range of spark ignition engines (say 10 to 1) is greater than compression ignition engines (say 5 to 1 for a truck engine). In addition the spark ignition engine is throttled, giving a further increase in the flow rate variation (say a 5 to 1 variation at a fixed speed). Thus there is a much wider variation in the air flowrate entering a spark ignition engine than a compression ignition engine. Turbochargers are dynamic flow devices, and for efficient operation the flow angles need to match the blade angles: this only occurs at one set of flow/rotor speed combinations.

Spark ignition engines also have a lower moment of inertia than compression ignition engines, which means that the engine speed can change more rapidly. When this is combined with the higher gas flowrate variation, then this increases the significance of the tubocharger's dynamic response.

At high loads (bmep), spark ignition engines are also susceptible to self ignition of the unburned mixture which leads to combustion 'knock'. A turbocharger will raise the temperature of the trapped charge (as well, of course, as the pressure), and this increases the susceptibility of the engine to knock. This may necessitate the use of: a reduced compression ratio, higher octane rating fuels, and retarded ignition timing.

Superchargers are appropriate when:

a) The transient response is important. The supercharger is a compressor driven directly from the engine crankshaft, so there is no equivalent of turbolag The finite inertia of the turbocharger rotor means that after any change in engine operating condition (even at constant speed), a finite time is needed for the turbocharger to accelerate, since the increased kinetic energy of the rotor can only come from the exhaust gas stream.

b) An approximately uniform increase in torque is required across the whole speed range. Superchargers are usually positive displacement compressors (a notable exception being radial flow compressors used on high performance aircraft engines) with direct drive from the engine crankshaft, so that the fractional increase in air flow is essentially independent of speed. In contrast, the fractional increase in air flow through a turbocharger is highly dependent on engine speed, until the wastegate (if fitted) starts to open and thereby control the pressure ratio.

c) Fuel economy is not of great importance. The power to drive the supercharger has to come from the crankshaft, and this imposes a fuel consumption penalty. In contrast, the turbocharger utilises the exhaust stream energy. Since the supercharger will gives a relatively greater increase in bmep at low engine speeds, then there is an increased need to take measures to avoid knock. Lowering the compression ratio, and retarding the ignition timing both ameliorate knock, but at the expense of lowering the engine brake efficiency.

9.3* Why do compression ignition engines have greater potential than spark ignition engines for improvements in power output and fuel economy as a result of turbocharging? When is it most appropriate to specify an inter-cooler [consider Eq. 9.10 to illustrate the answer].

Compression ignition engines have greater potential than spark ignition engines for increasing the power output because:

a) The bmep is inherently lower in naturally aspirated compression ignition engines than for spark ignition engines (say 7.5 bar compared to 10 bar), so a fixed improvement is more significant.

b) At high loads (bmep), spark ignition engines are susceptible to self ignition of the unburned mixture which leads to combustion 'knock'. A turbocharger will raise the temperature of the trapped charge (as well, of course, as the pressure), and this increases the susceptibility of the engine to knock. This may necessitate the use of: a reduced compression ratio, higher octane rating fuels, and retarded ignition timing. Compression ignition engines do not suffer these combustion difficulties, and the maximum boost pressure will be limited by the thermal loading and the maximum cylinder pressure. The maximum cylinder pressure will be limited to 150 or 160 bar in the highest output engines; the maximum cylinder pressure is also indicative of the thermal loading, and of course pressure is much easier to measure. To limit the maximum cylinder pressure, the compression ratio can be reduced. In some large engines (bore of say 0.25m and above) the compression ratio may be as low as 12:1, which can lead to difficulty in starting, and in low load operation. At low loads the ignition delay can be excessive, so that a substantial quantity of fuel vaporises and forms a flammable mixture with the air. When ignition does occur there is a very rapid pressure rise that can damage the piston in the same way as gasoline knock.

The fuel economy of compression ignition engines is usually improved by turbocharging because the frictional losses do not rise in proportion to the output. In other words, the mechanical efficiency of the engine is improved. To a first order, for every 10% increase in output, there will be about a 1% reduction in the minimum brake specific fuel consumption of the engine. These improvements could also occur with spark ignition engines if high octane rating fuels (that is, with a high resistance to 'knock') are available. However, the compression ratio of a spark ignition engine is maximised, so as to fully exploit the available octane rating. Thus to avoid knock in spark ignition engines it is necessary to use a combination of a reduced compression ratio, and a retarded ignition timing, both of which have fuel economy penalties.

Intercoolers become more appropriate as the boost pressure is raised, and or when the compressor isentropic efficiency is low. This can be demonstrated by an examination of Eq. 9.10:

$$\frac{\rho_3}{\rho_1} = \frac{p_2}{p_1}\left[1 + (1 - \epsilon)\frac{(p_2/p_1)^{(\gamma - 1)/\gamma} - 1}{\eta_c}\right]^{-1} \qquad (9.10$$

Substitution of $\epsilon = 0$ will give us the density ratio with no intercooler, and this divided into Eq. 9.10 will give us the fractional increase in density attributable to the intercooler (I), and using the following definition of the isentropic temperature ratio (θ):

$$\theta = p_2/p_1^{(\gamma-1)/\gamma} \qquad \text{and}$$

$$I = \frac{1 + \dfrac{(\theta - 1)}{\eta_c}}{1 + (1 - \epsilon)\dfrac{\theta - 1}{\eta_c}}$$

or

$$I = \frac{\eta_c + (\theta - 1)}{\eta_c + (1 - \epsilon)(\theta - 1)}$$

Since $0 < \epsilon < 1$, then the denominator is always smaller than the numerator, and $I > 1$

a) As the compressor isentropic efficiency is reduced, the reduction in the denominator is greater than the numerator, and I increases, ie the benefit of having an intercooler increases.

b) As the pressure ratio is increased (and the isentropic temperature ratio, θ, will be increased), the increase in the denominator is less than the numerator, and I increases, ie the benefit of having an intercooler increases.

9.4* Derive an expression that relates compressor delivery pressure (p_2) to turbine inlet pressure (p_3) for a turbocharger with a mechanical efficiency η_{mech}, and compressor and turbine isentropic efficiencies η_c and η_t, respectively. The compressor inlet conditions are p_1, T_1, the turbine inlet temperature is T_3, and the outlet pressure is p_4. The air/fuel ratio (AFR) and the differences between the properties of air (suffix a) and exhaust (suffix e) must all be considered.

By assuming the compressor and turbine to both be adiabatic, and neglecting changes in the kinetic energy and potential energy, the Steady Flow Energy Equation reduces to:

$$h_1 = h_2 + w \qquad \text{and, for Perfect Gas behaviour we can write: } c_pT_1 = c_pT_2 + w \ \text{ or } w = c_p(T_1 - T_2)$$

Thus on the T-s plot (Fig. 9.29) the vertical distances are proportional to work or heat flow, and an inspection of Fig. 9.29 provides a useful reminder of the definitions of isentropic efficiencies. (An irreversible adiabatic process will lead to an increase in entropy, so the path will always slope to the right. Thus, because the isobars diverge on the T-s plot, the compressor work input is increased, and the turbine work output is reduced.

The compressor work input (W_c) is: $W_c = m_a c_{p,a}(T_2 - T_1)$

where: m_a is the mass of air flowing through the compressor

We need to determine temperature T_2 in terms of the pressure ratio and the compressor isentropic efficiency (η_c):

$$T_{2s} = T_1 (p_2/p_1)^{(\gamma a-1/\gamma a)}$$

Using the following definition of the isentropic temperature ratio across the compressor (θ_c):

$$\theta_c = [p_2/p_1]^{(\gamma a-1)/\gamma a} \qquad \text{gives: } T_{2s} = T_1\theta_c$$

For Perfect Gas behaviour, the isentropic compressor efficiency (η_c) is:

$$\eta_c = (T_{2s} - T_1)/(T_2 - T_1) \qquad \text{so } (T_2 - T_1) = (T_{2s} - T_1)/\eta_c = T_1(\theta_c - 1)/\eta_c$$

Finally, the compressor work input (W_c) is: $W_c = m_a c_{p,a}(T_2 - T_1) = m_a c_{p,a} T_1(\theta_c - 1)/\eta_c$ (A

The turbine work output (W_t) is: $W_t = m_{ex} c_{p,ex}(T_3 - T_4)$

where: m_{ex} is the mass of exhaust flowing through the turbocharger.

We need to determine temperature T_4 in terms of the pressure ratio across the turbine and the turbine isentropic efficiency (η_t):

$$T_{4s} = T_3(p_4/p_3)^{(\gamma ex-1/\gamma ex)}$$

Using the following definition of the isentropic temperature ratio across the turbine (θ_t):

$$\theta_t = [p_3/p_4]^{(\gamma ex-1)/\gamma ex} \qquad \text{gives: } T_{4s} = T_3/\theta_t$$

For Perfect Gas behaviour, the isentropic turbine efficiency (η_t) is:

$$\eta_t = (T_3 - T_4)/(T_3 - T_{4s}) \qquad \text{so } (T_3 - T_4) = (T_3 - T_{4s})\eta_t = T_3(1 - 1/\theta_t)\eta_t$$

Finally, the turbine work output (W_t) is: $W_t = m_{ex} c_{p,ex}(T_3 - T_4) = m_{ex} c_{p,ex} T_3(1 - 1/\theta_t)\eta_t$ (B

The mass flows through the turbocharger are related by the air/fuel ratio (AFR):

$$m_{ex} = m_a + m_f = m_a(1 + m_f/m_a) = m_a(1 + 1/\text{AFR}) \qquad \text{(C}$$

The work balance equation for the turbocharger is: $W_c = \eta_{mech} W_t$ (D

Substitution of Equations A and B gives:

$$m_a c_{p,a} T_1(\theta_c - 1)/\eta_c = \eta_{mech} m_{ex} c_{p,ex} T_3(1 - 1/\theta_t)\eta_t$$

Incorporating Eq. (D) gives:

$$c_{p,a}T_1(\theta_c - 1)/\eta_c = \eta_{mech}c_{p,ex}T_3(1 - 1/\theta_t)\eta_t(1 + 1/\mathrm{AFR}) \qquad \text{(E}$$

or

$$\theta_c - 1 = \eta_c\eta_{mech}\eta_t(c_{p,ex}/c_{p,a})(T_3/T_1)(1 - 1/\theta_t)(1 + 1/\mathrm{AFR}) \qquad \text{(F}$$

Substitution for θ_c and θ_t gives;

$$[p_2/p_1]^{(\gamma a-1)/\gamma a} - 1 = \eta_c\eta_{mech}\eta_t(c_{p,ex}/c_{p,a})(T_3/T_1)(1 - [[p_3/p_4]^{(\gamma ex-1)/\gamma ex}]^{-1})(1 + 1/\mathrm{AFR}) \qquad \text{(G}$$

or

$$[p_2/p_1]^{(\gamma a-1)/\gamma a} - 1 = \eta_c\eta_{mech}\eta_t(c_{p,ex}/c_{p,a})(T_3/T_1)(1 - [p_4/p_3]^{(\gamma ex-1)/\gamma ex})(1 + 1/\mathrm{AFR})$$

9.5* Why do turbochargers most commonly use radial flow compressors and turbines with non-constant pressure supply to the turbine?

Radial flow compressors are used in preference to axial flow compressors because:

a) The desired pressure ratio can easily be obtained from a single stage of compression.

b) With a vaneless diffuser (or variable geometry diffuser) they are tolerant of a wider flow range.

c) Although the efficiency of radial flow compressors is inherently lower than for axial flow compressors because of higher secondary losses. Secondary losses are caused by secondary flows, which are flows that occur in addition to the desired (primary) flows. In the case of radial compressors, Coriolis accelerations are a source of secondary flows that are not present in axial flow compressors. In the flow range needed for IC engines, the effects of scale reduce the efficiency of axial compressors more than radial flow compressors. These effects are associated with leakage flows, such as past the ends of the blades.

The expansion ratios in tubocharger turbines can be accommodated by a single axial turbine stage (stator and rotor), and above a certain size the inherently higher efficiency of an axial flow turbine compensates for the greater sensitivity to losses associated with small sizes. Axial flow turbines are likely to be encountered in engines over about 1 MW, for which the turbine power will be about 100 kW.

Constant pressure turbine arrangements are used because:

a) The more compact exhaust manifold is easier to accommodate, and will give a more rapid transient response.

b) Although the turbine will have a lower efficiency when subject to a pulsating flow, full use is made of the pressure pulsations from exhaust 'blow-down' as the exhaust valve is opened.

Constant pressure turbocharging can be advantageous with very high boost pressures (say pressure ratios above 3), but such engines with constant pressure turbocharging will not have a good performance at part load.

9.6* Why does turbocharging a compression ignition engine normally lead to an improvement in fuel economy, while turbocharging a spark ignition engine usually leads to decreased fuel economy?

The fuel economy of compression ignition engines is usually improved by turbocharging because the frictional losses do not rise in proportion to the output. In other words, the mechanical efficiency of the engine is improved. To a first order, for every 10% increase in output, there will be about a 1% reduction in the minimum brake specific fuel consumption of the engine.

Consider a turbocharged diesel engine, for which the imep is 12 bar, and the fmep is 1.5 bar. This will give a bmep of 10.5 bar. Suppose the bmep is raised to 11.5 bar (an increase of 9.5%). With no changes to the frictional losses, the imep will be 13 bar. Suppose there is no change in the indicated efficiency, so that the fuel flow rate is proportional to the imep. The brake efficiency (η_b) of the engine is thus proportional to:

bmep/imep or the mechanical efficiency of the engine.

Using * to denote the performance of the higher output engine build:

$$\eta_b \; \alpha \; 10.5/12 = 0.875 \qquad \eta_b{}^* \; \alpha \; 11.5/13 = 0.885$$

This is an improvement of (0.885 - 0.875)/0.875, or 1.1%

Such improvements could also occur with spark ignition engines if high octane rating fuels (that is, with a high resistance to 'knock') are available. At high loads (bmep), spark ignition engines are susceptible to self-ignition of the unburned mixture which leads to combustion 'knock'. When the unburnt mixture is self-ignited the ensuing rapid pressure rise can cause structural oscillations that are audible as 'knock'. Self-ignition occurs when the unburnt mixture has been at a high enough temperature for sufficient time. A turbocharger will raise the temperature of the trapped charge (as well, of course, as the pressure), and this increases the susceptibility of the engine to knock. This may necessitate the use of: a reduced compression ratio, higher octane rating fuels, and retarded ignition timing. Knock is undesirable, since the pressure waves in the combustion chamber disrupt the thermal boundary layers, and this can lead to overheating of components. Compression ignition engines do not suffer these combustion difficulties, and the maximum boost pressure will be limited by the thermal loading and the maximum cylinder pressure.

However, the compression ratio of a spark ignition engine is maximised, so as to fully exploit the available octane rating. Thus to avoid knock in spark ignition engines it is necessary to use a combination of a reduced compression ratio, and a retarded ignition timing, both of which have fuel economy penalties.

9.7* Show that the density ratio across a compressor and intercooler is given by

$$\frac{\rho_3}{\rho_1} = \frac{p_2}{p_1}\left[1 + (1 - \epsilon)\frac{(p_2/p_1)^{(\gamma - 1)/\gamma} - 1}{\eta_c}\right]^{-1}$$

where 1 refers to compressor entry
2 refers to compressor delivery
3 refers to inter-cooler exit
η_c compressor isentropic efficiency
ϵ inter-cooler effectiveness = $(T_2 - T_3)/(T_2 - T_1)$.

Neglect the pressure drop in the inter-cooler, and state any assumptions that you make.

Plot a graph of the density ratio against effectiveness for pressure ratios of 2 and 3, for ambient conditions of 1 bar, 300 K, if the compressor isentropic efficiency is 70 per cent.
What are the advantages and disadvantages in using an intercooler? Explain under what circumstances it should be used?

We will assume Perfect Gas behaviour, so from the Equation of State we can write:

$$\frac{\rho_3}{\rho_1} = \frac{p_3\, T_1}{p_1\, T_3} = \frac{p_2\, T_1}{p_1\, T_3} \qquad \text{(A}$$

Since we can ignore the pressure drop in the intercooler (thus $p_3 = p_2$).

We now need to find temperature T_3 in terms of T_1, and we do this by first finding temperature T_2. For an isentropic process:

$$T_{2S} = T_1\ (p_2/p_1)^{(\gamma-1/\gamma)} = \phi T_1 \qquad \text{where: } \phi = (p_2/p_1)^{(\gamma-1/\gamma)}$$

Assuming that the compressor is adiabatic, the isentropic compressor efficiency (η_c) is:

$$\eta_c = (T_{2S} - T_1)/(T_2 - T_1)$$

or

$$T_2 = T_1 + (T_{2S} - T_1)/\eta_c \qquad \text{(B}$$

Substituting for T_{2s}, and dividing both sides by T_1 gives:

$$T_2/T_1 = 1 + (\phi - 1)/\eta_c \qquad \text{(C}$$

We now have to rearrange the equation that defines the intercooler effectiveness ($\epsilon = (T_2 - T_3)/(T_2 - T_1)$)

$$T_3 = T_2(1 - \epsilon) + \epsilon T_1 \quad \text{or dividing both sides by } T_1 \text{ gives: } T_3/T_1 = (T_2/T_1)(1 - \epsilon) + \epsilon \qquad \text{(D}$$

Substituting for T_2/T_1 gives: $T_3/T_1 = (1 + (\phi - 1)/\eta_c)(1 - \epsilon) + \epsilon$

$$T_3/T_1 = 1 - \epsilon + ((\phi - 1)/\eta_c)(1 - \epsilon) + \epsilon = 1 + ((\phi - 1)/\eta_c)(1 - \epsilon) \qquad \text{(E}$$

Substitution of T_3/T_1 into Eq A, and $\phi = (p_2/p_1)^{(\gamma-1/\gamma)}$ gives:

$$\frac{\rho_3}{\rho_1} = \frac{p_2}{p_1}\left[1 + (1 - \epsilon)\frac{(p_2/p_1)^{(\gamma - 1)/\gamma} - 1}{\eta_c}\right]^{-1}$$

Next we need to evaluate the density ratio for the two cases:

i) $\eta_c = 0.7 \quad p_2/p_1 = 2$

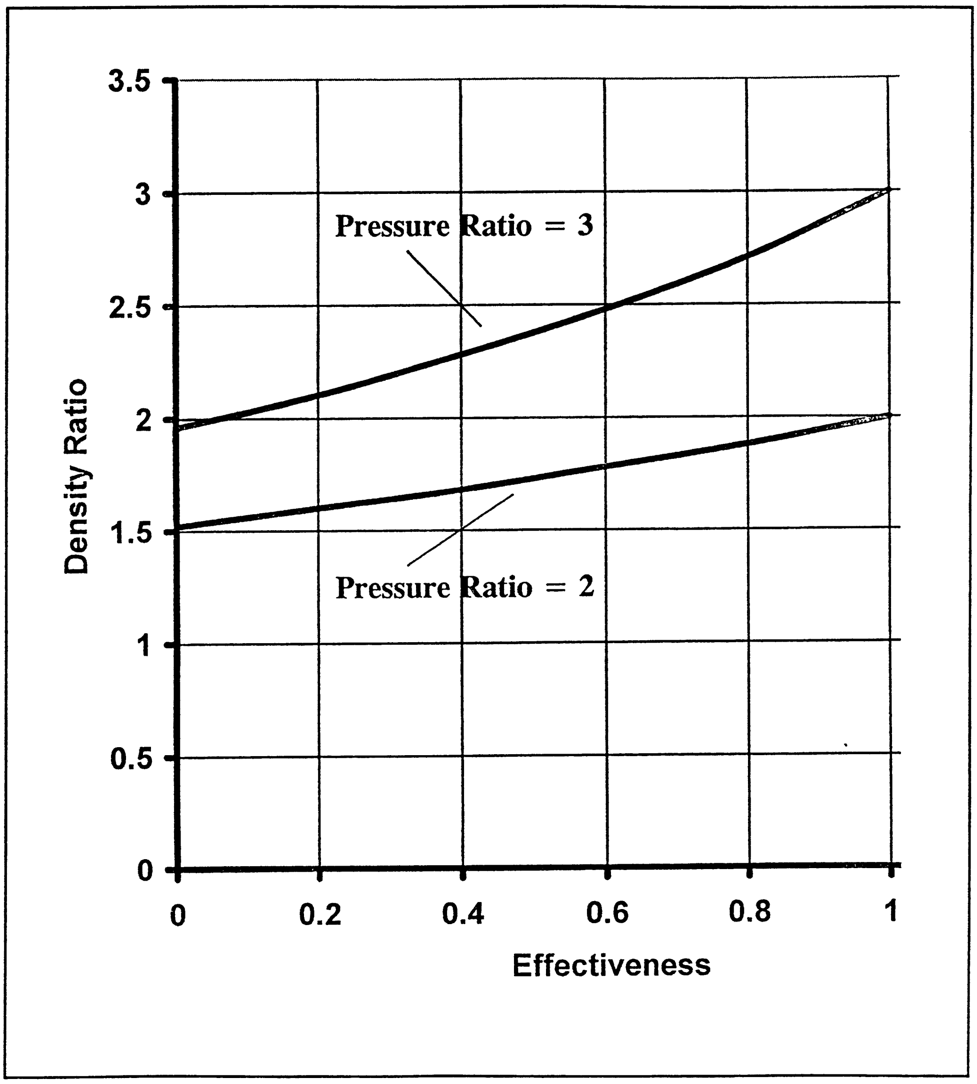
$$\left[\frac{(p_2/p_1)^{(\gamma - 1)/\gamma} - 1}{\eta_c}\right] = \frac{2^{(1.4 - 1)/1.4} - 1}{0.7} = 0.313$$

ii) $\eta_c = 0.7 \quad p_2/p_1 = 3$

$$\left[\frac{(p_2/p_1)^{(\gamma - 1)/\gamma} - 1}{\eta_c}\right] = \frac{3^{(1.4 - 1)/1.4} - 1}{0.7} = 0.527$$

We can now construct a table of the density ratio (ρ_3/ρ_1) for different values of the effectiveness (ϵ):

	effectiveness, ϵ					
p_3/p_1	0.0	0.2	0.4	0.6	0.8	1.0
case (i)	1.52	1.60	1.68	1.78	1.88	2.00
case (ii)	1.96	2.11	2.28	2.48	2.71	3.00



Advantages of intercooling are:

1) The mass flow rate of air is increased for a given pressure ratio, so this gives the option of increasing the fuel flowrate, thereby increasing the power output and efficiency (the efficiency will increase, since the mechanical losses do not rise in proportion to the brake power output).

2) The cooler air at the start of the compression process will lower the temperatures in all subsequent processes, and thus lower the heat transfer and thermal loading on the engine.

3) The lower combustion temperatures will lead to lower NOx emissions, since NOx formation is highly temperature dependant.

The disadvantages of intercooling are:

1) The space needed by the intercooler and its associated ductwork (for both the engine air, and the cooling medium).

2) The increased volume between the compressor and engine will worsen the transient response.

3) The lower temperatures during compression will increase the ignition delay. This will lead to an increase in the mass of flammable air/fuel mixture formed before self-ignition, and thus increase the initial rate of pressure rise and thence the combustion noise. This will be most significant at low loads, but the ignition delay can be reduced by using engine coolant as the cooling medium for the intercooler. This will infact heat the air under very low load conditions, thereby reducing the ignition delay period. The disadvantage is that the air will not be cooled as much by the intercooler at higher loads.

Intercoolers are widely used as a way of increasing the power output. Once the desired output can only be achieved by a pressure ratio of above about 2, then intercooling becomes an attractive option for compression ignition engines. Intercooling has the greatest impact when either the compressor isentropic efficiency is low, or the boost pressure ratio is high. Spark Ignition engines would only use intercooling with highly turbocharged engines, because the transient response is more important with spark ignition engines, and there is evaporative cooling by the fuel. Many turbocharged spark ignition engines in passenger vehicles do little more than compensate for the fall in volumetric efficiency at higher engine speeds. When spark ignition engines are conversions of diesel engines to run on natural gas, then the boost pressures will be higher. Natural gas has a very high octane rating (resistance to self-ignition), and there is of course no evaporative cooling effect.

9.8* **A turbocharged Diesel engine has an exhaust gas flow rate of 0.15 kg/s. The turbine entry conditions are 500°C at 1.5 bar, and the exit conditions are 450°C at 1.1 bar.**

(a) Calculate the turbine isentropic efficiency and power output.

The engine design is changed to reduce the heat transfer from the combustion chamber, and for the same operating conditions the exhaust temperature becomes 550°C. The pressure ratio remains the same, and assume the same turbine isentropic efficiency.

(b) Calculate the increase in power output from the turbine.

How will the performance of the engine be changed by reducing the heat transfer, in terms of: economy, power output an emissions?

Assume: ratio of specific heat capacities = 1.3, and c_p = 1.15 kJ/kgK.

Assuming the turbine to be adiabatic, with no mechanical loss of power, the turbine power output (W_t) is:

$$W_t = m_{ex}c_p(T_1 - T_2) = 0.15 \text{ x } 1.15 \text{ x } (500 - 450) = 8.625 \text{ kW}$$

Assuming Perfect Gas behaviour (so that $h = c_pT$), the isentropic turbine efficiency (η_t) is:

$$\eta_t = (T_1 - T_2)/(T_1 - T_{2s}) \quad \text{where:} \quad T_{2S} = T_1\,(p_2/p_1)^{(\gamma-1/\gamma)}$$

$$T_{2S} = (500 + 273)(1.1/1.5)^{([1.3 - 1]/1.3)} = 720 \text{ K or } 447°\text{C}$$

Thus: $\eta_t = (500 - 450)/(500 - 447) = 0.94$ [rather a high value, but never mind!]

For the low heat loss engine design, the turbine entry has been raised to 550°C

We need to recalculate the turbine isentropic expansion temperature:

$T_{2S} = T_1\ (p_2/p_1)^{(\gamma-1/\gamma)} = (550 + 273)(1.1/1.5)^{([1.3 - 1]/1.3)} = 766\ \text{K}$ or 493°C

Again assuming the turbine to be adiabatic, with no mechanical loss of power, the turbine power output (W_t) is:

$$W_t = m_{ex}c_p(T_1 - T_2) = m_{ex}c_p\eta_t(T_1 - T_{2s}) = 0.15 \text{ x } 1.15 \text{ x } 0.94 \text{ x } (550 - 493) = 9.24 \text{ kW}$$

an increase of **0.61 kW**

The reduced in-cylinder heat transfer will give higher gas temperatures during the expansion stroke, and this will increase the expansion work. The increased turbine work will give a higher compressor boost pressure, so that the pumping work will be reduced - it might even become a positive quantity: this will further increase the engine work output. (In reality there will also be a change in the turbine pressure ratio and mass flow, but the previous conclusion is none the less correct, with a reduction in the pumping losses.) The reduced cooling requirements permit a smaller cooling system, with reduced power requirements.

Since there has been no change to the fuelling rate of the engine, and the power output has increased, then the economy will be improved. The higher in-cylinder temperatures will tend to reduce the volumetric efficiency of the engine, but the increase in the compressor pressure ratio will dominate, so that there will be an increase in the air flow, and a weakening of the air/fuel ratio. The weaker air/fuel ratio will make the gases behave more like perfect gases, so that there will be an improvement in the cycle efficiency. If full load of the engine was restricted by smoke or particulate emissions, then the weaker air/fuel ratio will lead to more complete combustion and an improvement in the fuel economy. At part load the reduced power requirements of the cooling system will be more significant.

The higher combustion temperatures will lead to an increase in the NOx emissions, because these are very temperature sensitive. Carbon monoxide will remain negligible as the mixture is (very) weak. The unburnt hydrocarbons and particulates should reduce because the air fuel ratio will be weaker, and the higher temperatures during expansion will promote oxidation. The combustion noise should also be reduced, since the higher combustion chamber temperatures will lead to a shorter ignition delay period (this reduces the amount of flammable mixture in the pre-mixed combustion phase, and thus the maximum rate of pressure rise).

9.9* **A compressor with the performance characteristics shown in figure 9.31 is operating with a mass flow rate (m) of 49.5 g/s at an isentropic efficiency of 60 per cent. The compressor is fitted to a turbocharged and inter-cooled Diesel engine. Assume**

p	**(the compressor inlet pressure) is 95 kN/m^2**
T	**(the inlet temperature) is 291 K.**
γ	**(the ratio of gas specific heat capacities) is 1.4**
c_p	**1.01 kJ/kgK**

Calculate the pressure ratio, the compressor speed, the compressor delivery temperature, and the compressor power.

If the inter-cooler is removed and the air/fuel ratio is kept constant, how would the compressor operating point be affected? Neglecting any change in the compressor efficiency and pressure ratio, estimate the maximum increase in output that the inter-cooler could lead to. State clearly any assumptions that you make.

It must be appreciated that the compressor map parameters are not dimensionless, and thus the results that are obtained will depend on the units used. The question implies the relevant units, and these must be adhered to strictly.

Consider first the mass flow parameter:

$$m\sqrt{T}/p = 49.5\sqrt{[291]}/95 = 8.89$$

From the figure:

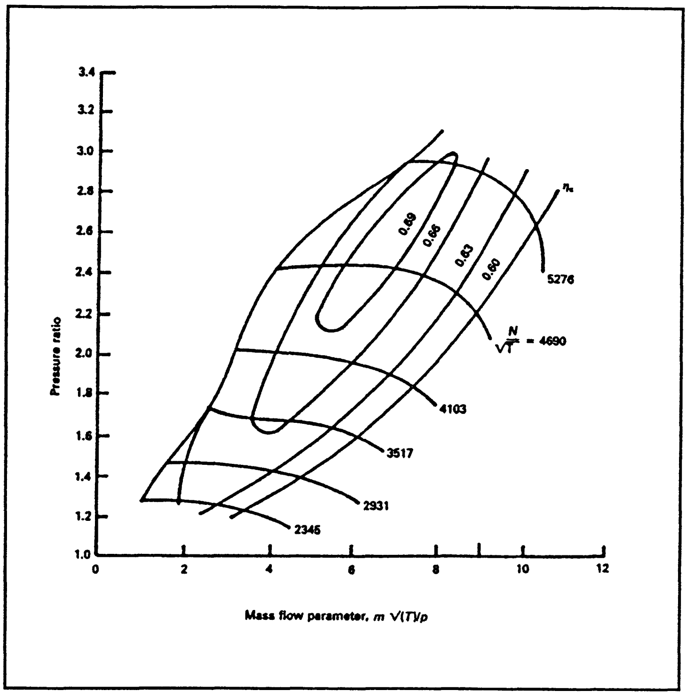
$$p_2/p_1 = 2.2,\ N/\sqrt{T} = 4690,\ \eta_c = 0.6$$

The speed, $N = 4690\sqrt{T}$
$= 4690\sqrt{291}$ = **80 000 rpm**

To determine the compressor exit temperature (T_2), we need to first calculate the isentropic compression temperature (T_{2s})

$T_{2s} = T_1\ (p_2/p_1)^{((\gamma-1)/\gamma)} = 291 \times 2.2^{([1.4-1]/1.4)}$
= **364.5 K**

Assuming Perfect Gas behaviour (so that $h = c_pT$), the isentropic compressor efficiency (η_t) is:



$$\eta_c = (T_{2S} - T_1)/(T_2 - T_1)$$

or

$$T_2 = T_1 + (T_{2S} - T_1)/\eta_c = 291 + (364.5 - 291)/0.6 = 413.5$$

The compressor work input (W_c) is: $W_c = m_a c_p (T_2 - T_1)$ where: m_a is the mass of air flow into the compressor
$= 49.5 \times 1.01 \times (413.5 - 291)$ = **6.13 kW**

If the intercooler is removed, then the mass flowrate into the engine will be reduced, and thus the mass flow parameter will be reduced. The higher inlet temperature to the engine, and the fixed air/fuel ratio, will mean a slightly higher turbine inlet temperature. Neglecting changes in the compressor and turbine efficiencies, this implies an increase in the turbine (and thus also the compressor) specific work, so the compressor pressure ratio will increase. The compressor operating point moves ↖, as indicated on the diagram. The increased pressure ratio will increase the mass flow rate of air, but not as much as the reduction caused by the lower density of the air entering the engine because of the higher air temperature when the intercooler has been removed.

To estimate the maximum increase in power output that an intercooler can lead to, we will assume: the same air/fuel ratio, the same volumetric efficiency, the same brake efficiency. In other words, we are assuming that the power output is proportional to the air mass flow rate. If the pressure ratio and the compressor isentropic efficiency remain the same, then the power output of the engine is proportional to the air density in the inlet manifold, which is inversely proportional to temperature. If the intercooler is ideal, then the air flow will be cooled from T_2 (413.5 K) to the ambient temperature T_1 (291 K).

Thus the percentage increase in power is [(413.5 - 291)/291] x 100% = 42%

There are some gross simplifications in the foregoing analysis, especially concerning the compressor operating point. The compressor operating point will move to a higher mass flow rate, and this will be accompanied by a fall in the isentropic efficiency, and a reduction in the pressure ratio. The 42% increase is thus an upper bound. More realistic assumptions that take into account the change in the compressor operating point are discussed by *Watson and Janota*[1], and an increase of about 30% is probably a more realistic assumption. However, the change is very dependant on the compressor characteristics, and the location of the initial operating point on the compressor map.

9.10* **A turbocharged six-cylinder Diesel engine has a swept volume of 39 litres. The inlet manifold conditions are 2.0 bar and 53°C. The volumetric efficiency of the engine is 95 per cent, and it is operating at a load of 16.1 bar bmep, at 1200 rpm with an air/fuel ratio of 21.4. The power delivered to the compressor is 100 kW, with entry conditions of 25°C and 0.95 bar. The fuel has a calorific value of 42 MJ/kg.**

Stating any assumptions, calculate :

(a) the power output of the engine
(b) the brake efficiency of the engine
(c) the compressor isentropic efficiency
(d) the effectiveness of the inter-cooler.

Estimate the effect of removing the inter-cooler on the power output and emissions of the engine, and the operating point of the turbocharger.

To find the brake power (W_b), we need to use Eq 2.38:

$$\text{Power, } W_b = p_b V_s N^* \qquad (2.17$$

where: p_b is the bmep (N/m^2)
V_s is the engine swept volume (m^3)
N^* is rpm/120 for a 4-stroke engine (s^{-1})

Thus: $W_b = 16.1\text{x}10^5 \text{ x } 39\text{x}10^{-3} \text{ x } 1200/120 =$ **628 kW**

To determine the brake efficiency (η_b), we need to find the fuel mass flow rate (m_f), from the air mass flow rate (m_a), and the air/fuel ratio (AFR):

The air mass flow rate (m_a) can be found from the volumetric efficiency (Eq. 2.42):

$\eta_v = V_a/(V_s N^*)$, where V_a is the volumetric flow rate of the air (m^3/s)

and: $m_a = \rho V_a = \rho \eta_v V_s N^*$ where: $\rho = p/(RT)$

thus: $m_a = \eta_v V_s N^* p/(RT) = 0.95 \text{ x } 39\text{x}10^{-3} \text{ x } (1200/120) \text{ x } 2\text{x}10^5/(287 \text{ x } [273 + 53]) = 0.792$ kg/s

$m_f = m_a/\text{AFR} = 0.792/21.4 = 0.037$ kg/s

The brake efficiency of the engine is the ratio of the work output, to the energy released by the combustion of the fuel:

$\eta_b = W_b/(m_f \text{ x CV}) = 628\text{x}10^3/(0.037 \text{ x } 42\text{x}10^6) = 0.404$ or **40.4%**

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[1] N Watson & M S Janota, 'Turbocharging the Internal Combustion Engine', Ch 9 - Charge Cooling, Macmillan, 1982.

Assuming Perfect Gas behaviour, with no pressure drop in the intercooler, and no heat transfer in the compressor, then the compressor work input (W_c) is:

$$W_c = m_a c_{p,a}(T_2 - T_1)$$

From this equation we can determine the temperature rise, for comparison with the temperature rise in an isentropic process:

$$(T_2 - T_1) = W_c/(m_a c_{p,a}) = 100\text{x}10^3/(0.792 \text{ x } 1.01\text{x}10^3) = 125 \text{ K}$$

We need to determine the isentropic compression temperature (T_{2s}) from the pressure ratio across the compressor:

$$T_{2s} = T_1 \, (p_2/p_1)^{((\gamma-1)/\gamma)} = (273 + 25) \text{ x } (2/0.95)^{((1.4 - 1)/1.4)} = 369 \text{ K}$$

The isentropic compressor efficiency (η_c) is (refer to Fig 9.29 in Qu 9.1):

$\eta_c = (T_{2s} - T_1)/(T_2 - T_1) = (369 - 298)/125 = 0.57$ or **57%**

The inter-cooler effectiveness (ϵ) is defined as:

$\epsilon = (T_2 - T_3)/(T_2 - T_1)$, where T_3 is the temperature after the intercooler.

Substitution of numerical values gives: $\epsilon = (423 - 326)/(423 - 298) =$ **0.78**

Removing the intercooler will reduce the density of the air at inlet to the engine, and thus the air mass flow rate. The air/fuel ratio of 21.4 is probably smoke limited, so that as the air flow is reduced, there will have to be a corresponding reduction in the fuel flow rate. A pessimistic assumption would be to assume that the pressure ratio across the compressor remained the same. If the brake efficiency of the engine is assumed to remain constant (a slightly optimistic assumption, since the frictional losses will become more significant), then the power output of the engine is directly proportional to the air mass flow rate.

The air mass flow rate would become: $m_a T_3/T_2 = 0.792 \text{ x } 326/423 = 0.61$ kg/s

and the power output would be reduced by T_3/T_2 (326/423 =) 0.77 or **77%** to (0.77 x 628 =) **484 kW**.

The constant air/fuel ratio and the higher inlet temperature will mean that all processes within the engine will occur at higher temperatures. This means:

i) The increased turbine entry temperature will mean that the turbine specific work output increases, and this in turn means a higher compressor delivery pressure (unless this is limited by a wastegate), so that the mass flow rate of air into the engine will not be decreased by as much as was assumed above.

ii) The NOx emissions will be increased, because the formation of NOx is strongly temperature dependant. A 10% increase in the in-cylinder temperature at inlet valve closure will cause something like a 30% increase in the NOx emissions.

iii) The combustion noise will be reduced, since higher in-cylinder temperatures will reduce the ignition delay period and the mass of flammable mixture formed prior to ignition.

9.11 A turbocharged diesel engine has a compressor operating point that is marked by a cross on the accompanying figure. If the compressor entry conditions are a pressure of 1 bar and a temperature of 20°C, determine the volume flow rate out of the compressor, and the power absorbed by the compressor. Assume the following properties for air: $\gamma = 1.4$, $c_p = 1.01$ kJ/kgK.

The fuelling rate to the engine is increased and the air mass flow rate into the engine is increased by 50%, and the volume flow rate out of the compressor increases by 22%. Stating any assumptions, establish approximately the new operating point for the compressor, its rotor speed, and the power that it is absorbing.

List briefly: **the advantages and disadvantages of turbocharging a diesel engine, and how the disadvantages can be ameliorated.**

m	**mass flow rate**	**(kg/s)**
T	**Temperature**	**(K)**
p	**pressure**	**(bar)**
N	**rotor speed**	**(rpm)**
η_c	**compressor isentropic efficiency**	

The initial operating point on the compressor map gives:

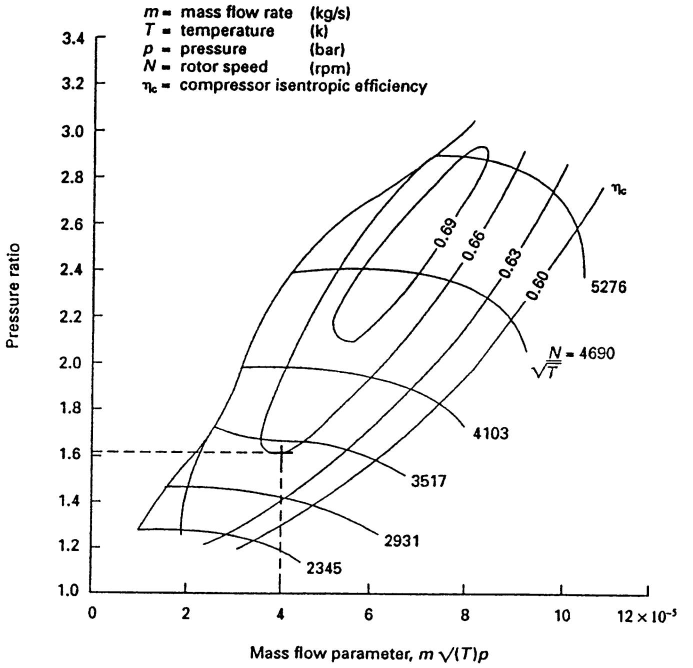
Pressure ratio, $p_2/p_1 = 1.62$
compressor isentropic efficiency, $\eta_c = 0.66$
mass flow parameter, $m\sqrt{T}/p = 4\text{x}10^{-5}$

To determine the volume flowrate out of the compressor, we can use the equation of state, once we know:

i) the compressor delivery pressure (p_2); this is obtained from the pressure ratio (r_p)

ii) the compressor delivery temperature (T_2); this is obtained from the pressure ratio and the compressor isentropic efficiency, and

iii) the mass flow rate; this is found from the mass flow parameter (mfp).



$$p_2 = p_1 r_p = 1 \text{ x } 1.62 = 1.62 \text{ bar} \qquad \text{(A}$$

To find the compressor delivery temperature, we start by finding the isentropic compression temperature, (T_{2S}).

$$T_{2S} = T_1\ (p_2/p_1)^{(\gamma-1/\gamma)} = 293(1.62)^{(1.4-1/1.4)} = 336 \text{ K} \qquad \text{(B}$$

The isentropic compressor efficiency (η_c) is:

$$\eta_c = (T_{2s} - T_1)/(T_2 - T_1)$$

or

$$T_2 = T_1 + (T_{2s} - T_1)/\eta_c = 293 + (336 - 293)/0.66 = 358 \text{ K} \qquad \text{(C}$$

finally, the mass flow rate comes from:

$$m = \text{mfp x } p\ /\sqrt{T} = 4\text{x}10^{-5} \text{ x } 1\ /\sqrt{293} = 0.234 \text{ kg/s.} \qquad \text{(D}$$

Using the equation of state, gives: $V = mRT/p = 0.234 \times 287 \times 358 / 1.62\text{X}10^5 =$ **148 L/s** (E

The power input to the compressor (W_c), (assuming it to be adiabatic) is:

$W_c = m_a c_p (T_2 - T_1) = 0.234 \times 1.01 \times (358 - 293) =$ **15.4 kW** (F

The new mass flow parameter will be (1.5 x 4=) 6, but we do not know what the pressure ratio will be. An analytical solution is not possible, so we have to guess the pressure ratio and compare:

i) the compressor delivery temperature, computed from the isentropic compressor efficiency (from the map) at this pressure ratio, with

ii) the delivery temperature implied by the increased mass flow rate at the pressure ratio.

We can record the results in a table, to summarise the results:

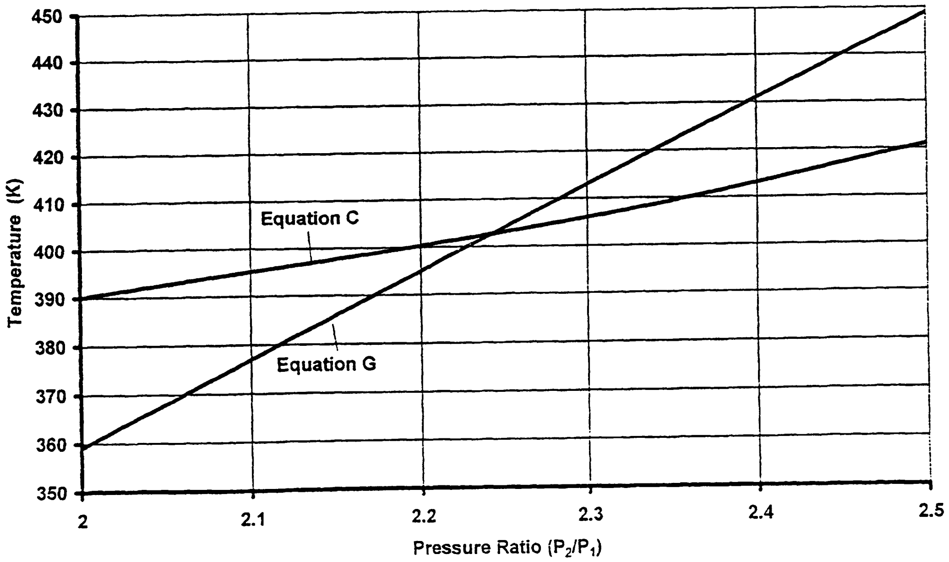
The new volume flow rate into the engine is: 148 x 1.22 = 181 L/s

The new mass flow rate into the engine is: 0.234 x 1.5 = 0.351 kg/s

Rearranging Eq E gives: $T_2 = pV/mR = p_2 \times 0.181 /(0.351 \times 287)$ (G

p_2/p_1 guess	η_c from the map	T_{2s} (K) Eq B	T_2 (K) Eq C	T_2 (K) Eq G
2.5	0.69	381	421	449
2.0	0.66	357	390	359
2.3	0.70	372	406	413

Plotting the results for T_2 from Eqs C and G against the pressure ratio, enables us to find the compressor operating point, as the pressure ratio where Eqs C and G give the same temperature.



From the graph the new compressor operating point is a pressure ratio of 2.24, and a delivery temperature of 402 K.

The new compressor operating point on the map is 62% of the way between the 4103 and 4690 speed parameter contours, thus

$$N/\sqrt{T} = 4103 + 0.62(4690 - 4103) = 4467$$

or $$N = 4467\sqrt{T} = 4467\sqrt{402} = \mathbf{89\ 562\ rpm}$$

The power input to the compressor (W_c) with the increased mass flowrate, (assuming it to be adiabatic) is:

$$W_c = m_a c_p (T_2 - T_1) = (0.234 \times 1.5) \times 1.01 \times (402 - 293) = \mathbf{38.6\ kW} \qquad \text{(F}$$

Advantages of turbocharging a diesel engine are:

a) Increasing the engine output: per kg, per unit cost, per unit volume.
b) Improves the efficiency (since the mechanical losses do not rise in proportion to the output).

Disadvantages of turbocharging a diesel engine are: Turbolag, increased NOx emissions and a higher thermal loading

The effect of turbolag can be reduced by:

a) minimising the manifold volumes,
b) undersizing the turbine to reduce its inertia (but using a wastegate to prevent over-speeding and too high a boost pressure),
c) use two (or more) turbochargers to replace one; the flow area $\alpha\ d^2$, while the inertia is $\alpha\ d^5$,
d) use an additional energy input to accelerate the turbocharger.

The increased NOx emissions and thermal loading can be both be reduced by intercooling. This will tend to increase the turbolag, but as well as increasing the engine output (kW/kg, kW/m^3 and kW/$) there will be a further improvement in the engine efficiency.

NOTE There are a number of alternative interpolation schemes for finding the new operating point, but it is probably most convenient to still interpolate for different pressure ratios. Equation C could have been used in reverse to compute T_{2s}, and then Eq B could have been used in reverse to compute η_c, which could then have been plotted as a comparison with the value from the map.

9.12 The Rolls Royce Crecy engine (for which some development was undertaken in the University of Oxford, Department of Engineering Science during the 1939-45 war by Ricardo) was intended for aircraft use.The Crecy was a supercharged 2-stroke engine with a swept volume of 26 litres. The predicted performance at an altitude of 4500 m and a speed of 792 km/h was:

supercharger pressure rise	**1.05**	**bar**
supercharger isentropic efficiency	**0.70**	
engine speed	**3000**	**rpm**
trapped gravimetric air/fuel ratio	**15:1**	
brake specific fuel consumption	**225**	**g/kWh**
brake power output	**1740**	**kW**
air flow rate	**5.4**	**kg/s**
exhaust temperature	**750**	**°C**
exhaust duct outlet area	**0.042**	**m^2**
mean molar mass of the exhaust products	**28.5**	**kg/kmol**

The engine had in-cylinder fuel injection, and the valve timing was such that a large flow of air (the scavenge flow) would not be trapped in the cylinder. You may neglect the pressure rise in the inlet system to the supercharger due to the forward motion of the aircraft. At 4500 m the ambient pressure is 0.578 bar, and the ambient temperature is 259 K.

Stating any other assumptions that you make:

1) **Calculate the scavenge flow as a percentage of the total flow into the supercharger.**

2) **If the frictional losses in the engine are equivalent to a frictional mean effective pressure (fmep) of 1 bar, calculate the indicated mean effective pressure (imep).**

3) **Determine the volumetric efficiency based on the inlet manifold conditions and the trapped mass in the cylinder.**

4) **Calculate the thrust from the exhaust, and compare this 'jet power' to the brake power of the engine,**

List 4 of the advantages/disadvantages of in-cylinder petrol injection.

1)

The scavenge flow is the difference between that entering the engine, and that which is trapped in the cylinder (m_t). The trapped mass can be found from the stated trapped air fuel ratio, and the calculated fuel flow rate:

$$m_f = \text{bsfc} \times W_b = (0.225/3600) \times 1740 = 0.109 \text{ kg/s}$$

Since the trapped air fuel ratio (AFR_t) is 15:1, the mass trapped in the cylinder is

$$m_t = m_f \times \text{AFR}_t = 0.109 \times 15 = 1.631 \text{ kg/s}$$

$$\text{scavenge flow} = (m_a - m_t)/m_a = 1 - 1.631/5.4 = 0.70 \text{ or } \mathbf{70\%}$$

2)

The indicated power (W_i) is found by adding the brake power (W_b), the power used to drive the supercharger (W_s), and the frictional power (W_f). The indicated power can then be converted to the imep.

$W_i = W_b + W_s + W_f$ or $p_i = (W_b + W_s)/(V_s \times N) + p_f$, where N is the number of firing revolutions each second

For the supercharger, $W_s = m_a \times c_p\,(T_{2s} - T_1)/\eta_c$

where the supercharger isentropic compression temperature: $T_{2S} = T_1\,(p_2/p_1)^{(\gamma-1/\gamma)}$

$$T_{2S} = 259 \times ([1.05 + 0.578]/0.578)^{(1.4-1/1.4)}$$

$$= 348 \text{ K}$$

For the supercharger, $W_s = 5.4 \times 1.01 \times (348 - 259)/0.7 = 693 \text{ kW}$

Remembering that it is a 2-stroke engine:

$$p_i = (W_b + W_s)/(V_s \times N) + p_f = (1740 + 693)\text{x}10^3/(26\text{x}10^{-3} \times 3000/60) + 1\text{x}10^5 = \mathbf{19.72\ bar}$$

3) To determine the volumetric efficiency of the engine, it is necessary to use the compressor delivery conditions.

$T_2 = T_1 + (T_{2S} - T_1)/\eta_c = 259 + (348 - 259)/0.7 = 386$ K

$p_2 = 0.578 + 1.05 = 1.628$ bar

The volume flowrate of the mass trapped in the cylinder (V_t) is obtained from applying then equation of state:

$V_t = m_t\, R\, T_2 \,/\, p_2 = 1.631 \text{ x } 287 \text{ x } 386 \,/\, 1.628\text{x}10^5 = 1.11 \text{ m}^3\text{/s}$

The swept volume rate (the air flow rate into a perfect engine) is: $V_s \text{ x } N = 26\text{x}10^{-3} \text{ x } 3000/60 = 1.3 \text{ m}^3\text{/s}$

The volumetric efficiency is thus 1.11/1.3 = 0.85 or **85%**

4) The thrust from the exhaust is the product of the exhaust mass flow rate and its velocity relative to the aircraft.

$m_{ex} = m_f + m_a = 0.109 + 5.4 = 5.509$ kg/s

$V_{ex} = m_{ex}RT/p$ where $R = R_o/M = 8314.3/28.5 = 292$ J/kgK

So $V_{ex} = 5.509 \text{ x } 292 \text{ x } (750 + 273)/0.578\text{x}10^5 = 28.47 \text{ m}^3\text{/s}$

The velocity is: $v_{ex} = V_{ex}/A = 28.47/0.042 = 678$ m/s

Finally, the thrust (F) is $F = m_{ex}(v_{ex} - v_{aircraft}) = 5.509 \text{ x } (678 - 792\text{x}10^3/3600) =$ **2523 N**

The 'jet power' of the engine W_F is the product of the exhaust thrust and the aircraft velocity:

$W_F = F \text{ x } v_{ex} = 2523 \text{ x } 792\text{x}10^3/3600 =$ **555 kW**

The jet power is thus (555/1740) 32% of the shaft power.

Advantages

a) No possibility of a 'short-circuiting' fuel loss, especially important for 2-stroke engines.

b) There is potential for stratified charge operation, so that overall very weak mixtures can be used. This improves the fuel economy at part load operation, since the thermodynamic efficiency is improved (consider the air standard fuel-air cycle results), and throttling losses can be avoided.

Disadvantages

a) Gasoline has low lubricity, so it is difficult to design the pump and injectors.

b) There is very little time for mixture preparation, so there is a risk of hydrocarbon and particulate emissions.

c) It is difficult to ensure a flammable mixture when and where the spark occurs.

9.13 A Sulzer RTA two-stroke diesel engine has a bore of 0.84 m and a stroke of 2.09 m; the bmep is 15.53 bar. If the engine operates at a speed of 70 rpm, calculate the power output per

cylinder. If the brake specific fuel consumption is 167 g/kWh calculate the fuel mass flow rate and the brake efficiency (assuming the fuel to have a calorific value of 42 MJ/kg.

Such engines are turbocharged and intercooled. Assuming the following data:

turbine isentropic efficiency	**0.90**
turbocharger mechanical efficiency	**0.98**
specific heat capacity of air	**1.01 kJ/kgK**
specific heat capacity of the exhaust products	**1.20 kJ/kgK**
ratio of the heat capacities of air (γ_a)	**1.4**
ratio of the heat capacities of the exhaust products (γ_{ex})	**1.3**
compressor entry pressure	**1.0 bar**
compressor entry temperature	**300 K**

Stating clearly any assumptions, determine the relationship between the compressor pressure ratio, and the turbine entry temperature, such that the compressor delivery pressure is always greater than the turbine entry pressure. Plot the results for pressure ratios in the range 2 to 3 (using a scale length of 100 mm) for compressor isentropic efficiencies of 0.65 and 0.75 - please use a scale of 1K/mm for the temperature axis.

Why, especially in a two-stroke engine, is it desirable for the compressor delivery pressure to be greater than the turbine entry pressure.

To calculate the brake power output we can use the definition of bmep Eq 2.38

$$W_b = p_b V_s N^*$$

where: p_b is the bmep (N/m^2)
V_s is the engine swept volume (m^3)
N^* is rpm/60 for a 2-stroke engine (s^{-1})

W_b = 15.53x10^5 x 2.09 x (π x 0.42^2) x (70/60) = **2.10 MW/cylinder**

m_f = W_b x bsfc = 2.1x10^6 x (0.167/3600) = **0.097 kg/s/cylinder**

η_b = $W_b/(m_f$ x $CV)$ = 2.1x10^6/(0.097 x 42x10^6) = **0.515**

.oOo.

Assuming: No pressure drop in the intercooler, no allowance for the difference in the mass flowrates in the compressor and turbine (since we do not know the air flowrate), an adiabatic compressor and turbine, and no pressure drop in the engine exhaust.

The isentropic turbine efficiency (η_t) is:

$$\eta_t = (T_4 - T_5)/(T_4 - T_{5s}) \quad \text{or} \quad T_4 - T_5 = \eta_t(T_4 - T_{5s}) \quad \text{where: } T_{5s} = T_4\ (p_5/p_4)^{(\gamma-1/\gamma)ex}$$

The turbine work <u>output</u> (W_t) is: $W_t = m_{ex}c_{p,ex}(T_4 - T_5) = m_{ex}c_{p,ex}\eta_t(T_4 - T_{5s}) = m_{ex}c_p\eta_t T_4(1 - \{p_5/p_4\}^{(\gamma-1/\gamma)ex})$ (A

The compressor is driven by the turbine, so a work balance (allowing for the mechanical efficiency is:

$$W_c = \eta_t W_t = m_a c_{p,a}(T_2 - T_1) = m_a c_{p,a}(T_{2s} - T_1)/\eta_c \quad \text{where: } T_{2s} = T_1\ (p_2/p_1)^{(\gamma-1/\gamma)a} \qquad \text{(B}$$

In the limiting case $p_2 = p_4$, and this will give the minimum value of T_4. Since we are neglecting any pressure drop in the exhaust, then the pressure ratio across the turbine and the compressor is the same, and we can denote it as β. If we substitute $\Gamma = (\gamma - 1)/\gamma$, and then combine Equations A & B, noting that there is assumed to be no difference in the compressor and turbine flowrates:

$$\eta_m(mc_{p,ex}\eta_t T_4(1 - 1/\beta^{\Gamma ex})) = mc_{p,a}\, T_1(\beta^{\Gamma a} - 1)/\eta_c$$

Rearranging gives:

$$T_4 = c_{p,a}T_1(\beta^{\Gamma a} - 1)/(\eta_c\eta_t\eta_m c_{p,ex}\eta_t(1 - 1/\beta^{\Gamma ex})) \qquad \text{(C}$$

Substitution of numerical values gives:

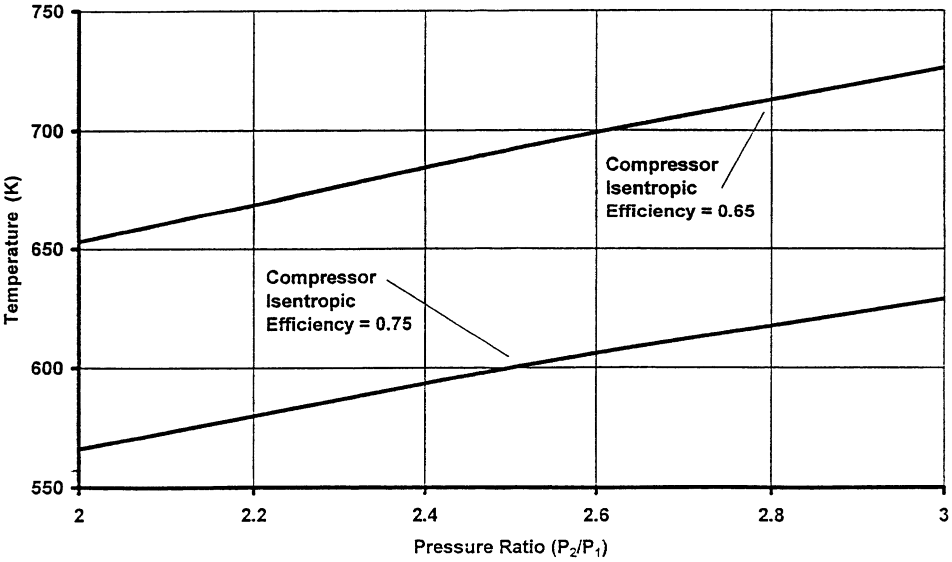
$$\Gamma_a = (1.4 - 1)/1.4 = 0.286, \qquad \Gamma_{ex} = (1.3 - 1)/1.3 = 0.231,$$

$$c_{p,a}T_1/(\eta_t\eta_m c_{p,ex}) = 300 \text{ x } 1.01/(0.90 \text{ x } 0.98 \text{ x } 1.2) = 286.3$$

$$T_4 = (286.3/\eta_c) \text{ x } (\beta^{0.286} - 1)/(1 - 1/\beta^{0.231})$$

Evaluation at two compressor isentropic efficiencies for three pressure ratio (β), gives the following table of the turbine entry temperature (T_4) necessary for the compressor boost pressure to be greater than the turbine back pressure:

pressure ratio ($\beta = p_2/p_1$)	2.0	2.5	3.0
$\eta_c = 0.65$:	653	692	726
$\eta_c = 0.75$:	566	600	629



Since a two-stroke engine does not have separate induction and exhaust strokes, then when the boost pressure is greater than the turbine back pressure there will be good scavenging.

9.14 A turbocharged 2 litre direct injection diesel engine operates on a four stroke cycle. At 2900 rpm and a bmep of 9.7 bar (full load), it is operating with a 22:1 gravimetric air fuel ratio and a brake specific fuel consumption of 230 g/kWh. The turbocharger is fitted with a waste-gate to regulate the pressure ratio to 2.0, and the compressor map is shown in the accompanying figure, for which: the pressure units are kN/m^2, the mass flow is in g/s, and the temperature units are K. The turbine entry temperature is 850K, its pressure ratio is also 2.0, and the turbine isentropic efficiency is 0.75.

The compressor entry conditions are 1 bar and 298 K, and you should assume the following thermodynamic properties:

	Air	**Exhaust**
Specific heat capacity at constant pressure, c_p (kJ/kgK)	**1.01**	**1.12**
Ratio of heat capacities, γ	**1.4**	**1.33**

a) **Stating any assumptions that you make, calculate the brake power output of the engine, its volumetric efficiency (based on inlet manifold conditions), and the fraction of the exhaust gas that passes through the turbine.**

b) **Explain, by means of annotated sketch, how the wastegate operates to control the boost pressure.**

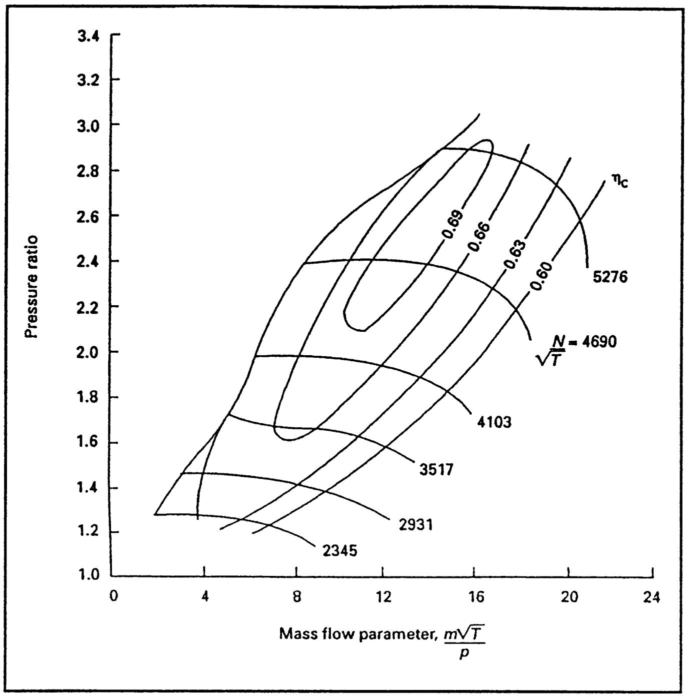


Fig 9.33

c) **Suggest ways of increasing the bmep of this engine in order of increasing complexity, with an indication of the likely increase in output (and how this would be calculated). Comment on how other aspects of the engine performance would be affected.**

To calculate the brake power output we can use the definition of bmep (Eq 2.38)

where: p_b is the bmep (N/m^2)
V_s is the engine swept volume (m^3)
N^* is rpm/120 for a 4-stroke engine (s^{-1})

$$W_b = p_b V_s N^* = 9.7\text{x}10^5 \text{ x } 2.0\text{x}10^{-3} \text{ x } (2900/120) = \mathbf{46.9\ kW}$$

To determine the volumetric efficiency of the engine, we need to know the air mass flow rate into the engine, and the compressor delivery conditions. The compressor delivery conditions depend on: the inlet conditions, the pressure ratio (all of which are known) and the compressor isentropic efficiency, which we have to deduce from the operating point on the compressor map. This in turn depends on the pressure ratio and the air flow rate, so a good way to proceed is to calculate the air mass flow rate next.

Since we know the power output and the engine's brake specific fuel consumption (bsfc), we can calculate the fuel mass flow rate (m_f), and then use the air fuel ratio (AFR) to calculate the air mass flow rate (m_a).

$$m_f = \text{bsfc} \times W_b = 230(\text{g/kWh}) \times 46.9\ (\text{kW}) = 10787\ \text{g/h} \quad \text{or} \quad 10787/3600 = 2.996\ \text{g/s}$$

$$m_a = \text{AFR} \times m_f = 22 \times 2.996 = 65.9\ \text{g/s air.}$$

Next we need to find the value of the compressor mass flow parameter (m^*), taking careful note of the units since the mass flow parameter is not dimensionless:

$$\text{m}^* = m_a\ (\text{g/s}) \times \sqrt{T}\ (\text{K})\ /\ p\ (\text{kN/m}^2) = 65.9 \times \sqrt{298}\ /\ 100 = 11.38$$

The intersection of the 11.38 mass flow parameter and the pressure ratio of 2.0 gives (by interpolation) a compressor isentropic efficiency of 0.67. We can now find the compressor delivery temperature, but first we need the isentropic compression temperature (T_{2s}) from the pressure ratio across the compressor:

$$T_{2s} = T_1\ (p_2/p_1)^{((\gamma-1)/\gamma)} = 298 \times (2.0)^{((1.4 - 1)/1.4)} = 363\ \text{K}$$

The isentropic compressor efficiency (η_c) is (refer to Fig 9.29 in Qu 9.1):

$$\eta_c = (T_{2s} - T_1)/(T_2 - T_1) \quad \text{or} \quad \text{T2} = (T_{2s} - T_1)/\eta_c + T_1 = (363 - 298)/0.67 + 298 = 395\ \text{K}$$

The volumetric efficiency (Eq. 2.42):

$\eta_v = V_a/(V_s N^*)$, where V_a is the volumetric flow rate of the air (m^3/s)

and: $V_a = m_a/\rho$ where: $\rho = p/(RT)$

thus: $\eta_v = m_a(RT/p)/(V_s N^*) = 0.0659\ (287 \times 395/2\text{x}10^{5})/(2.0\text{x}10^{-3} \times 2900/120) = \mathbf{0.77}$

To find out what fraction of the exhaust flow passes through the turbine, we need to calculate the power absorbed by the compressor. Assuming it to be adiabatic, then the compressor work input (W_c) is:

$$W_c = m_a c_{p,a}(T_2 - T_1) = 0.0659 \times 1.01\text{x}10^{-3}\ (395 - 298) = 6.46\ \text{kW}$$

Assuming that the turbine is also adiabatic, and that there are no mechanical losses, then a power balance can be written to define the mass flow through the turbine (m_t):

$W_c = m_t c_{p,ex}(T_3 - T_4)$ where 3 is the turbine entry, and 4 is its exit.

We have been given the turbine entry temperature (T_3), but we will have to calculate T_4 from the turbine pressure ratio and its isentropic efficiency:

$(T_3 - T_4) = \eta_t\ (T_3 - T_{4s})$ where: $T_{4s} = T_3\ (p_4/p_3)^{((\gamma-1)/\gamma)} = 850 \times 2.0^{(1.33 - 1)/1.33} = 716\ \text{K}$

So: $(T_3 - T_4)_{-} = 0.75(850 - 716) = 100.5$ K, and $W_c = m_t c_{p,ex}\ 100.5$

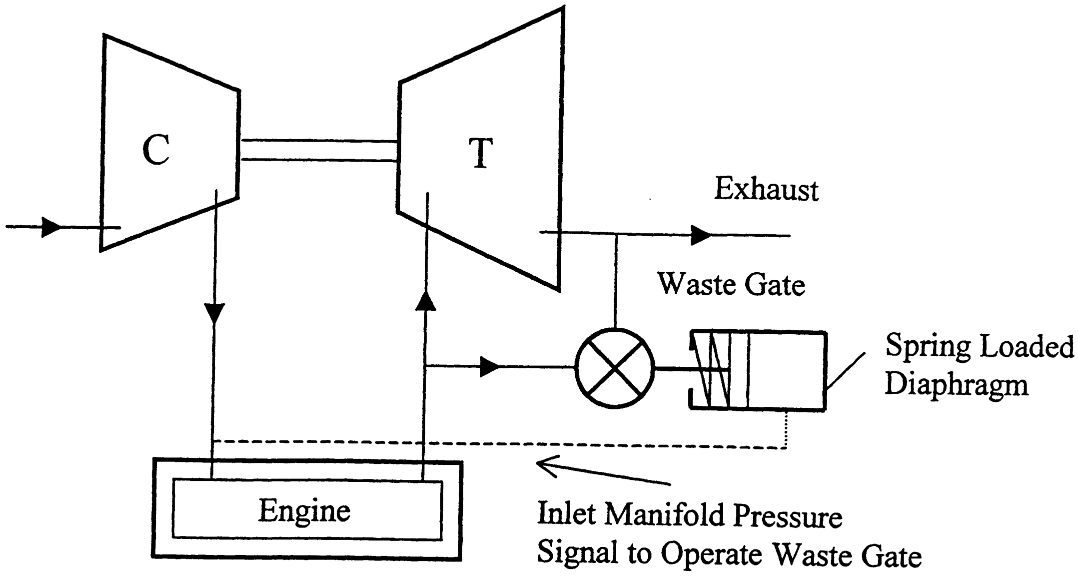
or $m_t = W_c/(c_{p,ex}\ 100.5) = 6460/(1120 \times 100.5) = 57.4$ g/s

We have to compare this with the mass flow rate of the exhaust (m_{ex})

$$m_{ex} = m_a + m_f = m_a(1 + 1/\text{AFR}) = 65.9(1 + 1/22) = 68.9\ \text{g/s}$$

The fraction of the exhaust flowing through the turbine is $m_t/m_{ex} = 57.4/68.9 = 0.833$ or **83.3%**

b)



c)

i) Increasing the boost pressure (and increasing the fuelling rate to maintain the same air fuel ratio) will lead to an increase in output. Since the fuel injection pump should be fitted with a boost control unit, to limit the maximum fuelling rate according to the inlet manifold pressure (and possibly temperature), then for small increases in boost pressure, there should be a corresponding increase in the fuelling rate. However, there will be a corresponding increase in the maximum combustion pressures and the thermal loading. We can estimate the possible increase in output by estimating the increase in the turbine output. We will need to make a number of assumptions:

a) The turbine isentropic efficiency is unchanged (there might be a slight increase)
b) The turbine entry temperature does not increase (it will, so this is a conservative assumption)
c) The volumetric efficiency of the engine is unchanged.

The calculation procedure will be iterative:

a) Estimate by how much the pressure ratio across the compressor will increase
b) Assuming the same compressor isentropic efficiency, calculate the air mass flow rate into the compressor and engine.
c) Identify the operating point on the compressor map, and if the estimate of the compressor isentropic efficiency was wrong, then recalculate the air flow rate. Repeat until satisfactory.
d) Calculate the power input required to drive the compressor.
e) Assuming the same pressure ratio across the turbine and compressor, calculate the power output from the turbine.
f) Compare the power output of the turbine, with the power requirement of the compressor, and make a better estimate of the compressor pressure ratio.
g) Repeat steps a) to f) until satisfactory convergence.

In this case, if alLof the exhaust flows through the turbine, then there is an increase from 57.4 to 68.9 g/s (an increase of 20%); this suggests that the air mass flow might be increased by about 20%, with a similar increase in the engine output. However, there are practical considerations that might limit the increase in air flow: Firstly, the maximum pressure and temperature already referred to, and secondly, the compressor operating point will move closer to the surge line. An increase in 10% might be a more realistic limit to the increase in output.

ii) Intercooling lowers the temperature of the air, thereby increasing its density. The mass flow rate of air is increased for a given pressure ratio, so this gives the option of increasing the fuel flowrate, thereby increasing the power output and efficiency (the efficiency will increase, since the mechanical losses do not rise in proportion to the brake power output). To a first order, the air mass flowrate will be increased in inverse proportion to the absolute temperature (since we can ignore the pressure drop in the intercooler).

Temperature after the compressor	395 K
Ambient Temperature	298 K

With an effectiveness of 1.0, the temperature after the intercooler would be 298 K. More realistically, with an effectiveness of 0.7, the temperature after the intercooler would be:

$$395 - 0.7(395 - 298) = 327 \text{ K}$$

and the **increase in output** would be: $(1/327 - 1/395)/(1/395) = (395 - 327)/327 = 0.21$, or **21%**

Since the mass flowrate through the compressor and the turbine both will have increased, and the pressure ratio across the compressor is limited to 2.0 (by the wastegate), then the compressor operating point will move to the right. The reduction in the compressor isentropic efficiency means an increase in the compressor specific work, so the fraction of the flow through the wastegate might be reduced slightly.

The cooler air at the start of the compression process will lower the temperatures in all subsequent processes, and thus lower the heat transfer and thermal loading on the engine. The lower combustion temperatures will lead to lower NOx emissions, since NOx formation is highly temperature dependant.

The disadvantages of intercooling are:

a) The space needed by the intercooler and its associated ductwork (for both the engine air, and the cooling medium).

b) The increased volume between the compressor and engine will worsen the transient response.

c) The lower temperatures during compression will increase the ignition delay. This will lead to an increase in the mass of flammable air/fuel mixture formed before self-ignition, and thus increase the initial rate of pressure rise and thence the combustion noise. This will be most significant at low loads, but the ignition delay can be reduced by using engine coolant as the cooling medium for the intercooler. This will infact heat the air under very low load conditions, thereby reducing the ignition delay period. The disadvantage is that the air will not be cooled as much by the intercooler at higher loads. Alternatively, hot EGR at part load will help to maintain a higher inlet manifold temperature.

9.15 In a turbocharged engine, it is desirable for the compressor boost pressure to be greater than the back pressure from the turbine. Assuming steady flow, and the following locations:

entry to the compressor	**1**
exit from the compressor	**2**
entry to the turbine	**3**
exit from the turbine	**4**

devise an expression for the pressure ratio p_2/p_3 in terms of:

the temperature ratio, T_3/T_1
the pressure ratio, p_2/p_1
the compressor isentropic efficiency, η_c

the turbine isentropic efficiency, η_t
the turbocharger mechanical efficiency, η_m
the air fuel ratio, AFR.

Assume that the air and exhaust products behave as perfect gases with the same property values, but allow for any differences in the mass flows through the compressor and turbine. State clearly any additional assumptions that you make.

Comment briefly on all of the assumptions. What might the effect of a compact exhaust manifold be, when using steady flow turbocharger performance data, for predicting the performance of a turbocharged Diesel engine?

The isentropic turbine efficiency (η_t) is:

$$\eta_t = (T_3 - T_4)/(T_3 - T_{4s}) \quad \text{or} \quad T_3 - T_4 = \eta_t(T_3 - T_{4s}) \quad \text{where:} \quad T_{4s} = T_3\ (p_4/p_3)^{(\gamma-1/\gamma)ex}$$

The turbine work <u>output</u> (W_t) is: $W_t = m_{ex}c_{p,ex}(T_3 - T_4) = m_{ex}c_{p,ex}\eta_t(T_3 - T_{4s}) = m_{ex}c_p\eta_tT_3(1 - \{p_4/p_3\}^{(\gamma-1/\gamma)ex})$(A

The compressor is driven by the turbine, so a work balance (allowing for the mechanical efficiency is:

$$W_c = \eta_tW_t = m_ac_{p,a}(T_2 - T_1) = m_ac_{p,a}(T_{2s} - T_1)/\eta_c \quad \text{where:} \quad T_{2s} = T_1\ (p_2/p_1)^{(\gamma-1/\gamma)a} \qquad \text{(B}$$

In the limiting case $p_2 = p_3$, and this will give the <u>minimum</u> value of T_3. Since we are neglecting any pressure drop in the exhaust, then the pressure ratio across the turbine and the compressor is the same, and we can denote it as β.

Noting that the compressor and turbine flowrates are related by the air fuel ratio (AFR):

$$m_{ex} = m_a(1 + 1/\text{AFR}) \quad \text{or} \quad \text{AFR}m_{ex} = m_a(1 + \text{AFR})$$

If we substitute $\Gamma = (\gamma - 1)/\gamma$, and then combine Equations A & B, noting that we are allowed to assume the same thermodynamic properties for the air and exhaust properties:

$$\eta_m(1 + \text{AFR})c_p\eta_tT_3(1 - 1/\beta^\Gamma) = \text{AFR}c_pT_1(\beta^\Gamma - 1)/\eta_c$$

or:

$$\eta_c\eta_m(1 + \text{AFR})\eta_tT_3(1 - 1/\beta^\Gamma) = \text{AFR}T_1(\beta^\Gamma - 1)$$

Multiplying both sides by β^Γ gives:

$$\eta_c\eta_m(1 + \text{AFR})\eta_tT_3(\beta^\Gamma - 1) = \text{AFR}T_1(\beta^\Gamma - 1)\beta^\Gamma$$

or:

$$\beta = p_2/p_1 = [\eta_c\eta_m\eta_t(T_3/T_1)(1 + \text{AFR})/\text{AFR}]^{\gamma/(\gamma - 1)}$$

Ignoring the pressure drop in the compressor is probably acceptable, but assuming the same thermodynamic properties for the air and exhaust products is unlikely to be acceptable.

A compact exhaust manifold causes unsteady flow (in other words there will be pressure fluctuations) into the turbine. This means that the isentropic efficiency will be lower than in the steady flow tests.

9.16 **The Sabre Marathon engine is a two-stage turbocharger conversion of the Ford Dover Diesel engine, with intercoolers after each compressor. Figure 9.26 shows the arrangement of the turbochargers and intercoolers, figure 9.27 shows the compressor maps. The engine has an output of 448 kW at 2400 rpm, from a swept volume of 6.8 litres. At this operating point the bsfc is 268 g/kWh, the air fuel ratio is 21.9:1, and the operating points of the turbochargers are:**

Turbocharger Performance	Low Pressure	High Pressure
Temperature before compressor	25	64 °C
Temperature after compressor	168	217 °C
Temperature after cooler	64	49 °C
Compressor pressure ratio	2.14	2.50
Turbine entry temperature	716	790 °C
Exhaust temperature	601°C	

a) **Calculate the power used by each compressor, and its isentropic efficiency.**

b) **Compare the compressor operating points with those shown on the compressor maps in figure 9.27 (note that the air flow rates need to be pseudo non-dimensionalised as $(\dot{m}\sqrt{T})/p$); assume that the compressor maps have a datum pressure of 1 bar.**

c) **Determine the effectiveness of the intercoolers, assuming a cooling media is available at 15°C.**

d) **If the overall pressure ratio is 5.1 (after allowing for pressure drops in the intercoolers), what is the volumetric efficiency of the engine?**

e) **Assuming no mechanical losses in the turbochargers, calculate the apparent value for the heat capacity of the exhaust gases in each turbocharger, and comment on these values.**

Data: **Calorific Value of diesel fuel - 42 MJ/kg**
For air, take c_p = 1.01 kJ/kgK and c_v = 0.721 kJ/kgK .

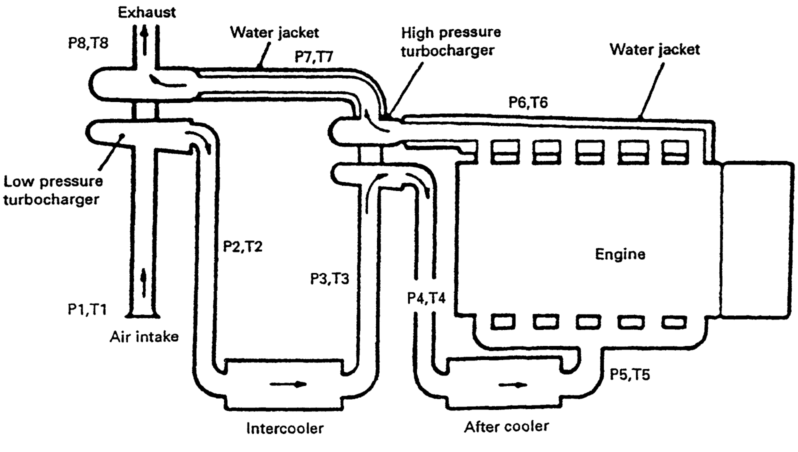


Fig 9.27 Arrangement for the two-stage turbocharging

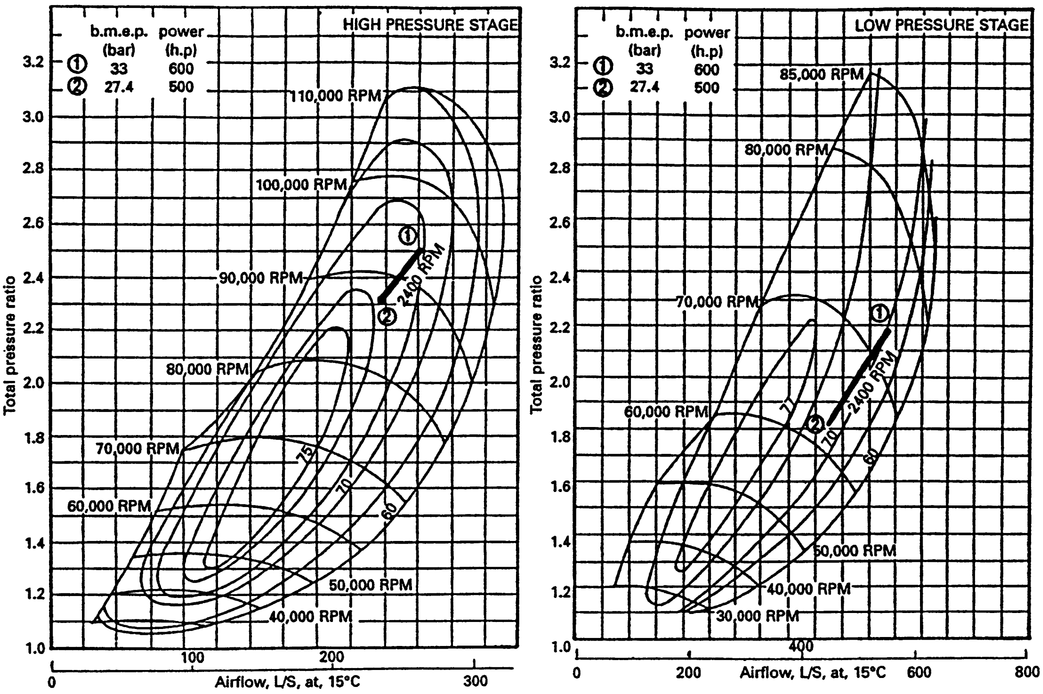


Fig 9.28 Low and high pressure compressor maps

Solution

a)

Since we know the power output and the engine's brake specific fuel consumption (bsfc), we can calculate the fuel mass flow rate (m_f), and then use the air fuel ratio (AFR) to calculate the air mass flow rate (m_a).

$$m_f = \text{bsfc x } W_b = 268(\text{g/kWh}) \text{ x } 448 \text{ (kW)} = 120\ 064 \text{ g/h or } 120\ 064/3600 = 33.35 \text{ g/s}$$

$$m_a = \text{AFR x } m_f = 21.9 \text{ x } 33.35 = 730.4 \text{ g/s air.}$$

For the low pressure compressor (assuming it is adiabatic):

$$W_{c,12} = m_a c_{p,a}(T_2 - T_1) = 0.7304 \text{ x } 1.01\ (168 - 25) = 105.5 \text{ kW}$$

The isentropic compressor efficiency (η_c) is (refer to Fig 9.20 in Qu 9.1):

$$\eta_c = (T_{2s} - T_1)/(T_2 - T_1)$$

We now need to find the isentropic compression temperature (T_{2s}) from the pressure ratio across the compressor, for which we need to evaluate the ratio of the specific heat capacities:

$$\gamma = c_p/c_v = 1.01/0.721 = 1.40$$

$$T_{2s} = T_1\ (p_2/p_1)^{((\gamma-1)/\gamma)} = 298 \text{ x } (2.14)^{((1.4 - 1)/1.4)} = 370.5 \text{ K}$$

So $$\eta_c = (370.5 - 298)/(168 - 25) = \mathbf{0.68}$$

For the high pressure compressor (assuming it is adiabatic):

$$W_{c.34} = m_a c_{p.a}(T_4 - T_3) = 0.7304 \text{ x } 1.01\ (217 - 63.5) = 113.2 \text{ kW}$$

The isentropic compressor efficiency (η_c) is (refer to Fig 9.29 in Qu 9.1):

$$\eta_c = (T_{4s} - T_3)/(T_4 - T_3)$$

We now need to find the isentropic compression temperature (T_{4s}) from the pressure ratio across the compressor:

$$T_{4s} = T_3\ (p_4/p_3)^{([\gamma-1]/\gamma)} = (63.5 + 273.15) \text{ x } (2.5)^{([1.4 - 1]/1.4)} = 437.4 \text{ K}$$

So $\eta_c = (437.4 - 336.7)/(217 - 63.5) = \mathbf{0.66}$

b) Next we need to find the value of the compressor mass flow parameter (m^*) for the low pressure compressor, taking careful note of the units since the mass flow parameter is not dimensionless:

$$m^* = m_a \text{ (kg/s) x} \sqrt{T} \text{ (K) / } p \text{ (bar)} = 0.7304 \text{ x} \sqrt{298} \text{ / } 1 = 12.61$$

We now need to find the equivalent mass flowrate (m') at the compressor map conditions of 15°C and 1 bar:

$$m^* = m' \text{ (kg/s) x} \sqrt{T} \text{ (K) / } p \text{ (bar)} = m' \text{ x} \sqrt{288} \text{ / } 1 = 12.61$$

or $m' = 12.61/\sqrt{288} = 0.743$ kg/s

This needs to be expressed as a volume flowrate (at the map datum conditions), so using the equation of state:

$$V' = m'RT/p = 0.743 \text{ x } 287 \text{ x } 288 \text{ / } 10^5 = 614 \text{ L/s}$$

From the compressor map, the equivalent ambient flowrate of 614 L/s with a pressure ratio of 2.14, indicates a compressor isentropic efficiency of 0.63 - this is quite close to the value of 0.68 calculated from the temperatures.

Next we need to find the value of the compressor mass flow parameter (m^*) for the high pressure compressor, taking careful note of the units since the mass flow parameter is not dimensionless:

$$m^* = m_a \text{ (kg/s) x} \sqrt{T} \text{ (K) / } p \text{ (bar)} = 0.7304 \text{ x} \sqrt{337} \text{ / } 2.14 = 6.266$$

We now need to find the equivalent mass flowrate (m') at the compressor map conditions of 15°C and 1 bar:

$$m^* = m' \text{ (kg/s) x} \sqrt{T} \text{ (K) / } p \text{ (bar)} = m' \text{ x} \sqrt{288} \text{ / } 1 = 6.266$$

or $m' = 6.266/\sqrt{288} = 0.369$

This needs to be expressed as a volume flowrate (at the datum conditions of the map), so using the equation of state:

$$V' = m'RT/p = 0.369 \text{ x } 287 \text{ x } 288 \text{ / } 10^5 = 305 \text{ L/s}$$

From the compressor map, the equivalent ambient flowrate of 305 L/s with a pressure ratio of 2.50, indicates a compressor isentropic efficiency of 0.65 - this is very close to the value of 0.66 calculated from the temperatures.

c) The effectiveness of the low pressure intercooler is given by:

$$\epsilon = (T_2 - T_3)/(T_2 - T_o) = (168 - 63.5)/(168 - 15) = 0.67$$

The effectiveness of the high pressure intercooler is given by:

$$\epsilon = (T_4 - T_5)/(T_4 - T_o) = (217 - 49)/(217 - 15) = 0.85$$

d) The volumetric efficiency (Eq. 2.42):

$\eta_v = V_a/(V_s N^*)$, where V_a is the volumetric flow rate of the air (m^3/s)

and: $V_a = m_a/\rho$ where: $\rho = p/(RT)$

thus: $\eta_v = m_a(RT/p)/(V_s N^*) = 0.730\ (287 \text{ x } [273.15 + 49] / 5.1\text{x}10^{-5})/(6.8\text{x}10^{-3} \text{ x } 2400/120) = \mathbf{0.97}$

Rather a high value of volumetric efficiency.

e) We will assume that the turbine is adiabatic, and that there are no mechanical losses, so that a power balance can be written to define the mass flow through the turbine (m_t). We first need to calculate the mass flow rate of exhaust through the turbines, by using the air fuel ratio:

$$m_t = m_a (1 + AFR)/AFR = 0.730\ (1 + 21.9)/21.9 = 0.764 \text{ kg/s}$$

For the low pressure turbine:

$W_c = m_t c_{p,ex}(T_7 - T_8)$ where 7 is the turbine entry, and 8 is its exit.

or $c_{p,ex} = W_c /[m_t(T_7 - T_8)] = 105.5/[0.764(716 - 601)] = \mathbf{1.20}$ kJ/kgK - a reasonable value

For the high pressure turbine:

$W_c = m_t c_{p,ex}(T_6 - T_7)$ where 6 is the turbine entry, and 7 is its exit.

or $c_{p,ex} = W_c /[m_t(T_6 - T_7)] = 113.2/[0.764(790 - 716)] = \mathbf{2.00}$ kJ/kgK - a very high value.

The high pressure turbine entry temperature is perhaps a bit low. The thermocouples will indicate too low a temperature if there are radiation losses to the water-cooled exhaust manifold. The radiation effects will be most significant at the highest temperature.

9.17 The Ford Essex V6 spark ignition engine was the subject of a turbocharging study, using an Airesearch T-04B turbocharger; the carburettor was placed downstream of the compressor. The compression ratio was reduced from 9.1:1 to 7.6:1, so as to avoid combustion 'knock', and it may be assumed that the reduction in the indicated efficiency is 1½ times that of the reduction in the corresponding Otto cycle. At 3000 rpm, the bmep was increased from 9.6 bar (when naturally aspirated) to 11.1 bar when turbocharged with a boost pressure ratio of 1.4. [*The frictional mean effective pressure is (independent of load) 1.2 bar, and the air flowrate into the turbocharged engine is 105 g/s.* Omitted by error from the 1st printing of the 3rd edition of the book.]

Assuming that the air fuel ratio, the pumping work, and the volumetric efficiency are unchanged, then calculate the density of the air leaving the compressor and the compressor isentropic efficiency (assuming an ambient temperature of 25°C). Determine and comment on the change in the brake specific fuel consumption, and any other assumptions that have been made.

The air standard Otto cycle efficiency is given by (equation 2.22):

$$\eta_{Otto} = 1 - \frac{1}{r_v^{\gamma-1}}$$

Substitution of the values:

compression ratio, $r_v = 9.1$, and
ratio of heat capacities, $\gamma = 1.4$, gives

$$\eta_{Otto} = 1 - \frac{1}{9.1^{1.4-1}} = 0.587$$

$$\eta_{\mathrm{Otto}} = \mathbf{58.7\%}$$

compression ratio, $r_v = 7.6$

$$\eta_{Otto} = 1 - \frac{1}{7.6^{1.4-1}} = 0.556$$

$$\eta_{\mathrm{Otto}} = \mathbf{55.6\%}$$

The change in indicated efficiency is:

$\eta_i = 1.5 \times (1 - 0.556/0.587) = 0.079$

The mass flow rate of air (m_a) will be proportional to both the imep (p_i) and the indicated efficiency (η_i):

$m_a \ \alpha \ p_i \times \eta_i$

Noting that: $p_i = p_b + p_f$

where: p_b is the bmep, and p_f is the fmep.

Thus:

$m_{a,7.6}/m_{a,9.1} = [(11.1 + 1.2)/(9.1 + 1.2)] \times 1.079 = 1.229$

There is thus a 22.9% in the air flowrate with the turbocharged engine, and with no change in the volumetric efficiency, then the increase in density is also 1.229.

The boost pressure ratio is 1.4, so by applying the equation of state with the density ratio, the temperature at the compressor delivery can be determined.

or

The isentropic compressor efficiency (η_c) is:

$$\frac{\rho_2}{\rho_1} = \frac{p_2}{p_1} \times \frac{T_1}{T_2}$$

$$\frac{T_2}{T_1} = \frac{p_2}{p_1} \times \frac{\rho_1}{\rho_2} = \frac{1.4}{1.229} = 1.139$$

$$\eta_c = (T_{2S} - T_1)/(T_2 - T_1)$$

For an isentropic compression process: $T_{2S} = T_1\ (p_2/p_1)^{(\gamma-1/\gamma)}$

$$T_{2S} = T_1(1.4/1)^{(1.4-1/1.4)} = 1.101\ T_1$$

We can now substitute into the expression for the isentropic compressor efficiency:

$$\eta_c = (T_{2S} - T_1)/(T_2 - T_1) = (1.101T_1 - T_1)/(1.229T_1 - T_1) = 0.886$$

The compressor work input (W_c) is:

$$W_c = m_a c_p(T_2 - T_1) = 0.105 \text{ x } 1.01 \text{ x } (1.229 - 1) \text{ x } 298.15 = 4.39 \text{ kW}$$

Since the air fuel ratio is assumed to be unchanged, then the fuel flowrate will change in proportion to the air flow rate. Thus:

The change in fuel flowrate is proportional to the air flow rate => an increase of 1.229

The change in output of the engine (the bmep) is 11.1/9.6, an increase of 1.159.

The increase in brake specific fuel consumption is 1.229/1.159 = 1.060, an increase of 6%. This reduction in engine efficiency is a result of the loss in efficiency (caused by the reduced compression ratio) outweighing the reduced significance of the mechanical losses.

In reality the engine showed a negligible change in fuel economy. A possible explanation is that no account has been taken of the changes in the pumping work. In the naturally aspirated engine at full throttle, the pumping mean effective pressure (pmep) is negative, say about 0.1 bar. In contrast, with the turbocharged engine the compressor boost pressure will be greater than the turbine back pressure, and the pmep will be positive (say about 0.2 bar). It is of course possible that the air fuel ratio will be different, and the turbocharged engine may be on a less rich air fuel ratio.

9.18 A 4 litre swept volume spark ignition engine is supercharged using a Roots blower to give a pressure ratio of 1.5. At maximum power, the engine output is 240 kW at 5000 rpm.

The operation of a Roots blower is described by figure 9.34 A volume of air ΔV is trapped at ambient pressure, and the pressure is unchanged until this trapped volume is transported to the high pressure side. At the instant that the high pressure port is un-covered (once rotor I has turned a little more), then the air in the rotor is compressed by the irreversible reverse flow of the high pressure air from downstream of the Roots blower. The work done is thus the rectangular area *abcd* in figure 9.34. This work is executed as the rotor turns, to displace the volume (ΔV) of high pressure gas (corresponding to the trapped volume of the rotor) out of the Roots blower. This model assumes that the downstream volume is sufficiently large compared to the trapped volume, for the delivery pressure to remain constant. Show that the type

efficiency of the Roots blower (the work required from a perfect Roots blower, divided by the work required in an isentropic compressor) is:

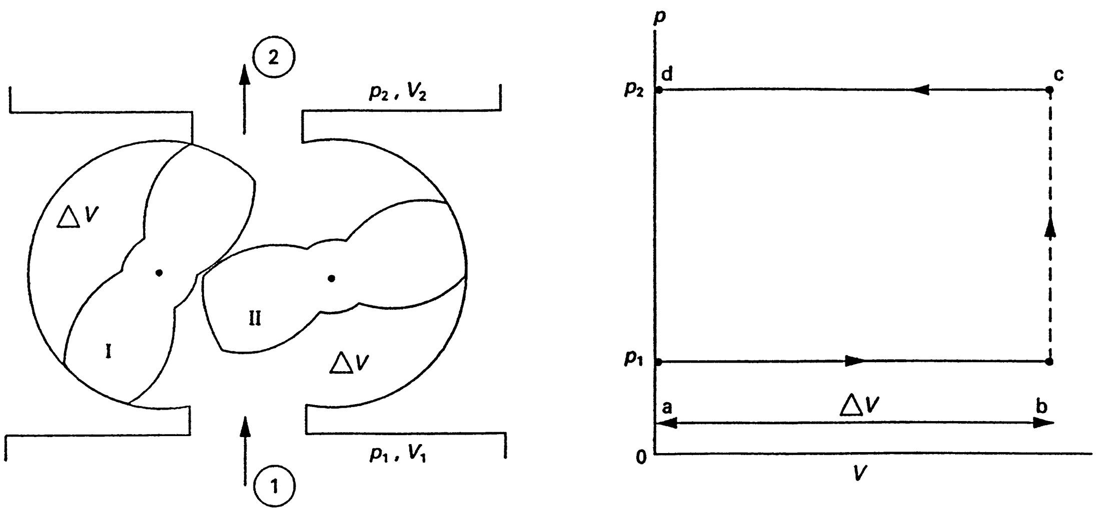


Fig 9.34 Operation of a Roots blower

The performance of a Roots compressor is further compromised by its mechanical losses, and its volumetric efficiency. Because of losses (including internal leakage), the volume flow rate into the compressor is reduced, but the work is still area *abcd* in figure 9.34. If the air mass flow rate is 243 g/s at ambient conditions of 1 bar and 25°C, calculate the power requirement of a Roots compressor with a pressure ratio of 1.5, for mechanical and volumetric efficiencies both of 80%. What would the exit air temperature be from the Roots blower?

After intercooling the air temperature is reduced to 50°C, neglecting any pressure drop in the intercooler, calculate the volumetric efficiency of the engine.

The indicated work (from the pressure-volume diagram) is $V\Delta p$, or

$$W_R = V\Delta p = V(p_2 - p_1)$$

For an isentropic compressor:

$$W_s = mc_p(T_{2s} - T_1) = mT_1[(p_2/p_1)^{(\gamma-1/\gamma)} - 1]$$

Applying the equation of state gives:

$$W_s = (p_1 V/R)c_p[(p_2/p_1)^{(\gamma-1/\gamma)} - 1]$$

The ratio of isentropic work to Roots compressor work is thus:

$$W_s/W_R = (p_1 V/R)c_p[(p_2/p_1)^{(\gamma-1/\gamma)} - 1] \,/\, Vp_1(p_2/p_1 - 1)$$

$$= R/c_p[(p_2/p_1)^{(\gamma-1/\gamma)} - 1] \,/\, [(p_2/p_1 - 1)]$$

$R = c_p - c_v$, so $R/c_p = (c_p - c_v)/c_p = \gamma/(\gamma - 1)$, since $c_p/c_v = \gamma$

Thus $W_s/W_R = \{\gamma/(\gamma - 1)\}\{[(p_2/p_1)^{(\gamma-1/\gamma)} - 1] \,/\, [(p_2/p_1 - 1)]\}$

To find the volume flowrate of air (V_a) into the supercharger, we can apply the equation of state:

$$V_a = mRT/p = 0.243 \text{ x } 287 \text{ x } (273 + 25)/10^5 = 0.208 \text{ m}_3\text{/s}$$

The indicated work is: $W_R = V\Delta p = V(p_2 - p_1)$,

but only 80% (η_v) of the volume trapped by the Roots rotors is air flowing from the inlet to the compressor.

The actual compression work is thus: $W = (V_a/[\eta_v \eta_m])(p_2 - p_1)$

$$W = (0.208/[0.8 \text{ x } 0.8](1.5 - 1)10^5 = \mathbf{16.25 \text{ kW}}$$

By assuming the compressor to be adiabatic, we can apply the steady flow energy equation:

$W = mc_p(T_2 - T_1)$, or $T_2 = T_1 + W/mc_p = 25 + 16.25/(0.243 \text{ x } 1.01) = \mathbf{91\ °C}$

To find the volumetric efficiency of the engine (η_v), we need to calculate the volume flowrate of air after the intercooler ($V_{a,2}$).

$$V_{a,2} = mRT_2/p_2 = 0.243 \text{ x } 287 \text{ x } (50 + 273)/1.5\text{x}10^5 = 0.150 \text{ m}^3\text{/s}$$

Finally, $\eta_v = V_{a,2}/(V_s[N/120]) = 0.150/(4\text{x}10^{-3} \text{ x } 5000/120) = \mathbf{0.90}$

Comment

This question is based on the Jaguar AJ6 engine, for which the maximum power to drive the supercharger is 34 kW (this also leads to a significantly higher compressor delivery temperature). The SAE Paper 870355 'Development of the Eaton Supercharger' by L H Uthoff & J W Yakimow, indicates that volumetric efficiencies of 55% might be more realistic.

11 Mechanical Design Considerations

11.1 The Rover K4 single cylinder research engine has a reciprocating mass of 1.53 kg in optical mode, the stroke is 89 mm, and the connecting rod length/crank throw ratio (*L/R*) is 3.6. What product of mass (*m*) and eccentricity (*e*) should be used for the primary and secondary balance masses, and how should they be deployed?

Equation 11.10 gives the standard approximation for the axial primary and secondary forces:

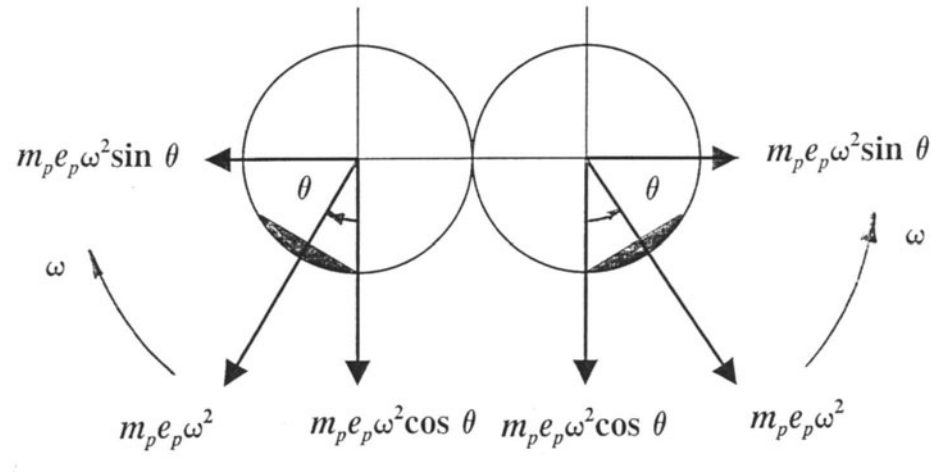
$$F_r \approx m_r\,\omega^2\,r\,(\cos\theta + r/L\,\cos 2\theta)$$

Where: θ is the crankshaft rotation measured from top dead centre (tdc)

m_r is the reciprocating mass, 1.53 kg

r is the crank throw = stroke/2 = 0.089/2 = 0.0445 m and $r/L = 1/3.6$

The primary out of balance force ($F_p = m_r\,\omega^2\,r\cos\theta$) can be balanced by a pair of counter-rotating balance masses at the same angular velocity (ω) as the crankshaft. As can be seen below, two counter-rotating balance masses are needed to eliminate the horizontal components of their forces.



$$F_p = m_r\,\omega^2\,r\cos\theta = 2(m_pe_p)\,\omega^2\cos\theta$$

or

$$m_pe_p = m_rr/2 = 1.53 \times 0.0445/2 = \mathbf{34\ kg\ mm}$$

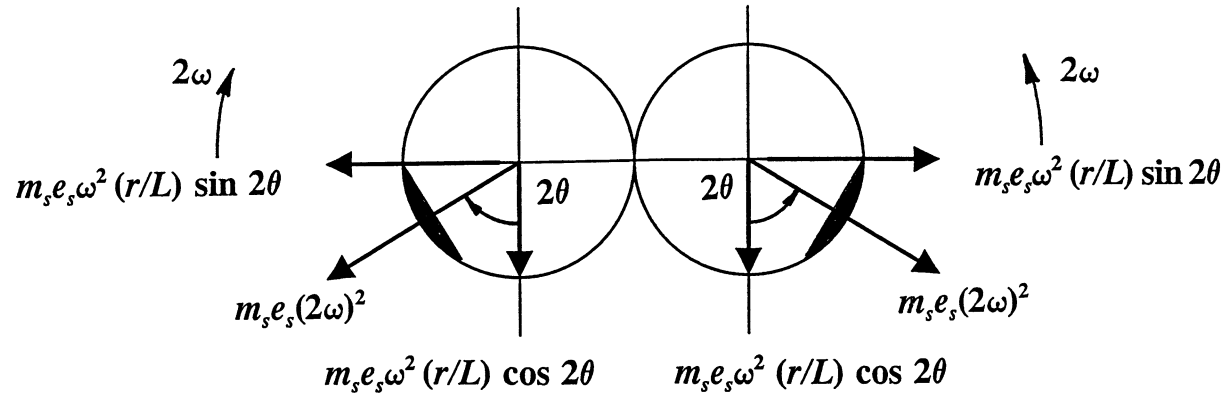
The secondary out of balance force ($F_s = m_r\,\omega^2(r/L)\,r\cos\theta$) can be balanced by a pair of counter-rotating balance masses at twice the angular velocity (ω) of the crankshaft. As can be seen below, two counter-rotating balance masses are needed to eliminate the horizontal components of their forces.

$$F_s = m_r\,\omega^2(r/L)\,r\cos 2\theta = 2(m_se_s)\,(2\omega)^2\cos 2\theta$$

or

$$m_se_s = m_rr\,(r/L)/8 = 1.53 \times 0.0445 \times (1/3.6)/8 = \mathbf{2.4\ kg\ mm}$$

The balance mass position has been measured from bottom dead centre (bdc) while the piston position has been measured from tdc, thus when the piston is at tdc, both the primary and secondary balance masses must be in their datum positions (that is, as far from the piston as possible).



11.2 A 3 cylinder 2-stroke engine uses uniflow scavenging through overhead valves. The reciprocating mass for each cylinder is 0.3 kg, the stroke is 70 mm, the connecting rod length/crank throw ratio (*L/R*) is 3.5, and the inter-cylinder bore spacing is *C*. Show that, with a 120° firing interval, the primary and secondary forces are balanced. If the balance masses are for eliminating the primary moments are a distance *D* from the bore of the centre cylinder, what product of mass (*m*) and eccentricity (*e*) should be used, and what will the unbalanced secondary moments be? How should the balance masses be configured?

Equation 11.10 (the standard approximation for the axial primary and secondary forces) has to be modified for a multicylinder engine, by introducing ϕ_n, the phase separation between cylinder *n* and the reference cylinder:

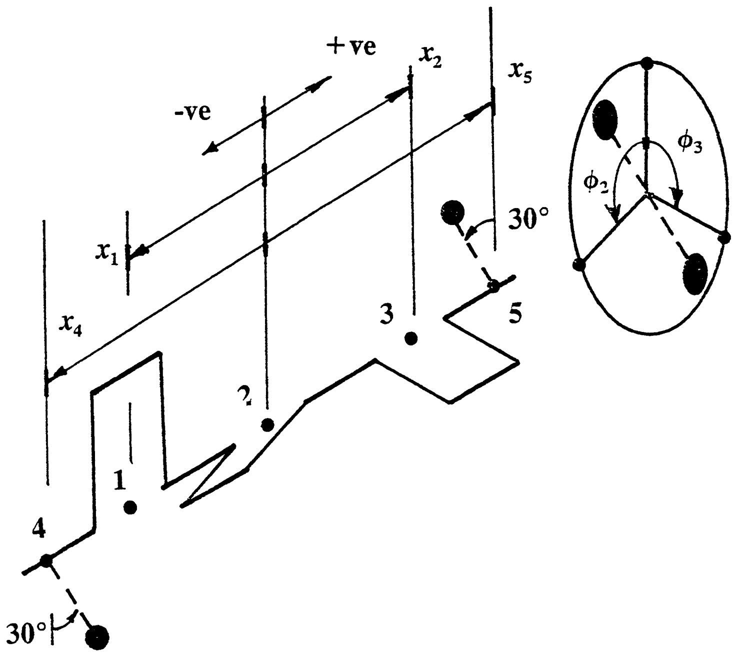
$$F_{r,n} \approx m_r\, \omega^2\, r\, (\cos\, [\theta + \phi_n] \;+\; r/L\, \cos\, 2[\theta + \phi_n])$$

Where: θ is the crankshaft rotation measured from top dead centre (tdc), $r/L = 1/3.5$

m_r is the reciprocating mass, 0.3 kg, and r is the crank throw = stroke/2 = 0.070/2 = 0.035 m

With the crank throws 120° apart and only 3 cylinders their order does not matter. As shown below, cylinder number 1 will be the reference cylinder, and as drawn it is at top dead centre ($\theta = 0$): at this stage the counterbalance masses in planes 4 and 5 should be ignored.

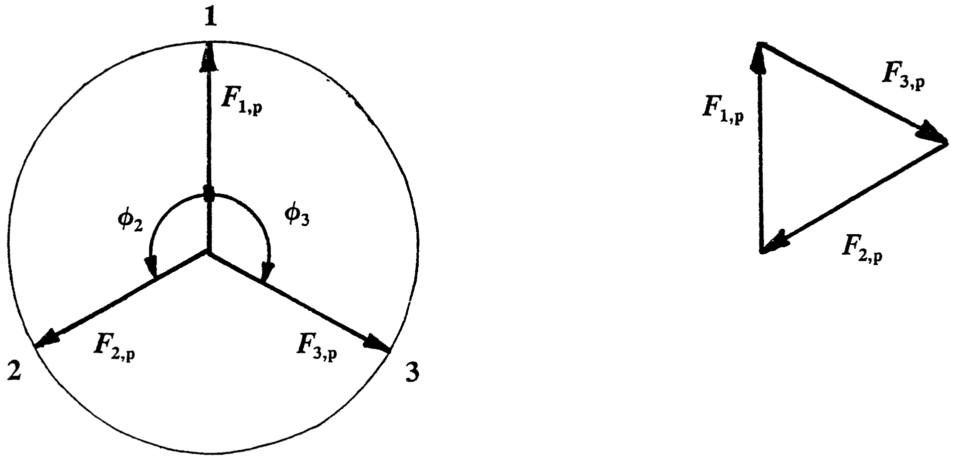
Isometric Sketch of the Crankshaft



The phasor approach will be used here, in which if the polygon of forces is closed, then the forces will be balanced for all positions of the reference crank (that is, all values of θ). The primary and secondary forces can only act along a cylinder axis, so for a particular value of θ only the force components along the cylinder axis need to be balanced. However, a new value of θ is equivalent to rotating the polygon of forces, and again only the force components along the cylinder axis need to be considered, so if the original polygon of forces is closed, then the forces will be balanced for any crankshaft position.

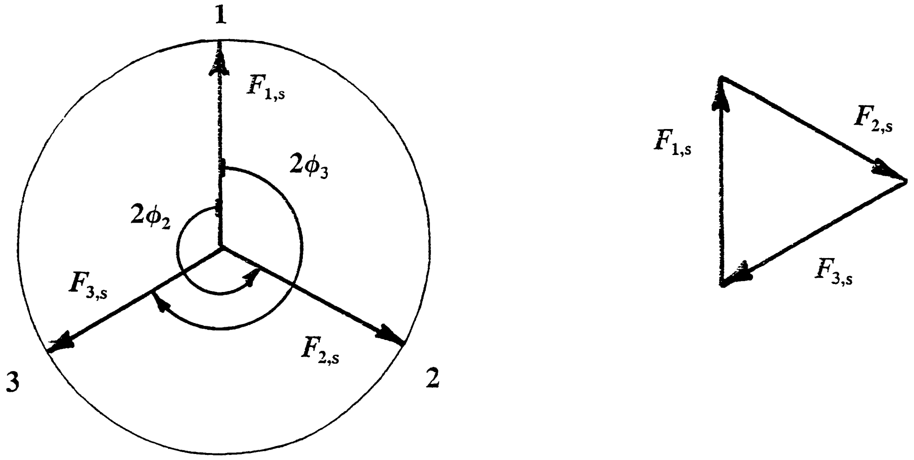
Considering first the primary out of balance forces $F_{p,n} = m_r \, \omega^2 \, r \cos [\theta+\phi_n]$, it can be seen that they are balanced:

Primary Forces



Considering next the secondary out of balance forces $F_{s,n} = m_r \, \omega^2(r/L) \, r \cos 2[\theta+\phi_n]$, it can be seen that they too are balanced:

Secondary Forces

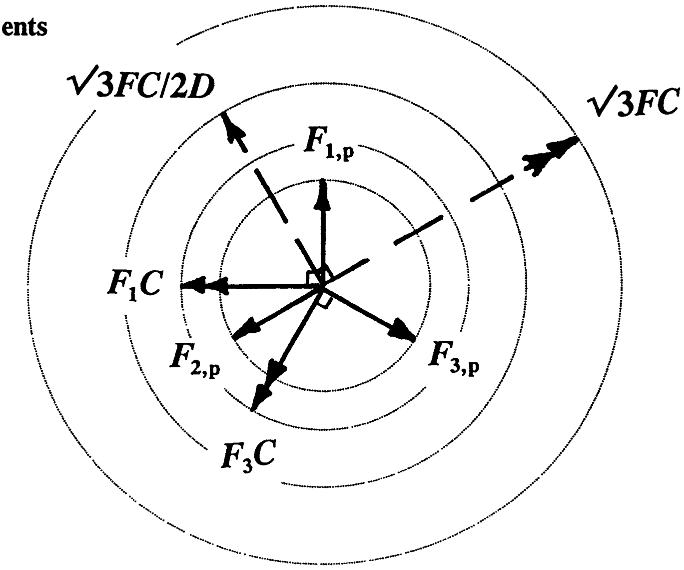


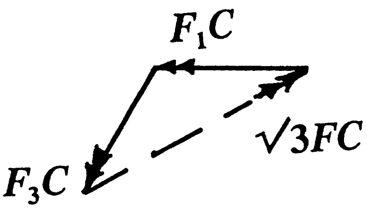
Greater care is needed with the evaluation of the out of balance moments, since it is easy to make mistakes in determining the direction of a moment. It should also be noted that the shape of the polygon of moments depends on the point where the moments are taken about, although of course the resultant moment (if any) will be the same. This will be illustrated by taking moments about both points 1 and 2.

The double headed arrow convention will be used here to denote moments, and looking along the arrow towards its head would be a clockwise moment. The positive direction along the crankshaft axis has to be defined, as can be seen in the isometric sketch of the crankshaft. In the phasor diagrams the moments and forces shown with broken lines should initially be ignored, since they arise form the balance masses.

For the primary moments, taking moments about point 2, gives the following phasor diagram:

Primary Moments about 2

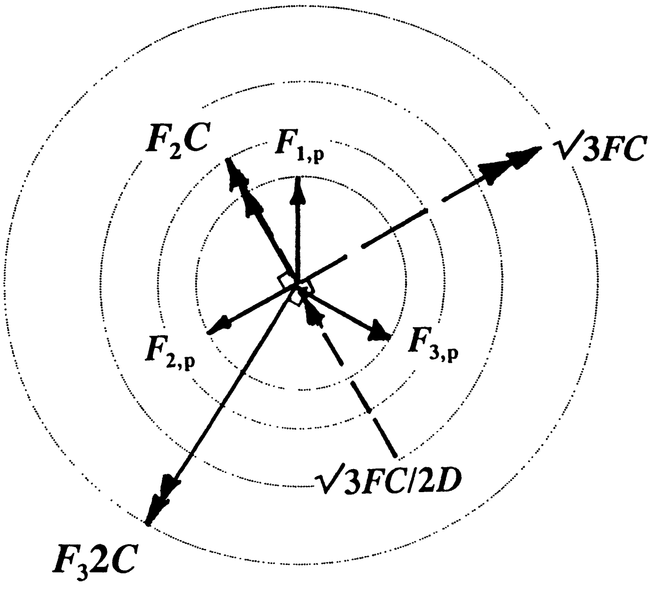


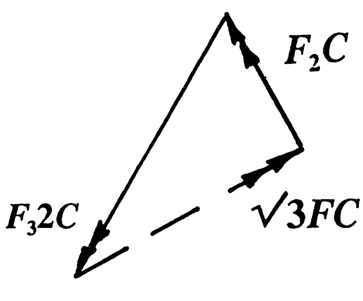


It should be remembered that the direction of the moment is at right-angles to the force it was produced by, and that its direction depends on the position of the forces plane relative to the reference plane. In this particular case, the distance $x_2 = -C$.

For the primary moments, taking moments about point 1, gives the following phasor diagram (noting that $x_3 = 2C$):

Primary Moments about 1





In both polygons of moments it can be seen that the moment required to close the polygon (and thus balance the moments) is the same in magnitude and direction. The simplest way that a moment can be balanced, without introducing any out of balance forces, is by a pair of balance masses that are separated along the crankshaft axis, and phased 180° apart.

The out of balance moment is: $(\sqrt{3})FC$

So the force from each balance mass has to be: $\sqrt{3}FC/(2D)$ since the masses are $2D$ apart.

The plane containing these masses is of course perpendicular to the direction of the moment. This leads to the orientation of the balance masses that is shown in the original sketch of the crankshaft. As might be expected, these balance masses are in a plane that is perpendicular to the crank throw for the centre cylinder.

However, it is only the component of force along the cylinder axes that is required, while the rotating balance masses will produce a moment that has components perpendicular to the cylinder axis. It is thus necessary to introduce a counter-rotating shaft that contains another pair of balance masses, which will be a mirror image of balance masses on the crankshaft. (The use of counter rotating shafts was illustrated in problem 11.1).

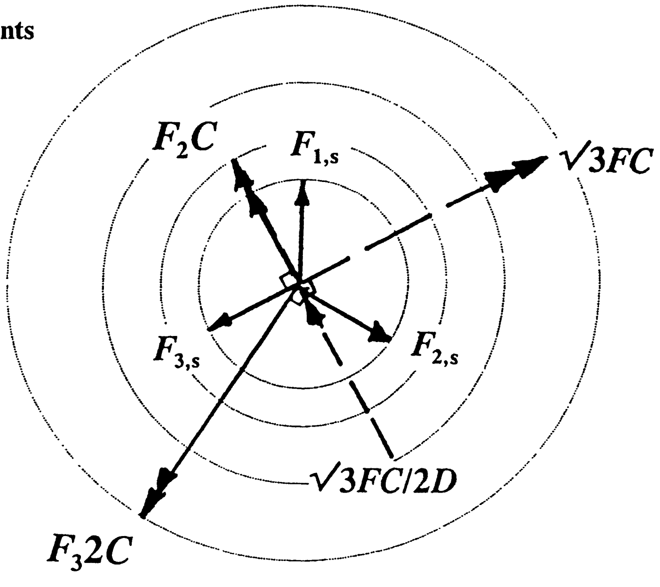
So finally, the force from each balance mass needs to be: $(\sqrt{3}/4)m_r\,\omega^2\,r\cos\theta\;C/D = (m_pe_p)\,\omega^2\cos\theta$

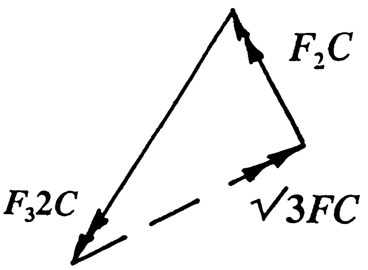
or: $m_pe_p = (\sqrt{3}/4)C/D\;m_rr = (\sqrt{3}/4)C/D \times 0.3 \times 0.035 = \mathbf{4.55}\boldsymbol{C/D}$ **kg mm**

Both masses on the crankshaft have to lie in a plane perpendicular to that containing the number 2 cylinder crank throw. The mass at the number 1 cylinder end has to be phased 150°ca from the number 1 crank, and the mass at the number 3 cylinder end has to be phased 150°ca from the number 3 crank. The balance shaft has to counter-rotate at engine speed, and the two balance masses have to be the mirror images of those on the crankshaft.

For the secondary out of balance moment it can be seen that the secondary force from cylinder number 2 lies in the direction of the primary force from cylinder number 3 and vice versa. Taking moments about cylinder number 1 thus gives the following polygon of moments:

Secondary Moments about 1





Noting that the secondary force is: $F_s = m_r\,\omega^2(r/L)\,r\cos 2\theta$

gives: $M_s = (\sqrt{3})\,m_r\omega^2\,C\,r\,(r/L)\cos 2\theta$

13 Experimental Facilities

13.1 Experiments are being conducted on a 3.9 litre 4 stroke diesel engine, which is being operated with three different inlet conditions:

- **i) naturally aspirated with air at an inlet temperature of 30°C**
- **ii) naturally aspirated with air at an inlet temperature of 150°C**
- **iii) naturally aspirated, but with a mixture of 30% O_2 and 70% CO_2 (molar basis) at an inlet temperature of 150°C.**

At a speed of 2000 rpm in mode (iii), the following data were obtained:

Brake power	**16.2**	**33.2**	**kW**
bsfc	**405.9**	**345.0**	**g/kWh**
oxygen level in the exhaust	**18.0**	**7.8**	**% dry gas**

At a bmep of 2.6 bar, the engine performance for cases (ii) and (iii) are:

	(ii)	**(iii)**	
Pressure at the end of compression	**38**	**31**	**bar**
Effective phasing of combustion	**0**	**12**	**°atdc**

a) Use the Willans' line construction to estimate the fmep of the engine.

b) Stating clearly any assumptions, calculate the volumetric efficiency of the engine, and comment on the result.

Assume that the effective compression ratio of the engine is 14:1 (instead of the nominal value of 15.5:1, to allow for the inlet valves closing slightly after bottom dead centre).

c) If the pressure at the start of compression is 1 bar, calculate the value of the polytropic index, and compare this with the value for the ratio of the specific heat capacities (use the data from the tables in Appendix A.

d) By assuming that the combustion can be treated as instantaneous at the 'effective phasing of combustion', use an Otto cycle analysis to apportion the reduction in cycle efficiency form case (i) to case (ii), between the effects of: the lower value of the ratio of the heat capacities, and (ii) the increased ignition delay.

a)

To construct the Willans' line, we need to calculate the bmep and fuel mass flow rate (m_f) for each of the operating points. The bmep is found from a rearrangement of equation 2.17:

$$\text{bmep} = \text{brake power}/(V_s \times N^*)$$

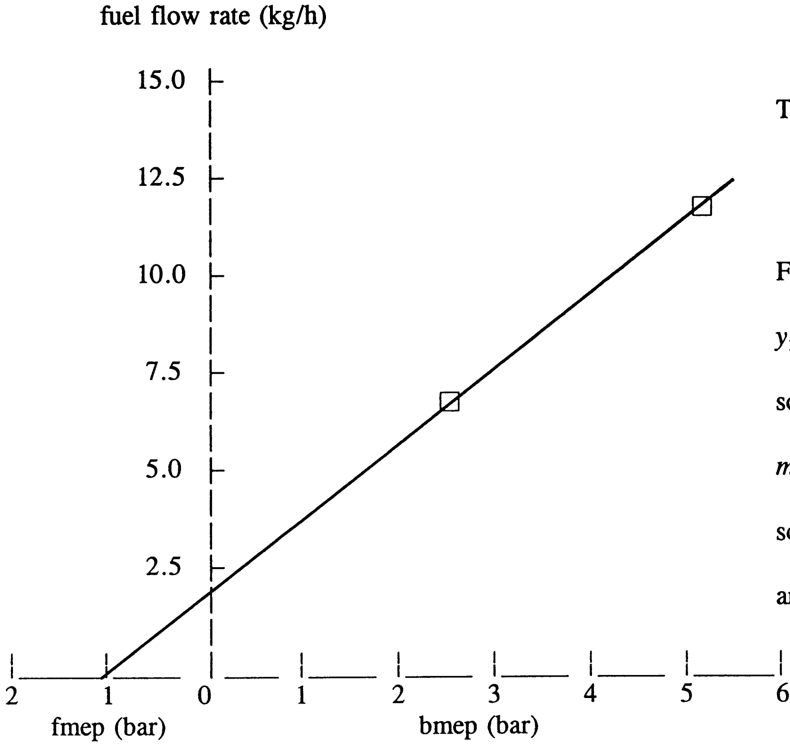
where: V_s = swept volume, and
N^* = number of times the swept volume is exchanged per second, remembering that this is a four-stroke engine, in which the volume is exchanged in alternate revolutions.

$$V_s \times N^* = 3.9\text{x}10^{-3} \times 2000/120 = 0.065 \text{ m}^3/\text{s}$$

The fuel mass flowrate is the product of the brake power (W_b) and the brake specific fuel consumption (bsfc):

$$m_f = W_b \text{ x bsfc}$$

	Load I	Load II	
Brake power	16.2	33.2	kW
bsfc	405.9	345.0	g/kWh
bmep	2.49	5.11	bar
fuel mass flow rate (m_f)	6.58	11.45	kg/h



The straight line can be fitted by:

$$y = mx + c$$

For the two data points:

$y_1 = mx_1 + c$ and $y_2 = mx_2 + c$

so $m = (y_1 - y_2)/(x_1 - x_2)$

$m = (11.45 - 6.58)/(5.11 - 2.49) = 1.859$

so $c = y_1 - mx_1 = 11.45 - 1.859 \text{x} 5.11$

and $c = 1.95$. Fmep is when $y = 0$

bmep $= -c/m = -1.95/1.859$

fmep $=$ -bmep $= 1.05$ bar

b)

To calculate the volumetric efficiency, we need to assume complete combustion, and that the fuel composition can be represented by $C_xH_{1.8x}$. We can then calculate the gravimetric 'air' fuel ratio, and as we have already calculated the fuel mass flow rate, this gives us the 'air' mass flow rate, from which we can calculate the volumetric efficiency. 'Air' is in quotes because its molar composition is 30% O_2 and 70% CO_2.

The generalised combustion equation, for 1 kmol of fuel is:

$$C_xH_{1.8x} + zx(0.3\ O_2 + 0.70\ CO_2) \rightarrow x(1 + 0.7z)CO_2 + 0.9xH_2O + x(0.3z - 1.45)O_2$$

In a dry gas analysis, the mole fraction of oxygen in the exhaust (a) is:

$$a = x(0.3z - 1.45)/[x(1 + 0.7z) + x(0.3z - 1.45)]$$

or

$$a = (0.3z - 1.45)/(z - 0.45)$$

or

$$az - 0.45a = 0.3z - 1.45$$

or

$$z = (1.45 - 0.45a)/(0.3 - a)$$

Since the 'air' is measured on a volumetric basis, while the fuel consumption has been measured on a mass basis, we will use the following unconventional definition of AFR:

The 'air' fuel ratio (kmols of gas/kg of fuel): $zx(0.3 + 0.7) : x(M_C + 1.8M_H)$

or $z : (12 + 1.8 \times 1)$ or $z/13.8 : 1$

For Load I: $a = 0.18$, so $z = (1.45 - 0.45 \times 0.18)/(0.3 - 0.18) = 11.41$, and $\text{AFR} = z/13.8 = 0.827$

the molar flow rate of 'air', $n_{a,I} = m_f \times \text{AFR} = 6.58 \times 0.827 = 5.44$ kmol/h or 1.51 gmol/s

For Load II: $a = 0.078$, so $z = (1.45 - 0.45 \times 0.078)/(0.3 - 0.078) = 6.37$, and $\text{AFR} = z/13.8 = 0.462$

the molar flow rate of 'air', $n_{a,II} = m_f \times \text{AFR} = 11.45 \times 0.462 = 5.29$ kmol/h or 1.47 gmol/s

As would be expected in a diesel engine, the molar (and thus volume) flowrate into the engine has decreased slightly as the engine load has increased.

The volume flow rate of 'air', $V = n_a R_o T/p$

and the volumetric efficiency, $\eta_{vol} = V/(Vs \times N/120) = 120 n_a R_o T/(p \times Vs \times N/120)$, so:

$$\eta_{vol,I} = 120 \times 1.51\text{x}10^{-3} \times 8314.3 \times (273.15 + 150)/(10^5 \times 3.9\text{x}10^{-3} \times 2000) = \mathbf{0.817}$$

$$\eta_{vol,II} = 120 \times 1.47\text{x}10^{-3} \times 8314.3 \times (273.15 + 150)/(10^5 \times 3.9\text{x}10^{-3} \times 2000) = \mathbf{0.796}$$

c)

The pressure at the end of compression is solely due to piston motion, since in both cases (ii) and (iii) the combustion does not commence until after top dead centre.

For a polytropic process, pv^n = const, or $p_1V_1^n = p_2V_2^n$

Taking logs and rearranging gives: $n = \ln(p_2/p_1)/\ln(V_1/V_2)$

For case (ii), $n = \ln(38)/\ln(14) = 1.38$, for case (iii), $n = \ln(31)/\ln(14) = 1.30$

To estimate the mean value of the ratio of specific heat capacities, we need to know the temperature range. If we assume the start of compression to be at 150°C, then we can apply the equation of state (assuming no leakage) to estimate the temperature at the end of compression.

$$p_1V_1/T_1 = p_2V_2/T_2 \quad \text{or} \quad T_2 = p_2V_2T_1/(p_1V_1)$$

For case (ii), $T_2 = 38 \times (150 + 273.15)/14 = 1149$ K; for case (iii), $T_2 = 31 \times (150 + 273.15)/14 = 937$ K.

Both these temperatures are rather high (since the 'air' will be cooled during the induction process), and because of the approximations in their evaluation, it will be sufficient to approximate the temperature ranges over which the ratio of the heat capacities is evaluated.

For case (ii) air, 400 to 1100 K:

$$C_p = (H_{1100} - H_{400})/(1100 - 400) = (24.984 - 2.973)/700 = 31.44 \text{ kJ/kmolK}$$

$$C_v = C_p - R_o = 31.44 - 8.3143 = 23.130 \text{ kJ/kmolK}$$

$$\gamma = C_p/C_v = 31.44 -22.13 = 1.36 \text{ (compared to 1.38 for the polytropic index)}$$

For case (iii), 30% O_2 and 70% CO_2, 400 to 900 K:

$$\begin{aligned} C_p &= (0.3H_{900,O2} + 0.7H_{900,CO2} - 0.3H_{900,O2} - 0.7H_{900,CO2})/(900 - 400) \\ &= (0.3\text{x}19.244 + 0.7\text{x}[-365.477] - 0.3\text{x}3.028 - [-389.509])/500 = 43.37 \text{ kJ/kmolK} \end{aligned}$$

$$C_v = C_p - R_o = 43.37 - 8.3143 = 35.06 \text{ kJ/kmolK}$$

$$\gamma = C_p/C_v = 43.37 - 35.06 = 1.24 \text{ (compared to 1.30 for the polytropic index)}$$

Since the polytropic index is higher than the ratio of heat capacities, then this suggests that the estimate of the effective compression ratio is low.

d)

With a compression ratio (r_v) of 14:

Otto cycle efficiency for case (ii) with $\gamma = 1.36$ is: $1 - 1/14^{1.36 - 1} = 0.613$

Otto cycle efficiency for case (iii) with $\gamma = 1.24$ is: $1 - 1/14^{1.24 - 1} = 0.469$

If the combustion is phased 12°atdc, and we assume simple harmonic motion for the piston, then the clearance volume has increased by:

$$V_s(1 - \cos 12°)/2 = 0.011V_s$$

the clearance volume was originally $V_s/(r_v - 1) = 0.077V_s$, so the new clearance volume is $0.088V_s$

The start of the expansion stroke is delayed, so the effective swept volume is $0.989V_s$

The compression ratio with delayed combustion is thus: $1 + 0.989/0.088 = 12.2$.

The Otto cycle efficiency for case (iii) is now: $1 - 1/12.2^{1.24 - 1} = 0.451$

The Otto cycle efficiency is thus lowered 14.4 %points by the reduced ratio of heat capacities, and by a further 1.8 %points by the delayed combustion.

.oOo.

This question has been based on experimental data in 'The Effects of Non-Air Mixtures on the Operation of a Diesel Engine by Experiment and Simulation', by J G Hawley, S J Ashcroft and M A Patrick, *Proc Instn Mech Engrs*, Vol 212 No A1, pp 55-68, 1998. The pressure volume diagrams show quite clearly the loss of work associated with the delayed combustion in case (iii).

APPENDIX A

THERMODYNAMIC DATA

A.1 Introduction

The thermodynamic tables presented here for enthalpy and internal energy differ from those that are usually available, since they incorporate the enthalpy of formation. This means that there is no need for separate tabulations of calorific values, and it will be found that energy balances for combustion calculations are greatly simplified. The enthalpy of formation (H_f^o) is perhaps more familiar to physical chemists than engineers.

> The **enthalpy of formation** (H_f^o) of a substance is the standard reaction enthalpy for the formation of the compound from its elements in their reference state.
>
> The **reference state** of an element is its most stable state (eg carbon atoms , but oxygen molecules) at a specified temperature and pressure, usually 298.15 K and a pressure of 1 bar. In the case of atoms that can exist in different forms, it is necessary to specify their form, for example, carbon is as graphite, not diamond.

Combustion calculations are most readily undertaken by using absolute (sometimes known as sensible) internal energies or enthalpy. In steady flow systems where there is displacement work then enthalpy should be used; this has been illustrated by Figure 3.8. When there is no displacement work then internal energy should be used (Figure 3.7). Consider now Figure 3.8 in more detail. With an adiabatic combustion process from reactants (R) to products (P) the enthalpy is constant, but there is a substantial rise in temperature.

Fig 3.7 Constant volume combustion

Fig 3.8 Constant pressure combustion

$$H_{IR} = H_{2P} \quad , \quad T_2 > T_1 \tag{A.1}$$

In the case of the isothermal combustion process ($IR \rightarrow IP$) the temperature (T) is obviously constant, and the difference in enthalpy corresponds to the isobaric calorific value ($-\Delta H_T^o$).

$$\Delta H_T^o = H_{R,T} - H_{P,T} \tag{A.2}$$

A.2 THERMODYNAMIC PRINCIPLES

In the following sections, it will be seen how the thermodynamic data for: internal energy, enthalpy, entropy and Gibbs function, can all be determined from measurements of heat capacity, and phase change enthalpies (or internal energies). Furthermore, when the energy change associated with a chemical reaction is measured, then the enthalpy of formation can be deduced. This in turn leads to 'absolute' values of internal energy, enthalpy, entropy and Gibbs function, from which it is possible to derive the equilibrium constant for any reaction.

A.2.1 Determination of: Internal Energy, Enthalpy, Entropy and Gibbs Function

Figure 3.8 shows that the enthalpies of both reactants and products are in general non-linear functions of temperature. The Absolute Molar Enthalpy tables presented here, use a datum of ***zero enthalpy for elements when they are in their standard state at a temperature of 25°C***. The enthalpy of any substance at 25°C will thus correspond to its enthalpy of formation, ΔH_f°. The use of these tables will be illustrated, after a description of how they have been developed.

Tables are not very convenient for computational use, so instead molar enthalpies and other thermodynamic data are evaluated from analytical functions; a popular choice is a simple polynomial. For species *i*

$$H_i(T) = A_i + B_iT + C_iT^2 + D_iT^3 + E_iT^4 + F_iT^5 \tag{A.3}$$

from which it can be deduced (since $\mathrm{d}H = C_\mathrm{p}\mathrm{d}T$) that:

$$C_{p,i}(T) = B_i + 2C_iT + 3D_iT^2 + 4E_iT^3 + 5F_iT^4 \tag{A.4}$$

As $U = H - RT$

$$U_i(T) = A_i + (B_i - R_o)T + C_iT^2 + D_iT^3 + E_iT^4 + F_iT^5 \tag{A.5}$$

and $\mathrm{d}U = C_\mathrm{v}\mathrm{d}T$

$$C_{v,i}(T) = (B_i - R_o) + 2C_iT + 3D_iT^2 + 4E_iT^3 + 5F_iT^4 \tag{A.6}$$

and as

$$dH = C_p dT = TdS$$

$$dS = (C_p/T)dT,$$

integrating gives equation A.4 gives:

$$S_i^o = B_i \ell n(T) + 2C_iT + 3/2D_iT^2 + 4/3E_iT^3 + 5/4F_iT^4 + G_i \quad \text{(A.7}$$

where G_i is an integration constant that is used to set the zero datum, e.g. 0 K by Rogers and Mayhew (1988) - the same datum does not have to be used as for enthalpy.

A more common choice is to use a polynomial function to describe the specific heat capacity variation, and to divide through by the Molar Gas Constant (R_o). Equation A.4 becomes

$$C_{p,i}(T)/R_o = a_i + b_iT + c_iT^2 + d_iT^3 + e_iT^4 \quad \text{(A.8}$$

where $a_i \equiv B_i/R_o$, $b_i \equiv 2C_i/R_o$, $c_i \equiv 3D_i/R_o$ etc.

$$\textit{Thus:} \quad H_i(T)/R_o = a_iT + b_iT^2/2 + c_iT^3/3 + d_iT^4/4 + e_iT^5/5 + f_i \quad \text{(A.9}$$

$$\textit{and:} \quad S_i^o(T)/R = a_i \ell n(T) + b_iT + c_i/2T^2 + d_i/3T^3 + e_i/4T^4 + g_i \quad \text{A.10} \quad ($$

Table A.1 Coefficients in Equations A.8 A.9 and A.10, for the evaluation of thermodynamic data from Gordon and McBride (1971), except Argon, from Reid et al (1987).

N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H
1000 - 5000 K										
0.28963e1	0.36220E1	0.31002E1	0.29841E1	0.44608E1	0.27168E1	0.31890E1	2.5016	0.29106E1	0.25421E1	2.5
0.15155e-2	0.73618E-3	0.51119E-3	0.14891E-2	0.30982E-2	0.29451E-2	0.13382E-2	0	0.95932E-3	-0.27551E-4	0
-0.57235e-6	-0.19652E-6	0.52644E-7	-0.57900E-6	-0.12393E-5	-0.80224E-6	-0.52899E-6	0	-0.19442E-6	-0.31028E-8	0
0.99807e-10	0.36202E-10	-0.34910E-10	0.10365E-9	0.22741E-9	0.10227E-9	0.95919E-10	0	0.13757E-10	0.45511E-11	0
-0.65224e-14	-0.28946E-14	0.36945E-14	-0.69354E-14	-0.15526E-13	-0.48472E-14	-0.64848E-14	0	0.14225E-15	-0.43681E-15	0
-0.90586e3	-0.12020E4	-0.87738E3	-0.14245E5	-0.48961E5	-0.29906E5	0.98283E4	-745.852	0.39354E4	0.29231E5	0.25472E5
0.61615e1	0.36151E1	-0.19629E1	0.63479E1	-0.98636E0	0.66306E1	0.67458E1	0.43529E1	0.54423E1	0.49203E1	-0.460120E0
300 - 1000 K										
0.36748E1	0.36256E1	0.30574E1	0.37101E1	0.24008E1	0.40701E1		2.5016			
-0.12082E-2	-0.18782E-2	0.26765E-2	-0.16191E-2	0.87351E-2	-0.11084E-2		0			
0.23240E-5	0.70555E-5	-0.58099E-5	0.36924E-5	-0.66071E-5	0.41521E-5		0			
-0.63218E-9	-0.67635E-8	0.55210E-8	-0.20320E-8	0.20022E-8	-0.29637E-8		0			
-0.22577E-12	0.21556E-11	-0.18123E-11	0.23953E-12	0.63274E-15	0.80702E-12		0			
-0.10612E4	-0.10475E4	-0.98890E3	-0.14356E5	-0.48378E5	-0.30280E5		-745.852			
0.23580E1	0.43053E1	-0.22997E1	0.29555E1	0.96951E1	-0.32270E0		0.43529E1			

polynomial fit will only be satisfactory over a small temperature range (300 - 1000 K or 1000 - 5000 K), and such polynomial quations ought never to be used outside their range. As the specific heat capacity variation with temperature has a 'knee' etween 900 K and 2000 K, then a single polynomial is never likely to be satisfactory. Instead, two polynomials can be used which give identical values of C_p at the transition between the low range and the high range (the transition temperature is usually chosen between 1000 and 2000 K). Examples of such polynomials are presented by Gordon and McBride (1971), and were used as the basis for constructing the tables used here. The coefficients for the evaluation of the thermodynamic tables are summarised in Table A.1.

The tables at the end of this Appendix present: the enthalpy (H), internal energy (U), entropy (S) and Gibbs energy (G) for gaseous species (Table A.4) and fuels (Table A.5). The tables have been extrapolated below 300 K, and these data should be used with caution. The entropy datum of zero at 0 K cannot be illustrated by the evaluation of equation A.10, since there is a singularity in this equation at 0 K, and in ny case there will be phase changes. Phase changes will lead to isothermal changes in entropy, and each different phase will have a different temperature/entropy relationship. Instead, use is made of the values of entropy for substances at 25°C in their standard state at a pressure of 1 bar (WARNING - Many sources use a datum pressure of 1 atm).

The entropy can be evaluated at other pressures from:

$$S = S^\circ - R_o \ln(p/p^\circ) \qquad \text{(A.11}$$

The Internal Energy (U) and Gibbs Function (G) are by definition:

$$H = U + pV = U + R_oT \qquad \text{and} \qquad G^\circ = H^\circ - TS^\circ \qquad \text{(A.12}$$

With the superscript ° referring to the datum pressure (p°) of 1 bar. The Gibbs function can be evaluated at other pressures in a similar way to the entropy (Equation A.11), and through the use of this equation:

$$G = G^\circ + (H - H^\circ) - T(S - S^\circ) = G^\circ + R_oT \ln(p/p^\circ) \qquad \text{(A.13}$$

The changes in S and G between state 1 (p_1, T_1) and state 2 (p_2, T_2), for a gas or vapour, are given by:

$$S_2 - S_1 = (S_2 - S_2^\circ) + (S_2^\circ - S_1^\circ) + (S_1^\circ - S_1)$$

$$S_2 - S_1 = (S_2^\circ - S_1^\circ) - R_o \ln(p_2/p_1) \qquad \text{(A.14}$$

and

$$G_2 - G_1 = (G_2 - G_2^\circ) + (G_2^\circ - G_1^\circ) + (G_1^\circ - G_1)$$

$$G_2 - G_1 = (G_2^\circ - G_1^\circ) + R_oT_2\ln(p_2/p^\circ) - R_oT_1\ln(p_1/p^\circ) \qquad \text{(A.15}$$

When the entropy and Gibbs Function of a mixture is being evaluated, then the properties of the individual constituents are summed, but the pressures (p_1 and p_2) now refer to the partial pressures of each constituent.

The use of these tables in combustion calculations, is best illustrated by an example.

EXAMPLE a mixture of carbon monoxide and 10% excess air at 25°C is burnt at constant pressure, and it is assumed that no carbon monoxide is present in the products. Treat air as 19% nitrogen and 21% oxygen, and estimate the adiabatic flame temperature.

Solution

The stoichiometric equation is: $CO + x(O_2 + 79/21\ N_2) \rightarrow CO_2 + 79x/21\ N_2$

Balancing of the oxygen <u>atoms</u> gives: $1 + 2x = 2$

With 10% excess air the combustion equation is:

$$CO + 0.55(O_2 + 79/21\ N_2) \rightarrow CO_2 + 0.05O_2 + 2.07N_2$$

At 25°C, the enthalpy of the reactants (H_R) is: H_R = -110.525 + 0.55(0 + 0) = -110.525 MJ/kmol_CO

Since the flame is adiabatic, then $H_P = H_R$ = -110.525 MJ/kmol_CO

Thus a temperature has to be found, at which the enthalpy of the products will sum to -110.525 MJ/kmol.

1st Guess 2000 K

$H_{P,2000} = 1 \times -302.128 + 0.05 \times 59.171 + 2.07 \times 56.114 = -183.013$

2nd Guess 3000 K

$H_{P,3000} = 1 \times -240.621 + 0.05 \times 98.116 + 2.07 \times 92.754 = -43.714$

The 3rd guess can be based on linear interpolation:

$$T_3 = 2000 + 1000\times(-110.525 + 183.013)/(-43.714 + 183.013) = 2520 \text{ K}$$

More accurate interpolation of the tables would lead to a temperature of 2523 K, but this is of limited purpose, since dissociation results in a temperature of about 2350 K.

A.2.2 Equilibrium Constants

Chemical reactions move towards an equilibrium in which both the reactants and products are present. If the concentration of the products is much greater than that of the reactants, then the reaction is said to be 'complete'. However, at the elevated temperatures associated with combustion there may be reactants, products, and partial products of combustion (eg CO) all present. Chemical reactions proceed in such a way as to minimise the Gibbs energy of the system, since this is the requirement for any system to be in equilibrium. This can be established by considering equation 2.11:

$$W_{REV} = G_{R0} - G_{P0} = -\Delta G_0 \qquad (2.11)$$

If a system has the capability for doing work, then the Gibbs energy will be reduced, thus when no more work can be done, the system will be in equilibrium and the Gibbs energy will be a minimum. For reacting mixtures it is helpful to introduce a parameter to define the extent of a reaction (ξ).

At a constant temperature and pressure, consider a reaction in which A is in equilibrium with B:

$$\mathrm{A} \rightleftharpoons \mathrm{B}$$

For an infinitesimal change dξ of A into B:

the change in amount of A present is $dn_A = -d\xi$, and
the change in amount of B present is $dn_B = +d\xi$. (A.16

The change in Gibbs energy at constant temperature and pressure, when the concentration of a species changes (with no other changes in composition of the mixture) is known as its chemical potential (μ). Thus

$$\mu = (\partial G/\partial n)_{T,p,nj} \qquad \text{(A.17}$$

The subscript n_j indicating that there is no change in the amounts of any of the other species that might be present.

For our simple system with only substances A and B, then the change in Gibbs energy is given by:

$\mathrm{d}G = (\partial G/\partial n)_{T,p,n\mathrm{B}}\mathrm{d}n_\mathrm{A} + (\partial G/\partial n)_{T,p,n\mathrm{A}}\mathrm{d}n_\mathrm{B} = \mu_\mathrm{A}\mathrm{d}n_\mathrm{A} + \mu_\mathrm{B}\mathrm{d}n_\mathrm{B}$
$= -\mu_\mathrm{A}\mathrm{d}\xi + \mu_\mathrm{B}\mathrm{d}\xi$ (A.18

The change in Gibbs energy with a change in the extent of the reaction is:

$(\partial G/\partial \xi)_{T,p} = -\mu_\mathrm{A} + \mu_\mathrm{B},$ (A.19

and at equilibrium $(\partial G/\partial \xi)_{T,p} = 0.$ (A.20

Since the Gibbs energy is now a minimum, there can be no scope for the system to do any work, and the system will be at equilibrium.

This now needs to be extended to a multi-component reaction, in which *a* kmols of species A, *b* kmols of species B and so on react to produce *c* kmols of species C, *d* kmols of species D:

$a\mathrm{A} + b\mathrm{B} \rightleftharpoons c\mathrm{C} + d\mathrm{D}$ or, $a\mathrm{A} + b\mathrm{B} - c\mathrm{C} - d\mathrm{D} = 0$

This can be generalised as: $\Sigma \nu_i A_i = 0$ (A.21

where ν_i is the stoichiometric coefficient of species A_i.

When the extent of the reaction changes by $\mathrm{d}\xi$, the amounts of the reactants and products change by:

$\mathrm{d}n_\mathrm{A} = -a\mathrm{d}\xi$, $\mathrm{d}n_\mathrm{B} = -b\mathrm{d}\xi$, $\mathrm{d}n_\mathrm{C} = +c\mathrm{d}\xi$, and $\mathrm{d}n_\mathrm{D} = +d\mathrm{d}\xi$, (A.22

and in general $\mathrm{d}n_\mathrm{i} = -\nu_i\mathrm{d}\xi.$ (A.23

So, at constant pressure and temperature, the change in Gibbs energy is:

$\mathrm{d}G = \mu_\mathrm{A}\mathrm{d}n_\mathrm{A} + \mu_\mathrm{B}\mathrm{d}n_\mathrm{B} + \mu_\mathrm{C}\mathrm{d}n_\mathrm{C} + \mu_\mathrm{D}\mathrm{d}n_\mathrm{D} = (-a\mu_\mathrm{A} - b\mu_\mathrm{B} + c\mu_\mathrm{C} + d\mu_\mathrm{D})\mathrm{d}\xi$ (A.24

and in general: $\mathrm{d}G = (\Sigma \nu_i \mu_i)\mathrm{d}\xi$, and $(\partial G/\partial \xi)_{T,p} = (\Sigma \nu_i \mu_i)$ (A.25

and at equilibrium $(\partial G/\partial \xi)_{T,p} = 0$, so $\Sigma \nu_i \mu_i = 0.$ (A.26

For species *i*: $\mu_i = (\partial G/\partial n_i)_{T,p,nj}$ (A.17

For a pure substance, the chemical potential (μ_i) is simply the molar Gibbs energy G/n_i. For one mole of gas:

$G = G^\circ + R_oT\ln(p/p^\circ)$ (A.13

so $\mu = \mu^\circ + R_oT\ln(p/p^\circ)$ (A.27

where the superscript ° refers to the use of a pressure datum of 1 bar.

For gaseous species *i* with ideal gas behaviour (enthalpy is not a function of pressure):

$\mu_i = \mu_i^\circ + R_oT\ln(p_i/p^\circ)$ (A.28

or $\mu_i = \mu_i^\circ + R_oT\ln(p^*_i)$ (A.29

where p^*_i represents the numerical value of the partial pressure of component *i*, when the pressure is expressed in units of **bar**.

For the mixture at equilibrium: $\Sigma \nu_i \mu_i = 0$ (A.26

Combining equations A.26 and A.29 gives: $\Sigma \nu_i(\mu_i^\circ + R_o T \ln(p*_i)) = \Sigma \nu_i(G_i^\circ + R_o T \ln(p*_i)) = 0$

or $\Delta G^\circ = -R_o T \Sigma(\nu_i \ln p*_i) = -R_o T \ln K_p$ (A.30

where $\Delta G^\circ = \Sigma \nu_i G_i^\circ$, the change in Gibbs (or free) energy for the reaction,

and $\Sigma(\nu_i \ln p*_i) = K_p$, (A.31

where K_p is the equilibrium constant of the reaction.

This is more frequently expressed as $K_p = \Pi p*_i^{\nu i}$, with Π denoting the product of the terms that follow. The equilibrium constant has a strong temperature dependency, so it is convenient to tabulate $\ln K_p$. Although it has no pressure dependency, it is essential to use the appropriate pressure units for the partial pressures unless $\Sigma \nu_i = 0$.

For the multicomponent reaction $a\text{A} + b\text{B} \rightleftharpoons c\text{C} + d\text{D}$:

$$K_p = \Pi p*_i^{\nu i} = (p*_\text{C}^{\text{c}} \times p*_\text{D}^{\text{d}})/(p*_\text{A}^{\text{a}} \times p*_\text{B}^{\text{b}}) \qquad (3.6$$

Remembering that $p*_i$ is the numerical value of the partial pressure of component i, when the pressure is expressed in units of **bar**.

The equilibrium constant can be determined from the change in Gibbs energy of the reaction at the relevant temperature:

$$\ln K_p = -\Delta G^\circ / R_o T, \text{ where } \Delta G^\circ = \Sigma \nu_i G_i^\circ \qquad (A.32$$

Thus the equilibrium constants can be calculated from the Gibbs energy values in Tables A.4 and A.5, and this is indeed how Table A.6 has been produced.

Tabulations of the equilibrium constants can be found in many sources (e.g. Howatson et al (1991), Haywood (1982) and Rogers and Mayhew (1988)). For calculations, an analytical expression is frequently more convenient, and an appropriate form can be found by dividing the equation for the Gibbs energy by $R_o T$. Such an equation was used by Olikara and Borman (1975).

$$\log_{10} K_p = A \ell n(T) + B/T + C + DT + ET^2 \qquad (A.33$$

Who evaluated these coefficients for a number of equilibria in the range 600 to 4000 K. Olikara and Borman used a temperature unit of kK and pressure units of atmospheres; in Table A.2 the pressure units have been converted to bar.

Regardless of the source of the equilibrium constant data, it is essential to pay strict attention to:

a) the pressure units
b) the form of the equation

Table A.2 **Coefficients for the evaluation of $Log_{10}K_p$; pressure units - bar, temperature units - kK**

Constants Reaction	A	B	C	D	E
½H_2 ⇄ H	0.432168	-0.112464 E2	0.266983 E1	-0.745744 E-1	0.242484 E-2
½O_2 ⇄ O	0.310805	-0.129540 E2	0.3214932 E1	-0.738336 E-1	0.344645 E-2
½N_2 ⇄ N	0.389716	-0.245828 E2	0.3142192 E1	-0.963730 E-1	0.585643 E-2
½O_2 + ½H_2 ⇄ OH	-0.141784	-0.213308 E1	0.853461	0.355015 E-1	-0.310227 E-2
½N_2 + ½O_2 ⇄ NO	0.150879 E-1	-0.470959 E1	0.646096	0.272805 E-2	-0.154444 E-2
H_2 + ½O_2 ⇄ H_2O	-0.752364	0.124210 E2	-0.262575 E1	0.259556	-0.162687 E-1
CO + ½O_2 ⇄CO_2	-0.415302 E-2	0.148627 E2	-0.475460 E1	0.124699	-900227 E-2

Consider now the equilibrium between H_2O, H and OH, which is not detailed in Table A.2.

$$H_2O \rightleftharpoons H + OH$$

$$K_p = \frac{p_H \, p_{OH}}{p_{H_2O}} \qquad \text{(A.34}$$

However, it will be shown how this can be reformulated in terms of the following tabulated equilibria: Equation 4.11 can be rewritten as:

$$\text{Thus} \qquad K_p = \frac{K_{p,H} * K_{p,OH}}{K_{p,H_2O}} \qquad \text{(A.35}$$

$$\tfrac{1}{2}H_2 \rightleftharpoons H \qquad K_{p,H} = p_H / p_{H_2}^{1/2}$$

$$\tfrac{1}{2}O_2 + \tfrac{1}{2}H_2 \rightleftharpoons OH \qquad K_{p,OH} = p_{OH} / \left(p_{H_2}^{1/2} * p_{O_2}^{1/2}\right)$$

$$H_2 + \tfrac{1}{2}O_2 \rightleftharpoons H_2O \qquad K_{p,H_2O} = p_{H_2O} / \left(p_{H_2} * p_{O_2}^{1/2}\right)$$

$$K_p = \frac{p_H p_{OH}}{p_{H_2O}} \times \frac{p_{H_2} p_{O_2}^{1/2}}{p_{H_2} p_{O_2}^{1/2}} = \frac{\dfrac{p_H}{p_{H_2}^{1/2}} * \dfrac{p_{OH}}{p_{H_2}^{1/2} * p_{O_2}^{1/2}}}{\dfrac{p_{H_2O}}{p_{H_2} * p_{O_2}^{1/2}}}$$

$$or \qquad \log_{10} K_p = \log_{10} K_{p,H} + \log_{10} K_{p,OH} - \log_{10} K_{p,H_2O}$$

This result can be generalised, and applied to the values of the equilibrium constants of formation of species (K_f) from the elements in their standard state. The JANAF Tables (1983) tabulate $log_{10}K_f$ for numerous species. For elements in their standard state (e.g. N_2, O_2, He etc) $log_{10}K_f$ is zero.

$$\log_{10}(K_p)_{reaction} = \sum_i \upsilon_i \log_{10}(K_f)_i \qquad \text{(A.36}$$

A.3 Thermodynamic Data

The following fuel properties have been obtained from the listings of 'Physical and Thermodynamic Properties of Pure Chemicals' by Daubert & Danner (1989). This comprehensive compilation covers the properties of solids, liquids and gases, with analytical expressions and coefficients that enable the temperature dependency of the following properties to be determined:

Solid density
Liquid density
Vapour pressure
Enthalpy of vaporisation
Solid specific heat capacity
Liquid specific heat capacity
Ideal gas specific heat capacity
Second virial coefficient (polynomials used in the Equation of State)
Liquid viscosity
Vapour viscosity
Liquid thermal conductivity
Vapour thermal conductivity
Surface tension

Table A.3 Boiling Points, Enthalpy of Vaporisation, Liquid Density and Specific Heat Capacity, Molar Masses, Standard Enthalpy of Formation, Standard State Entropy, and Calorific Values for fuels derived from Daubert & Danner (1989).

Fuel	Formula	Boiling Point at 1 atm (°C)	Enthalpy of Vaporisation[1] at 298.15K (MJ/kmol)	Density[1] (kg/m^3)	$C_{p,l}$[1,2] kJ/kmolK
Methane	CH_4	-161.5	8.171	422.5	57[a]
Propane	C_3H_8	-42.0	18.743	582.5	106.3[b]
Benzene	C_6H_6	80.1	33.790	872.9	135.6
Toluene	C_7H_8	110.6	38.341	864.7	156.1
n-Heptane	C_7H_{16}	98.4	36.630	681.5	224.7
Iso-octane (2,2,4-trimethylpentane)	C_8H_{18}	99.2	35.142	690.4	236.4
n-Hexadecane (Cetane)	$C_{16}H_{34}$	286.9	79.641	769.7	501.7
αMethylnaphthalene	$C_{10}H_7CH_3$	244.7	59.387	1017.2	224.4[c]
Methanol	CH_3OH	64.7	38.012	789.6	81.6
Ethanol	C_2H_5OH	78.3	42.512	785.9	113.0
Nitromethane	CH_3NO_2	101.2	38.365	1112.7	106.3

Fuel	Formula	M kg/kmol	H_f MJ/kmol	S^{o3} kJ/kmolK	Calorific Values[4] MJ/kmol	at 298.15K MJ/kg
Methane	CH_4	16.043	-74.52	186.27	802.64	50.031
Propane	C_3H_8	44.096	-104.68	270.2	2043.15	46.334
Benzene	C_6H_6	78.114	82.93	269.20	3169.47	40.575
Toluene	C_7H_8	92.141	50.00	319.74	3771.88	40.936
n-Heptane	C_7H_{16}	100.204	-187.65	427.98	4501.53	44.924
Iso-octane (2,2,4-trimethylpentane)	C_8H_{18}	114.231	-224.01	422.96	5100.50	44.651
n-Hexadecane (Cetane)	$C_{16}H_{34}$	226.446	-374.17	781.02	10033.03	44.307
αMethylnaphthalene	$C_{10}H_7CH_3$	142.2	116.86	377.44	5654.61	39.765
Methanol	CH_3OH	32.042	-200.94	239.88	676.22	21.104
Ethanol	C_2H5OH	46.069	-234.95	280.64	1277.55	27.731
Nitromethane	CH_3NO_2	61.040	-74.73	275.01	681.52	11.165

note 1 Properties have been evaluated at 25°C, except when a substance is a gas at this temperature, in which case the evaluation refers to the normal boiling point.

note 2 These data were obtained from the 'Handbook of Chemistry and Physics' (70th ed CRC Press, 1990), with the exception of the following data:

a Y S Touloukian & T Makita 'Specific Heat, nonmetallic liquids and gases', (Plenum, 1970)
b International Critical Tables, vol V, (McGraw Hill 1929)
c Daubert & Danner (1989)

note 3 The entropy values tabulated here for the standard state (S^o) refer to a pressure of 1 atm (1.01325 bar), whilst the entropy values evaluated in Tables A.4 and A.5 use a pressure of 1 bar as the datum; this accounts for the slight differences in the numerical values for entropy at 298.15K. The standard state values can refer to a hypothetical state, and this is indeed the case for many of these fuels, which cannot exist as a vapour at a pressure of 1 atm and a temperature of 298.15K.

note 4 The calorific values have been determined from the difference in the enthalpies of formation of the fuel and products, with all reactants and products in the vapour phase, this is known as the Net or Lower Calorific Value (LCV). When the water vapour in the products of combustion has been condensed to its liquid state, the calorific value of the fuel is known as the Gross or Higher Calorific Value (HCV), thus:

$$\text{HCV} = \text{LCV} + (n \times H_{fg})_{H2O}$$

where the enthalpy of condensation of **the water vapour, H_{fg} = 43.99 MJ/kmol_H_2O.**

Table A.4 Thermodynamic data for gaseous species

'ABSOLUTE' MOLAR ENTHALPY
(MJ/kmol)

T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
0	-8.774	-8.823	-8.709	-8.222	-119.363	-402.239	-251.763	81.717	-6.201	32.721	243.041	211.787	0
100	-5.784	-5.812	-5.755	-5.584	-116.336	-399.897	-248.414	84.423	-4.121	35.180	245.154	213.866	100
200	-2.855	-2.864	-2.858	-2.804	-113.387	-396.934	-245.097	87.231	-2.041	37.716	247.264	215.944	200
298.15	**0.0**	**0.0**	**0.0**	**0.0**	**-110.525**	**-393.512**	**-241.824**	**90.080**	**.000**	**40.277**	**249.333**	**217.984**	**298.15**
300	0.053	0.053	0.054	0.056	-110.471	-393.443	-241.761	90.135	.038	40.326	249.372	218.023	300
400	2.973	2.969	3.028	2.959	-107.550	-389.509	-238.371	93.125	2.118	43.005	251.477	220.101	400
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
500	5.930	5.909	6.089	5.880	-104.594	-385.208	-234.899	96.195	4.198	45.752	253.580	222.180	500
600	8.942	8.893	9.247	8.811	-101.584	-380.605	-231.326	99.337	6.278	48.564	255.681	224.259	600
700	12.018	11.934	12.500	11.750	-98.505	-375.753	-227.639	102.547	8.358	51.437	257.780	226.337	700
800	15.164	15.042	15.837	14.704	-95.353	-370.699	-223.831	105.817	10.438	54.369	259.876	228.416	800
900	18.379	18.219	19.244	17.681	-92.128	-365.477	-219.899	109.143	12.518	57.358	261.971	230.495	900
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
1000	21.655	21.459	22.708	20.686	-88.838	-360.112	-215.841	112.518	14.598	60.399	264.063	232.573	1000
1100	24.984	24.756	26.213	23.729	-85.496	-354.624	-211.652	115.939	16.678	63.492	266.154	234.652	1100
1200	28.357	28.100	29.754	26.814	-82.107	-349.051	-207.337	119.400	18.758	66.633	268.243	236.730	1200
1300	31.772	31.489	33.328	29.942	-78.676	-343.395	-202.904	122.897	20.838	69.820	270.330	238.809	1300
1400	35.224	34.917	36.934	33.112	-75.208	-337.664	-198.359	126.427	22.918	73.050	272.416	240.888	1400
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
1500	38.711	38.380	40.571	36.323	-71.707	-331.867	-193.711	129.986	24.998	76.322	274.501	242.966	1500
1600	42.228	41.876	44.237	39.574	-68.176	-326.012	-188.966	133.572	27.078	79.634	276.585	245.045	1600
1700	45.774	45.400	47.931	42.865	-64.618	-320.105	-184.131	137.180	29.158	82.982	278.668	247.124	1700
1800	49.345	48.949	51.652	46.194	-61.037	-314.151	-179.212	140.808	31.238	86.365	280.751	249.202	1800
1900	52.940	52.522	55.399	49.560	-57.435	-308.158	-174.215	144.454	33.318	89.781	282.833	251.281	1900
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
2000	56.556	56.114	59.171	52.962	-53.815	-302.128	-169.146	148.116	35.398	93.228	284.915	253.359	2000
2100	60.190	59.725	62.967	56.399	-50.178	-296.068	-164.009	151.792	37.478	96.705	286.997	255.438	2100
2200	63.842	63.351	66.787	59.870	-46.527	-289.981	-158.810	155.480	39.558	100.208	289.079	257.517	2200
2300	67.510	66.991	70.630	63.373	-42.863	-283.870	-153.553	159.179	41.638	103.738	291.162	259.595	2300
2400	71.192	70.644	74.495	66.908	-39.189	-277.737	-148.243	162.886	43.718	107.292	293.246	261.674	2400
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
2500	74.887	74.308	78.381	70.474	-35.504	-271.587	-142.883	166.602	45.797	110.868	295.330	263.753	2500
2600	78.595	77.981	82.288	74.068	-31.811	-265.420	-137.478	170.326	47.877	114.465	297.416	265.831	2600
2700	82.313	81.664	86.216	77.691	-28.111	-259.239	-132.031	174.055	49.957	118.083	299.503	267.910	2700
2800	86.041	85.354	90.163	81.341	-24.403	-253.045	-126.545	177.790	52.037	121.718	301.592	269.988	2800
2900	89.779	89.051	94.130	85.016	-20.689	-246.838	-121.022	181.531	54.117	125.371	303.684	272.067	2900
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
3000	93.527	92.754	98.116	88.716	-16.969	-240.621	-115.467	185.276	56.197	129.040	305.777	274.146	3000
3100	97.282	96.464	102.120	92.439	-13.244	-234.393	-109.881	189.026	58.277	132.724	307.872	276.224	3100
3200	101.046	100.179	106.142	96.185	-9.514	-228.155	-104.266	192.780	60.357	136.421	309.971	278.303	3200
3300	104.818	103.900	110.182	99.953	-5.778	-221.907	-98.625	196.538	62.437	140.132	312.072	280.382	3300
3400	108.597	107.625	114.238	103.741	-2.039	-215.650	-92.959	200.300	64.517	143.855	314.177	282.460	3400
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
3500	112.383	111.356	118.312	107.549	1.706	-209.383	-87.271	204.066	66.597	147.589	316.284	284.539	3500
3600	116.177	115.091	122.402	111.377	5.455	-203.106	-81.561	207.836	68.677	151.334	318.396	286.617	3600
3700	119.978	118.832	126.507	115.223	9.209	-196.819	-75.832	211.610	70.757	155.089	320.511	288.696	3700
3800	123.786	122.577	130.627	119.086	12.968	-190.522	-70.083	215.389	72.837	158.853	322.630	290.775	3800
3900	127.600	126.326	134.762	122.968	16.731	-184.215	-64.317	219.171	74.917	162.627	324.754	292.853	3900
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
4000	131.421	130.081	138.911	126.866	20.499	-177.898	-58.533	222.958	76.997	166.409	326.881	294.932	4000
4100	135.249	133.840	143.074	130.781	24.272	-171.570	-52.733	226.748	79.077	170.200	329.014	297.011	4100
4200	139.083	137.604	147.249	134.713	28.049	-165.232	-46.918	230.543	81.157	173.998	331.150	299.089	4200
4300	142.923	141.373	151.436	138.662	31.831	-158.884	-41.088	234.342	83.237	177.805	333.292	301.168	4300
4400	146.769	145.147	155.634	142.627	35.617	-152.526	-35.242	238.145	85.317	181.620	335.439	303.246	4400
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
4500	150.621	148.925	159.842	146.610	39.408	-146.159	-29.383	241.951	87.397	185.443	337.590	305.325	4500
4600	154.478	152.707	164.060	150.610	43.202	-139.783	-23.509	245.761	89.477	189.273	339.747	307.404	4600
4700	158.340	156.493	168.286	154.628	47.000	-133.400	-17.621	249.574	91.557	193.112	341.909	309.482	4700
4800	162.206	160.282	172.519	158.665	50.801	-127.012	-11.719	253.390	93.636	196.960	344.076	311.561	4800
4900	166.075	164.074	176.758	162.722	54.604	-120.619	-5.803	257.207	95.716	200.816	346.249	313.640	4900
5000	169.947	167.868	-181.001	166.800	58.409	-114.224	.127	261.025	97.796	204.682	348.427	315.718	5000
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)

Note

The term 'ABSOLUTE' Molar Enthalpy adopted here, uses a datum of ***zero enthalpy for elements when they are in their standard state at a temperature of 25°C***. The enthalpy of any molecule at 25°C will thus correspond to its enthalpy of formation, $\Delta H_f°$. The tables have been extrapolated below 300 K, and these data should be used with caution.

The enthalpies have been evaluated by the integration of a polynomial function that describes the molar specific heat capacity (C_p) variation with temperature. The difference in Enthalpy of Reactants and Products at 25°C will thus correspond to the Constant Pressure Calorific Value of the reaction.

'ABSOLUTE' MOLAR INTERNAL ENERGY

(MJ/kmol)

T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
0	-8.774	-8.823	-8.709	-8.222	-119.363	-402.239	-251.763	81.717	-6.201	32.721	243.041	211.787	0
100	-6.615	-6.643	-6.586	-6.415	-117.167	-400.729	-249.246	83.592	-4.953	34.349	244.322	213.034	100
200	-4.518	-4.527	-4.521	-4.467	-115.050	-398.597	-246.759	85.569	-3.704	36.053	245.601	214.281	200
298.15	**-2.480**	**-2.480**	**-2.479**	**-2.476**	**-113.004**	**-395.991**	**-244.303**	**87.601**	**-2.479**	**37.798**	**246.854**	**215.505**	**298.15**
300	-2.441	-2.441	-2.440	-2.438	-112.966	-395.937	-244.256	87.640	-2.456	37.831	246.877	215.528	300
400	-.352	-.356	-.298	-.367	-110.876	-392.835	-241.697	89.799	-1.207	39.680	248.151	216.776	400
500	1.773	1.752	1.931	1.723	-108.751	-389.366	-239.057	92.037	.041	41.595	249.423	218.023	500
600	3.953	3.904	4.258	3.822	-106.572	-385.594	-236.314	94.349	1.290	43.575	250.692	219.270	600
700	6.198	6.114	6.680	5.930	-104.325	-381.574	-233.459	96.727	2.538	45.617	251.959	220.517	700
800	8.513	8.390	9.186	8.053	-102.004	-377.351	-230.483	99.166	3.787	47.718	253.225	221.764	800
900	10.896	10.735	11.761	10.198	-99.611	-372.960	-227.382	101.660	5.035	49.874	254.487	223.012	900
1000	13.341	13.145	14.393	12.371	-97.153	-368.427	-224.155	104.204	6.284	52.085	255.749	224.259	1000
1100	15.838	15.610	17.067	14.583	-94.642	-363.770	-220.798	106.793	7.532	54.346	257.008	225.506	1100
1200	18.380	18.123	19.777	16.837	-92.084	-359.028	-217.315	109.422	8.781	56.655	258.265	226.753	1200
1300	20.963	20.680	22.519	19.133	-89.485	-354.204	-213.713	112.088	10.029	59.011	259.521	228.000	1300
1400	23.584	23.276	25.294	21.472	-86.849	-349.304	-210.000	114.787	11.278	61.410	260.776	229.247	1400
1500	26.239	25.908	28.099	23.851	-84.179	-344.339	-206.183	117.515	12.526	63.851	262.029	230.495	1500
1600	28.925	28.572	30.934	26.271	-81.479	-339.315	-202.270	120.268	13.775	66.330	263.282	231.742	1600
1700	31.639	31.265	33.796	28.730	-78.753	-334.239	-198.266	123.045	15.023	68.847	264.534	232.989	1700
1800	34.379	33.983	36.686	31.228	-76.003	-329.117	-194.178	125.842	16.272	71.399	265.785	234.236	1800
1900	37.143	36.724	39.601	33.762	-73.233	-323.955	-190.013	128.657	17.520	73.983	267.035	235.483	1900
2000	39.927	39.485	42.542	36.333	-70.444	-318.757	-185.775	131.487	18.769	76.599	268.286	236.730	2000
2100	42.730	42.264	45.507	38.938	-67.638	-313.529	-181.469	134.332	20.017	79.244	269.536	237.978	2100
2200	45.551	45.059	48.495	41.578	-64.819	-308.273	-177.102	137.188	21.266	81.916	270.787	239.225	2200
2300	48.387	47.868	51.507	44.250	-61.987	-302.993	-172.676	140.055	22.514	84.615	272.039	240.472	2300
2400	51.237	50.689	54.540	46.954	-59.144	-297.692	-168.198	142.932	23.763	87.337	273.291	241.719	2400
2500	54.101	53.521	57.595	49.688	-56.291	-292.373	-163.670	145.816	25.011	90.082	274.544	242.966	2500
2600	56.977	56.364	60.670	52.451	-53.429	-287.038	-159.096	148.708	26.260	92.848	275.798	244.213	2600
2700	59.864	59.214	63.767	55.242	-50.560	-281.688	-154.480	151.606	27.508	95.633	277.054	245.461	2700
2800	62.761	62.073	66.883	58.060	-47.683	-276.325	-149.825	154.510	28.757	98.438	278.312	246.708	2800
2900	65.667	64.939	70.018	60.904	-44.801	-270.950	-145.134	157.419	30.005	101.259	279.571	247.955	2900
3000	68.583	67.811	73.172	63.772	-41.913	-265.564	-140.410	160.333	31.254	104.096	280.833	249.202	3000
3100	71.507	70.689	76.345	66.664	-39.019	-260.168	-135.656	163.251	32.502	106.949	282.098	250.449	3100
3200	74.440	73.573	79.535	69.579	-36.120	-254.762	-130.872	166.173	33.751	109.815	283.364	251.697	3200
3300	77.380	76.462	82.744	72.515	-33.216	-249.345	-126.063	169.100	34.999	112.694	284.634	252.944	3300
3400	80.328	79.356	85.969	75.472	-30.308	-243.919	-121.229	172.031	36.248	115.585	285.907	254.191	3400
3500	83.283	82.255	89.211	78.448	-27.395	-238.484	-116.372	174.965	37.496	118.488	287.184	255.438	3500
3600	86.245	85.159	92.469	81.444	-24.477	-233.038	-111.494	177.904	38.745	121.402	288.464	256.685	3600
3700	89.214	88.068	95.743	84.459	-21.555	-227.583	-106.595	180.847	39.993	124.325	289.747	257.932	3700
3800	92.191	90.981	99.032	87.491	-18.627	-222.117	-101.678	183.794	41.242	127.258	291.035	259.180	3800
3900	95.174	93.900	102.336	90.541	-15.696	-216.642	-96.743	186.744	42.490	130.200	292.327	260.427	3900
4000	98.163	96.823	105.653	93.608	-12.759	-211.156	-91.791	189.700	43.739	133.151	293.623	261.674	4000
4100	101.160	99.751	108.984	96.692	-9.818	-205.659	-86.823	192.659	44.987	136.110	294.924	262.921	4100
4200	104.162	102.684	112.328	99.792	-6.872	-200.153	-81.839	195.622	46.236	139.077	296.229	264.168	4200
4300	107.171	105.621	115.684	102.909	-3.922	-194.636	-76.840	198.590	47.484	142.053	297.540	265.415	4300
4400	110.186	108.563	119.050	106.043	-.967	-189.109	-71.826	201.561	48.733	145.036	298.855	266.663	4400
4500	113.206	111.509	122.427	109.195	1.993	-183.574	-66.798	204.536	49.981	148.027	300.175	267.910	4500
4600	116.232	114.460	125.813	112.363	4.956	-178.030	-61.756	207.515	51.230	151.027	301.500	269.157	4600
4700	119.262	117.414	129.208	115.550	7.922	-172.479	-56.699	210.496	52.478	154.034	302.831	270.404	4700
4800	122.296	120.372	132.609	118.756	10.892	-166.921	-51.629	213.480	53.727	157.050	304.167	271.651	4800
4900	125.334	123.333	136.017	121.981	13.863	-161.360	-46.544	216.465	54.975	160.075	305.508	272.898	4900
5000	128.374	126.296	139.429	125.228	16.836	-155.797	-41.446	219.452	56.224	163.110	306.854	274.146	5000
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)

Note

The term 'ABSOLUTE' Molar Internal Energy adopted here, uses the same datum as the enthalpy table, namely a datum of ***zero enthalpy for elements when they are in their standard state at a temperature of 25°C***. The tables have been extrapolated below 300 K, and these data should be used with caution.

The difference in Internal Energy of Reactants and Products at 25°C will thus correspond to the Constant Volume Calorific Value of the reaction. When there is a difference in the number of kmols of gaseous reactants and products, the Constant Pressure Calorific Value (the difference in Enthalpy of Reactants and Products at 25°C) will differ from the Constant Volume Calorific Value .

'ABSOLUTE' MOLAR ENTROPY

(kJ/kmolK)

T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0
100	162.167	159.512	173.442	100.054	165.543	179.639	152.512	179.394	132.087	157.595	138.332	92.008	100
200	182.484	179.963	193.531	119.277	186.001	199.953	175.510	198.821	146.504	175.143	152.960	106.416	200
298.15	**194.096**	**191.614**	**205.150**	**130.689**	**197.646**	**213.811**	**188.820**	**210.398**	**154.809**	**185.550**	**161.376**	**114.715**	**298.15**
300	194.276	191.794	205.332	130.868	197.826	214.041	189.028	210.580	154.938	185.713	161.507	114.844	300
400	202.675	200.182	213.880	139.216	206.229	225.329	198.775	219.176	160.921	193.418	167.564	120.824	400
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
500	209.272	206.741	220.707	145.734	212.823	234.913	206.519	226.023	165.563	199.545	172.257	125.462	500
600	214.760	212.179	226.463	151.077	218.310	243.299	213.032	231.751	169.355	204.669	176.087	129.252	600
700	219.502	216.866	231.476	155.608	223.054	250.773	218.713	236.698	172.561	209.097	179.322	132.456	700
800	223.701	221.015	235.931	159.553	227.262	257.519	223.795	241.064	175.339	213.012	182.122	135.232	800
900	227.487	224.756	239.943	163.058	231.060	263.668	228.425	244.980	177.788	216.531	184.589	137.680	900
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
1000	230.938	228.170	243.591	166.224	234.525	269.319	232.700	248.536	179.980	219.735	186.793	139.870	1000
1100	234.111	231.312	246.935	169.127	237.712	274.541	236.693	251.796	181.962	222.682	188.786	141.851	1100
1200	237.046	234.222	250.015	171.811	240.661	279.390	240.447	254.807	183.772	225.415	190.604	143.660	1200
1300	239.779	236.934	252.876	174.315	243.407	283.917	243.995	257.606	185.437	227.965	192.275	145.324	1300
1400	242.337	239.474	255.548	176.664	245.976	288.163	247.362	260.222	186.978	230.359	193.821	146.864	1400
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
1500	244.743	241.863	258.057	178.879	248.392	292.162	250.569	262.678	188.413	232.617	195.259	148.298	1500
1600	247.013	244.119	260.423	180.977	250.671	295.941	253.631	264.991	189.756	234.754	196.604	149.640	1600
1700	249.162	246.255	262.662	182.972	252.827	299.522	256.562	267.179	191.017	236.783	197.867	150.900	1700
1800	251.204	248.284	264.789	184.875	254.874	302.925	259.373	269.253	192.206	238.717	199.057	152.088	1800
1900	253.147	250.216	266.815	186.694	256.822	306.166	262.075	271.224	193.330	240.564	200.183	153.212	1900
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
2000	255.002	252.058	268.750	188.439	258.679	309.258	264.675	273.102	194.397	242.332	201.251	154.278	2000
2100	256.775	253.820	270.602	190.116	260.453	312.215	267.181	274.896	195.412	244.028	202.267	155.292	2100
2200	258.474	255.507	272.379	191.731	262.152	315.047	269.600	276.611	196.379	245.658	203.235	156.259	2200
2300	260.104	257.125	274.087	193.288	263.780	317.763	271.936	278.255	197.304	247.227	204.161	157.183	2300
2400	261.671	258.680	275.732	194.793	265.344	320.373	274.196	279.833	198.189	248.739	205.048	158.068	2400
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
2500	263.180	260.175	277.318	196.248	266.848	322.884	276.384	281.350	199.038	250.199	205.899	158.916	2500
2600	264.634	261.616	278.851	197.658	268.296	325.302	278.504	282.810	199.854	251.610	206.717	159.732	2600
2700	266.037	263.006	280.333	199.025	269.693	327.635	280.560	284.218	200.639	252.975	207.505	160.516	2700
2800	267.393	264.348	281.768	200.352	271.041	329.888	282.555	285.576	201.395	254.297	208.264	161.272	2800
2900	268.705	265.645	283.160	201.642	272.345	332.066	284.493	286.889	202.125	255.579	208.998	162.001	2900
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
3000	269.975	266.901	284.512	202.896	273.606	334.173	286.376	288.159	202.830	256.823	209.708	162.706	3000
3100	271.206	268.117	285.825	204.117	274.827	336.216	288.208	289.388	203.513	258.031	210.395	163.388	3100
3200	272.401	269.296	287.102	205.306	276.012	338.196	289.990	290.580	204.173	259.205	211.061	164.048	3200
3300	273.562	270.441	288.345	206.466	277.161	340.118	291.726	291.736	204.813	260.347	211.708	164.687	3300
3400	274.690	271.554	289.556	207.597	278.277	341.987	293.417	292.860	205.434	261.458	212.336	165.308	3400
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
3500	275.788	272.635	290.736	208.701	279.363	343.803	295.066	293.951	206.037	262.540	212.947	165.910	3500
3600	276.857	273.687	291.889	209.779	280.419	345.571	296.675	295.013	206.623	263.595	213.542	166.496	3600
3700	277.898	274.712	293.013	210.832	281.448	347.294	298.245	296.047	207.193	264.624	214.121	167.065	3700
3800	278.913	275.711	294.112	211.863	282.450	348.973	299.778	297.055	207.747	265.628	214.687	167.620	3800
3900	279.904	276.685	295.186	212.871	283.427	350.612	301.275	298.037	208.288	266.608	215.238	168.160	3900
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
4000	280.872	277.635	296.237	213.858	284.381	352.211	302.740	298.996	208.814	267.566	215.777	168.686	4000
4100	281.817	278.564	297.264	214.825	285.313	353.773	304.172	299.932	209.328	268.502	216.303	169.199	4100
4200	282.741	279.471	298.271	215.772	286.223	355.301	305.573	300.847	209.829	269.417	216.818	169.700	4200
4300	283.644	280.357	299.256	216.701	287.113	356.795	306.945	301.741	210.318	270.313	217.322	170.189	4300
4400	284.529	281.225	300.221	217.613	287.984	358.256	308.289	302.615	210.797	271.190	217.816	170.667	4400
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
4500	285.394	282.074	301.167	218.508	288.836	359.687	309.606	303.470	211.264	272.049	218.299	171.134	4500
4600	286.242	282.905	302.094	219.387	289.669	361.088	310.897	304.308	211.721	272.891	218.773	171.591	4600
4700	287.072	283.719	303.002	220.251	290.486	362.461	312.163	305.128	212.168	273.717	219.238	172.038	4700
4800	287.886	284.517	303.894	221.101	291.286	363.806	313.406	305.931	212.606	274.527	219.695	172.476	4800
4900	288.684	285.299	304.768	221.938	292.071	365.124	314.625	306.718	213.035	275.322	220.142	172.904	4900
5000	289.466	286.066	305.625	222.762	292.839	366.416	315.823	307.489	213.455	276.103	220.582	173.324	5000
T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)

Note

The entropy is evaluated by the integration of $dS = (C_p/T)dT$. When C_p is described by a polynomial function there is a singularity at 0 K. The datum is provided by the values of entropy for substances at 25°C in their standard state at a pressure of 1 bar (**WARNING** - Many sources use a datum pressure of 1 atm). The entropy can be evaluated at other pressures from:

$$S = S^\circ - R \ln(p/p^\circ)$$

With the superscript ° referring to the datum pressure (p°) of 1 bar. When the entropy of a mixture is being evaluated, then the properties of the individual constituents are summed, but the pressure (p) now refers to the partial pressures of each constituent.

'ABSOLUTE' MOLAR GIBBS ENERGY

(MJ/kmol)

T(K)	Air	N_2	O_2	H_2	CO	CO_2	H_2O	NO	Ar	OH	O	H	T(K)
0	-8.77	-8.82	-8.70	-8.22	-119.36	-402.23	-251.76	81.71	-6.20	32.72	243.04	211.78	0
100	-22.00	-21.76	-23.09	-15.58	-132.89	-417.86	-263.66	66.48	-17.33	19.42	231.32	204.66	100
200	-39.35	-38.85	-41.56	-26.66	-150.58	-436.92	-280.19	47.46	-31.34	2.68	216.67	194.66	200
298.15	**-57.87**	**-57.13**	**-61.16**	**-38.96**	**-169.45**	**-457.25**	**-298.12**	**27.35**	**-46.15**	**-15.04**	**201.21**	**183.78**	**298.15**
300	-58.23	-57.48	-61.54	-39.20	-169.81	-457.65	-298.47	26.96	-46.44	-15.38	200.92	183.57	300
400	-78.09	-77.10	-82.52	-52.72	-190.04	-479.64	-317.88	5.45	-62.25	-34.36	184.45	171.77	400
500	-98.70	-97.46	-104.26	-66.98	-211.00	-502.66	-338.15	-16.81	-78.58	-54.02	167.45	159.44	500
600	-119.91	-118.41	-126.63	-81.83	-232.57	-526.58	-359.14	-39.71	-95.33	-74.23	150.02	146.70	600
700	-141.63	-139.87	-149.53	-97.17	-254.64	-551.29	-380.73	-63.14	-112.43	-94.93	132.25	133.61	700
800	-163.79	-161.77	-172.90	-112.93	-277.16	-576.71	-402.86	-87.03	-129.83	-116.04	114.17	120.23	800
900	-186.35	-184.06	-196.70	-129.07	-300.08	-602.77	-425.48	-111.33	-147.49	-137.52	95.84	106.58	900
1000	-209.28	-206.71	-220.88	-145.53	-323.36	-629.43	-448.54	-136.01	-165.38	-159.33	77.27	92.70	1000
1100	-232.53	-229.68	-245.41	-162.31	-346.97	-656.61	-472.01	-161.03	-183.48	-181.45	58.48	78.61	1100
1200	-256.09	-252.96	-270.26	-179.35	-370.90	-684.31	-495.87	-186.36	-201.76	-203.86	39.51	64.33	1200
1300	-279.94	-276.52	-295.41	-196.66	-395.10	-712.48	-520.09	-211.99	-220.23	-226.53	20.37	49.88	1300
1400	-304.04	-300.34	-320.83	-214.21	-419.57	-741.09	-544.66	-237.88	-238.85	-249.45	1.06	35.27	1400
1500	-328.40	-324.41	-346.51	-231.99	-444.29	-770.11	-569.56	-264.03	-257.62	-272.60	-18.38	20.51	1500
1600	-352.99	-348.71	-372.44	-249.98	-469.24	-799.51	-594.77	-290.41	-276.53	-295.97	-37.98	5.62	1600
1700	-377.80	-373.23	-398.59	-268.18	-494.42	-829.29	-620.28	-317.02	-295.57	-319.55	-57.70	-9.40	1700
1800	-402.82	-397.96	-424.96	-286.58	-519.81	-859.41	-646.08	-343.84	-314.73	-343.32	-77.55	-24.55	1800
1900	-428.03	-422.88	-451.54	-305.16	-545.39	-889.87	-672.15	-370.87	-334.00	-367.29	-97.51	-39.82	1900
2000	-453.44	-448.00	-478.32	-323.91	-571.17	-920.64	-698.49	-398.08	-353.39	-391.43	-117.58	-55.19	2000
2100	-479.03	-473.29	-505.29	-342.84	-597.13	-951.71	-725.08	-425.48	-372.88	-415.75	-137.76	-70.67	2100
2200	-504.80	-498.76	-532.44	-361.93	-623.26	-983.08	-751.92	-453.06	-392.47	-440.23	-158.03	-86.25	2200
2300	-530.73	-524.39	-559.77	-381.18	-649.55	-1014.72	-779.00	-480.80	-412.16	-464.88	-178.40	-101.92	2300
2400	-556.81	-550.18	-587.26	-400.59	-676.01	-1046.63	-806.31	-508.71	-431.93	-489.68	-198.86	-117.68	2400
2500	-583.06	-576.13	-614.91	-420.14	-702.62	-1078.79	-833.84	-536.77	-451.79	-514.63	-219.41	-133.53	2500
2600	-609.45	-602.22	-642.72	-439.84	-729.38	-1111.20	-861.58	-564.98	-471.74	-539.72	-240.04	-149.47	2600
2700	-635.98	-628.45	-670.68	-459.67	-756.28	-1143.85	-889.54	-593.33	-491.76	-564.95	-260.75	-165.48	2700
2800	-662.65	-654.82	-698.78	-479.64	-783.31	-1176.73	-917.69	-621.82	-511.87	-590.31	-281.54	-181.57	2800
2900	-689.46	-681.32	-727.03	-499.74	-810.48	-1209.82	-946.05	-650.44	-532.04	-615.80	-302.41	-197.73	2900
3000	-716.39	-707.94	-755.41	-519.97	-837.78	-1243.14	-974.59	-679.20	-552.29	-641.42	-323.34	-213.97	3000
3100	-743.45	-734.69	-783.93	-540.32	-865.20	-1276.66	-1003.32	-708.07	-572.61	-667.17	-344.35	-230.27	3100
3200	-770.63	-761.56	-812.58	-560.79	-892.75	-1310.38	-1032.23	-737.07	-592.99	-693.03	-365.42	-246.65	3200
3300	-797.93	-788.55	-841.35	-581.38	-920.41	-1344.29	-1061.32	-766.19	-613.44	-719.01	-386.56	-263.08	3300
3400	-825.35	-815.65	-870.25	-602.08	-948.18	-1378.40	-1090.57	-795.42	-633.95	-745.10	-407.76	-279.58	3400
3500	-852.87	-842.86	-899.26	-622.90	-976.06	-1412.69	-1120.00	-824.76	-654.53	-771.30	-429.03	-296.14	3500
3600	-880.50	-870.18	-928.39	-643.82	-1004.05	-1447.16	-1149.59	-854.21	-675.16	-797.60	-450.35	-312.76	3600
3700	-908.24	-897.60	-957.64	-664.85	-1032.14	-1481.80	-1179.33	-883.76	-695.85	-824.02	-471.73	-329.44	3700
3800	-936.08	-925.12	-986.99	-685.99	-1060.34	-1516.62	-1209.23	-913.42	-716.60	-850.53	-493.17	-346.18	3800
3900	-964.02	-952.74	-1016.46	-707.22	-1088.63	-1551.60	-1239.29	-943.17	-737.40	-877.14	-514.67	-362.97	3900
4000	-992.06	-980.46	-1046.03	-728.56	-1117.02	-1586.74	-1269.49	-973.02	-758.26	-903.85	-536.22	-379.81	4000
4100	-1020.20	-1008.27	-1075.71	-750.00	-1145.51	-1622.04	-1299.83	-1002.97	-779.16	-930.65	-557.83	-396.70	4100
4200	-1048.42	-1036.17	-1105.48	-771.53	-1174.08	-1657.49	-1330.32	-1033.01	-800.12	-957.55	-579.48	-413.65	4200
4300	-1076.74	-1064.16	-1135.36	-793.15	-1202.75	-1693.10	-1360.95	-1063.14	-821.13	-984.54	-601.19	-430.64	4300
4400	-1105.15	-1092.24	-1165.33	-814.87	-1231.51	-1728.85	-1391.71	-1093.36	-842.18	-1011.61	-622.95	-447.68	4400
4500	-1133.65	-1120.40	-1195.40	-836.67	-1260.35	-1764.75	-1422.60	-1123.66	-863.29	-1038.77	-644.75	-464.77	4500
4600	-1162.23	-1148.65	-1225.57	-858.57	-1289.27	-1800.78	-1453.63	-1154.05	-884.44	-1066.02	-666.61	-481.91	4600
4700	-1190.90	-1176.98	-1255.82	-880.55	-1318.28	-1836.96	-1484.78	-1184.52	-905.63	-1093.35	-688.51	-499.09	4700
4800	-1219.64	-1205.40	-1286.17	-902.62	-1347.37	-1873.28	-1516.06	-1215.07	-926.87	-1120.76	-710.45	-516.32	4800
4900	-1248.47	-1233.89	-1316.60	-924.77	-1376.54	-1909.72	-1547.46	-1245.71	-948.15	-1148.26	-732.44	-533.59	4900
5000	-1277.38	-1262.46	-1347.12	-947.00	-1405.78	-1946.30	-1578.99	-1276.42	-969.48	-1175.83	-754.48	-550.90	5000

Note

The Gibbs Function (G) is by definition: $G^\circ = H - TS^\circ$

With the superscript ° referring to the datum pressure (p°) of 1 bar. The Gibbs function can be evaluated at other pressures in a similar way to the entropy through the use of:

$$G = G^\circ + RT\ln(p/p^\circ)$$

When the Gibbs Function of a mixture is being evaluated, then the properties of the individual constituents are summed, but the pressure (p) now refers to the partial pressure of each constituent.

Table A.5 Thermodynamic data for fuels

ABSOLUTE MOLAR ENTHALPY
(MJ/kmol)

T(K)	CH_4	C_3H_8	C_6H_6	C_7H_8	C_7H_{16}	C_8H_{18}	$C_{16}H_{34}$	$C_{10}H_7CH_3$	CH_3OH	C_2H_5OH	CH_3NO_2	T(K)
0	-82.660	-115.697	74.264	36.827	-213.096	-183.604	-431.071	100.199	-210.113	-246.415	-84.821	0
100	-80.470	-114.640	73.170	36.863	-210.350	-188.380	-425.008	98.184	-207.653	-244.471	-83.125	100
200	-77.740	-110.826	76.290	41.489	-201.545	-201.761	-405.297	104.238	-204.545	-240.553	-79.660	200
298.15	**-74.520**	**-104.680**	**82.930**	**50.000**	**-187.650**	**-224.010**	**-374.170**	**116.860**	**-200.940**	**-234.950**	**-74.730**	**298**
300	-74.454	-104.543	83.086	50.195	-187.342	-224.521	-373.480	117.155	-200.867	-234.829	-74.624	300
400	-70.606	-96.060	93.061	62.502	-168.357	-257.379	-330.987	135.847	-196.714	-227.463	-68.200	400
500	-66.197	-85.627	105.760	77.961	-145.160	-301.001	-279.136	159.351	-192.197	-218.620	-60.563	500
600	-61.231	-73.475	120.774	96.150	-118.274	-355.997	-219.135	186.822	-187.444	-208.465	-51.871	600
700	-55.724	-59.814	137.734	116.679	-88.176	-422.921	-152.081	217.537	-182.602	-197.161	-42.272	700
800	-49.694	-44.836	156.315	139.186	-55.298	-502.273	-78.961	250.894	-177.834	-184.870	-31.901	800
900	-43.170	-28.713	176.235	163.340	-20.025	-594.497	-0.648	286.411	-173.320	-171.754	-20.880	900
1000	-36.185	-11.600	197.253	188.838	17.303	-699.983	82.093	323.729	-169.256	-157.974	-9.319	1000
1100	-28.779	6.370	219.172	215.406	56.392	-819.065	168.609	362.607	-165.858	-143.690	2.685	1100
1200	-21.000	25.083	241.839	242.801	96.994	-952.024	258.358	402.929	-163.357	-129.061	15.046	1200
1300	-12.902	44.443	265.142	270.810	138.908	-1099.083	350.910	444.696	-162.000	-114.245	27.692	1300
1400	-4.546	64.374	289.012	299.247	181.978	-1260.412	445.945	488.032	-162.055	-99.399	40.564	1400
1500	4.001	84.819	313.424	327.957	226.094	-1436.125	543.253	533.181	-163.803	-84.681	53.614	1500

ABSOLUTE MOLAR INTERNAL ENERGY
(MJ/kmol)

T(K)	CH_4	C_3H_8	C_6H_6	C_7H_8	C_7H_{16}	C_8H_{18}	$C_{16}H_{34}$	$C_{10}H_7CH_3$	CH_3OH	C_2H_5OH	CH_3NO_2	T(K)
0	-82.660	-115.697	74.264	36.827	-213.096	-183.604	-431.071	100.199	-210.113	-246.415	-84.821	0
100	-81.302	-115.471	72.339	36.032	-211.181	-189.212	-425.839	97.352	-208.484	-245.303	-83.957	100
200	-79.403	-112.489	74.628	39.826	-203.207	-203.424	-406.960	102.575	-206.208	-242.216	-81.323	200
298.15	**-76.999**	**-107.159**	**80.451**	**47.521**	**-190.129**	**-226.489**	**-376.649**	**114.381**	**-203.419**	**-237.429**	**-77.209**	**298.15**
300	-76.948	-107.037	80.592	47.701	-189.836	-227.015	-375.975	114.660	-203.362	-237.323	-77.118	300
400	-73.932	-99.386	89.735	59.177	-171.683	-260.705	-334.313	132.521	-200.040	-230.788	-71.526	400
500	-70.354	-89.785	101.603	73.804	-149.318	-305.159	-283.293	155.194	-196.354	-222.777	-64.720	500
600	-66.220	-78.464	115.785	91.161	-123.263	-360.986	-224.124	181.833	-192.433	-213.454	-56.859	600
700	-61.544	-65.634	131.914	110.859	-93.996	-428.741	-157.901	211.717	-188.423	-202.981	-48.092	700
800	-56.346	-51.487	149.664	132.535	-61.949	-508.924	-85.612	244.242	-184.486	-191.522	-38.552	800
900	-50.653	-36.197	168.752	155.857	-27.508	-601.980	-8.131	278.928	-180.803	-179.237	-28.363	900
1000	-44.499	-19.915	188.938	180.523	8.988	-708.297	73.778	315.414	-177.571	-166.289	-17.633	1000
1100	-37.925	-2.776	210.026	206.260	47.246	-828.211	159.463	353.461	-175.004	-152.836	-6.461	1100
1200	-30.977	15.106	231.862	232.824	87.016	-962.001	248.381	392.951	-173.334	-139.038	5.068	1200
1300	-23.711	33.634	254.333	260.001	128.099	-1109.892	340.101	433.887	-172.809	-125.054	16.883	1300
1400	-16.186	52.734	277.372	287.606	170.338	-1272.052	434.304	476.391	-173.695	-111.040	28.924	1400
1500	-8.471	72.348	300.952	315.485	213.622	-1448.597	530.781	520.709	-176.274	-97.153	41.143	1500

ABSOLUTE MOLAR ENTROPY

(kJ/kmol)

T(K)	CH_4	C_3H_8	C_6H_6	C_7H_8	C_7H_{16}	C_8H_{18}	$C_{16}H_{34}$	$C_{10}H_7CH_3$	CH_3OH	C_2H_5OH	CH_3NO_2	T(K)
0	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0
100	154.754	220.323	222.796	255.497	313.582	601.601	524.594	288.137	204.204	231.886	232.013	100
200	173.463	245.721	242.855	285.836	372.338	512.423	656.095	327.134	225.502	258.289	255.365	200
298.15	186.270	270.200	269.200	319.740	427.980	422.960	781.020	377.440	239.880	280.640	275.010	298.15
300	186.709	270.877	269.941	320.612	429.229	421.472	783.545	378.644	240.342	281.265	275.584	300
400	197.739	295.137	298.432	355.785	483.534	327.662	905.102	432.056	252.261	302.348	293.974	400
500	207.556	318.341	326.667	390.157	535.134	230.781	1020.442	484.322	262.329	322.022	310.969	500
600	216.594	340.454	353.982	423.250	584.058	130.834	1129.626	534.308	270.989	340.503	326.790	600
700	225.073	361.484	380.091	454.853	630.395	27.912	1232.860	581.597	278.452	357.907	341.570	700
800	233.117	381.467	404.880	484.880	674.259	-77.859	1330.416	626.103	284.821	374.305	355.408	800
900	240.796	400.444	428.328	513.312	715.779	-186.332	1422.599	667.914	290.143	389.745	368.382	900
1000	248.152	418.466	450.463	540.165	755.090	-297.349	1509.738	707.217	294.429	404.258	380.558	1000
1100	255.207	435.587	471.349	565.480	792.333	-410.742	1592.170	744.261	297.674	417.869	391.996	1100
1200	261.974	451.865	491.067	589.313	827.653	-526.343	1670.243	779.336	299.857	430.597	402.749	1200
1300	268.454	467.358	509.716	611.729	861.196	-643.977	1744.310	812.760	300.949	442.455	412.870	1300
1400	274.646	482.126	527.403	632.801	893.109	-763.469	1814.728	844.868	300.916	453.457	422.409	1400
1500	280.541	496.230	544.243	652.608	923.542	-884.642	1881.854	876.010	299.718	463.612	431.412	1500

ABSOLUTE MOLAR GIBBS ENERGY

(MJ/kmol)

T(K)	CH_4	C_3H_8	C_6H_6	C_7H_8	C_7H_{16}	C_8H_{18}	$C_{16}H_{34}$	$C_{10}H_7CH_3$	CH_3OH	C_2H_5OH	CH_3NO_2	T(K)
0	-82.660	-115.697	74.264	36.827	-213.096	-183.604	-431.071	100.199	-210.113	-246.415	-84.821	0
100	-95.946	-136.672	50.891	11.314	-241.708	-248.541	-477.467	69.370	-228.073	-267.660	-106.326	100
200	-112.432	-159.970	27.719	-15.678	-276.012	-304.246	-536.516	38.811	-249.645	-292.211	-130.733	200
298.15	**-130.056**	**-185.240**	**2.668**	**-45.330**	**-315.252**	**-350.116**	**-607.031**	**4.326**	**-272.460**	**-318.623**	**-156.724**	**298.15**
300	-130.467	-185.806	2.104	-45.988	-316.111	-350.962	-608.544	3.561	-272.970	-319.208	-157.299	300
400	-149.702	-214.115	-26.312	-79.811	-361.771	-388.444	-693.028	-36.975	-297.618	-348.402	-185.790	400
500	-169.975	-244.798	-57.573	-117.118	-412.727	-416.392	-789.357	-82.810	-323.361	-379.631	-216.047	500
600	-191.188	-277.747	-91.615	-157.800	-468.709	-434.498	-896.911	-133.763	-350.037	-412.767	-247.945	600
700	-213.275	-312.853	-128.329	-201.718	-529.452	-442.460	-1015.083	-189.581	-377.519	-447.696	-281.371	700
800	-236.188	-350.009	-167.589	-248.718	-594.705	-439.985	-1143.293	-249.989	-405.691	-484.314	-316.227	800
900	-259.886	-389.113	-209.260	-298.641	-664.226	-426.798	-1280.988	-314.712	-434.448	-522.525	-352.424	900
1000	-284.336	-430.066	-253.211	-351.328	-737.787	-402.634	-1427.645	-383.488	-463.686	-562.232	-389.877	1000
1100	-309.507	-472.776	-299.311	-406.623	-815.175	-367.249	-1582.778	-456.080	-493.299	-603.346	-428.511	1100
1200	-335.368	-517.155	-347.441	-464.374	-896.190	-320.412	-1745.934	-532.275	-523.185	-645.777	-468.253	1200
1300	-361.892	-563.123	-397.489	-524.438	-980.647	-261.912	-1916.693	-611.892	-553.234	-689.437	-509.039	1300
1400	-389.049	-610.603	-449.353	-586.675	-1068.375	-191.555	-2094.674	-694.783	-583.337	-734.239	-550.808	1400
1500	-416.811	-659.526	-502.941	-650.956	-1159.219	-109.162	-2279.529	-780.833	-613.379	-780.100	-593.503	1500

Table A.6 EQUILIBRIUM CONSTANTS

At a given temperature, the standard (referring here to a pressure of 1 bar) free enthalpy of reaction or Gibbs Energy change (ΔG°), is related to the equilibrium constant (K_p) by:

$$\Delta G^\circ_T = -R_o T \ln K_p$$

and the following values of the equilibrium constants have been calculated from the Gibbs Energy tabulations in Tables A.4 and A.5.

The chemical reactions considered here are presented in the form:

$\Sigma \nu_i A_i = 0$, where: ν_i is the stoichiometric coefficient of the substance A_i.

The partial pressures of the species in equilibrium are found from:

$\ln K_p = \Sigma \nu_i \ln p_i^*$, where: the dimensionless quantity p_i^* is numerically equal to the partial pressure of substance A_i, in units of **bar**.

Reaction Number **Valid Range: 300 - 5000 K**

1 $- 2H + H_2 = 0$
2 $- 2O + O_2 = 0$
3 $- 2NO + N_2 + O_2 = 0$
4 $- H_2 - \frac{1}{2}O_2 + H_2O = 0$
5 $- \frac{1}{2}H_2 - OH + H_2O = 0$
6 $- CO - \frac{1}{2}O_2 + CO_2 = 0$
7 $- CO - H_2O + CO_2 + H_2 = 0$

ln K_p - bar

Reaction Number

T(K)	1	2	3	4	5	6	7	T(K)
100	511.058	584.208	213.879	284.475	331.098	328.849	44.375	100
200	250.154	285.590	105.451	139.970	162.100	159.694	19.723	200
298.15	**163.990**	**187.014**	**69.785**	**92.206**	**106.332**	**103.762**	**11.556**	**298.15**
300	162.906	185.774	69.337	91.604	105.630	103.058	11.454	300
400	119.151	135.735	51.277	67.320	77.322	74.670	7.350	400
500	92.822	105.639	40.433	52.689	60.291	57.617	4.928	500
600	75.220	85.531	33.199	42.896	48.908	46.244	3.349	600
700	62.612	71.139	28.027	35.875	40.758	38.124	2.249	700
800	53.130	60.326	24.146	30.591	34.632	32.037	1.447	800
900	45.735	51.902	21.126	26.468	29.858	27.308	.840	900
T(K)	1	2	3	4	5	6	7	T(K)

T(K)	1	2	3	4	5	6	7	T(K)
1000	39.803	45.153	18.709	23.160	26.031	23.528	.369	1000
1100	34.938	39.623	16.732	20.446	22.895	20.439	-.007	1100
1200	30.873	35.009	15.083	18.179	20.279	17.869	-.310	1200
1300	27.426	31.100	13.688	16.258	18.062	15.698	-.560	1300
1400	24.464	27.746	12.492	14.607	16.160	13.840	-.767	1400
1500	21.892	24.835	11.455	13.175	14.510	12.232	-.942	1500
1600	19.637	22.286	10.548	11.919	13.065	10.828	-1.091	1600
1700	17.643	20.035	9.748	10.810	11.790	9.591	-1.219	1700
1800	15.867	18.032	9.036	9.823	10.655	8.494	-1.330	1800
1900	14.275	16.238	8.400	8.940	9.640	7.514	-1.426	1900

T(K)	1	2	3	4	5	6	7	T(K)
2000	12.840	14.622	7.827	8.143	8.726	6.633	-1.510	2000
2100	11.540	13.160	7.309	7.422	7.899	5.838	-1.584	2100
2200	10.356	11.829	6.838	6.766	7.146	5.117	-1.649	2200
2300	9.273	10.613	6.408	6.167	6.460	4.460	-1.707	2300
2400	8.280	9.498	6.015	5.617	5.830	3.858	-1.759	2400
2500	7.364	8.471	5.653	5.111	5.251	3.306	-1.805	2500
2600	6.518	7.523	5.319	4.644	4.716	2.797	-1.847	2600
2700	5.733	6.645	5.010	4.211	4.221	2.327	-1.884	2700
2800	5.004	5.829	4.723	3.808	3.761	1.891	-1.918	2800
2900	4.324	5.069	4.457	3.433	3.333	1.486	-1.948	2900

T(K)	1	2	3	4	5	6	7	T(K)
3000	3.689	4.359	4.208	3.083	2.934	1.108	-1.975	3000
3100	3.095	3.695	3.976	2.756	2.560	.756	-2.000	3100
3200	2.537	3.072	3.758	2.449	2.210	.426	-2.022	3200
3300	2.012	2.487	3.554	2.160	1.881	.117	-2.043	3300
3400	1.518	1.936	3.363	1.888	1.572	-.173	-2.061	3400
3500	1.052	1.416	3.182	1.631	1.280	-.447	-2.078	3500
3600	.611	.925	3.012	1.389	1.005	-.705	-2.093	3600
3700	.194	.460	2.851	1.159	.744	-.948	-2.107	3700
3800	-.202	.020	2.699	.941	.497	-1.178	-2.120	3800
3900	-.577	-.397	2.555	.735	.263	-1.396	-2.131	3900

T(K)	1	2	3	4	5	6	7	T(K)
4000	-.934	-.794	2.419	.538	.041	-1.603	-2.141	4000
4100	-1.273	-1.172	2.289	.351	-.171	-1.799	-2.150	4100
4200	-1.597	-1.532	2.166	.173	-.372	-1.986	-2.159	4200
4300	-1.906	-1.875	2.049	.003	-.564	-2.163	-2.166	4300
4400	-2.201	-2.202	1.937	-.159	-.747	-2.332	-2.173	4400
4500	-2.482	-2.515	1.830	-.315	-.922	-2.494	-2.179	4500
4600	-2.752	-2.815	1.729	-.463	-1.090	-2.648	-2.185	4600
4700	-3.010	-3.101	1.632	-.606	-1.250	-2.795	-2.189	4700
4800	-3.258	-3.376	1.539	-.743	-1.403	-2.936	-2.193	4800
4900	-3.496	-3.640	1.450	-.874	-1.551	-3.071	-2.197	4900

T(K)	1	2	3	4	5	6	7	T(K)
5000	-3.724	-3.893	1.365	-1.000	-1.692	-3.200	-2.200	5000
5500	-4.740	-5.022	.988	-1.564	-2.322	-3.773	-2.209	5500
6000	-5.586	-5.964	.678	-2.037	-2.847	-4.247	-2.210	6000
T(K)	1	2	3	4	5	6	7	T(K)