An efficient generic method for calculating the properties of combustion products

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Abstract: A simple method for calculating the properties of combustion products is presented. The method is generic: the same equations apply to any fuel for any fuel–air ratio and temperature. The equations are suitable for both hand calculation and computer applications requiring repetitive property evaluations. The present equations offer accuracy comparable with the most elaborate method available but at a significantly reduced computational cost. The theory should find direct use in design-point and off-design performance calculations and optimization of internal combustion engines, e.g. gas turbine plants, calculation of the three-dimensional flowfield within a multistage turbine, and other applications requiring properties of combustion products.

Keywords: combustion, thermodynamic properties, internal combustion engine, gas turbine, fuel, real gas, specific heat capacity, turbomachinery, computational fluid dynamics (CFD), optimization, performance

NOTATION

A_i, B_i	constants
c_p	specific heat capacity at constant pressure
Δc_p	difference in values of c_p calculated by equation (10) and by equations (6), (7) and (1) expressed as a percentage
h	specific enthalpy
M	molecular weight
n_{air}	kmol of air used per kmol of fuel
n_C	number of carbon atoms in one molecule of fuel
n_H	number of hydrogen atoms in one molecule of fuel
n_O	number of oxygen atoms in one molecule of fuel
p	pressure
r_{c_p}	non-dimensional specific heat capacity [equation (8)]
r_{fa}	fuel–air ratio by mass
R	specific gas constant
s	specific entropy
S	characteristic ratio, depends on fuel and temperature [equation (7)]
T	temperature
y	mass fraction

γ	specific heat ratio
χ	ratio of enthalpy change of combustion products and that of air [equation (18)]
$\Delta\psi_{air}$	temperature function needed to calculate entropy $$= \int_{T_1}^{T_2} c_{p,\,air}\, dT/T$$
$\mathfrak{I}_0$, $\mathfrak{I}_1$, $\mathfrak{I}_2$, $\mathfrak{R}$	characteristic numbers of a fuel [equations (11) and (13)]

Subscripts

air	air
fuel	fuel
combust	combustion products

1 INTRODUCTION

Most power-producing and propulsion plants depend on the combustion of hydrocarbon fuels, be it coal, natural gas, gasoline, kerosene, diesel or alcohol. In the analysis of thermodynamic cycles on which these engines, particularly internal combustion engines, operate, it is often required to compute the physical properties of the products of combustion. These calculations are required

to study both design-point and off-design performances, and to determine optimum design parameters. The properties of combustion products are also required, for example, for accurate determination of the three-dimensional flowfield inside the blade passages of a multistage turbine (computational fluid dynamics, CFD). This article presents simple yet accurate formulae for calculating various thermodynamic properties of the products of combustion given the composition of the fuel.

The method presented is generic. The same equations apply to any fuel, any fuel–air ratio and temperature. The equations have a thermodynamic basis. They are very simple but produce results which are comparable in accuracy to that of the most elaborate and time-consuming method. It is thus profitable to use these equations in computer simulations requiring repetitive property evaluations. They can equally easily be incorporated in hand calculations.

The generic nature of the presented analysis gives it an amount of versatility as various engines use different fuels depending on application. Aero-engines almost exclusively use kerosene, marine gas turbines use diesel which also finds use in military applications, land-based power-generating gas turbines usually burn natural gas. Engines for natural gas pumping burn solely the gas tapped off the pipeline [1]. Reciprocating internal combustion engines use gasoline and diesel. Other fuels are also used in various circumstances; e.g. the small jet engine [2] used in the aeronautics laboratory of the University of Bristol uses propane as the fuel. (The engine is designed to propel unmanned aerial vehicles and model aircraft.) Methanol is sometimes used as a fuel in racing cars [3] and ethanol (a biomass synfuel) is sold in a mixture with gasoline for automotive use, especially in Brazil [3]. Other synthetic fuels (e.g. gasified or liquefied coal) are under development. The gas turbine in future combined power plants could be directly coal fired.

The numerical illustrations presented here are for lean (excess air) mixtures. For rich mixtures, when not all the fuel is burned, the chemistry of the combustion process can be complex. However, if the composition of the products of combustion is known, then the simple methodology of the present paper can be extended to deal with rich mixtures and would offer computational advantages over traditional methods.

2 VARIOUS METHODS OF DETERMINING THE PROPERTIES OF COMBUSTION PRODUCTS

The properties of combustion products can be determined in various ways with different levels of accuracy and computational cost. The following enumerates a few of the possibilities.

2.1 The simplest and least accurate method

In this method, constant values of properties are used that are suitable for the temperature range involved. This method is naturally restrictive, and the values should be changed depending on the fuel and the fuel–air ratio. For quick evaluation of thermodynamic cycles, especially for hand calculation, this method is, however, useful.

It is interesting to note the comments of Sir Frank Whittle, one of the inventors of jet engines, which he makes in the Preface (p. xi) to his book [4]:

> when, in jet engine design, greater accuracy was necessary for detail design, I worked in pressure ratios, used $\gamma = 1.4$ for compression and $\gamma = 1.33$ for expansion and assumed specific heats for combustion and expansion corresponding to the temperature range concerned. I also allowed for the increase of mass flow in expansion due to fuel addition (in the range 1.5–2 per cent). The results, despite the guesswork involved in many of the assumptions, amply justified these methods to the point where I was once rash enough to declare that 'jet engine design has become an exact science'. (This statement was inspired by the fact that on the first test of the W2/500 engine every experimental point fell almost exactly on the predicted curves of performance.)

2.2 The most accurate but computationally demanding method

In this method, at first, the composition of the combustion products is determined depending on the fuel and the particular value of the fuel–air ratio. This gives the mass fraction of each constituent gas in the combustion product. The properties of each constituent are then calculated at the prevalent temperature and are combined (weighted by individual mass fractions) to give the respective values for the mixture. The details are described in Section 3.

From their extensive experience of working with leading aero-engine manufacturers, Walsh and Fletcher [1] state that this method 'for performance calculations is now almost mandatory for computer 'library' routines in large companies'. For this purpose, Walsh and Fletcher express the specific heats of air and common gases in combustion products as eighth-order polynomials in temperature:

$$c_p = \sum_{i=0}^{n} A_i \left(\frac{T}{1000} \right)^i \tag{1a}$$

Walsh and Fletcher (reference [1], p. 115) provide the values shown in Table 1 for the coefficients, A_i, for various gases. Walsh and Fletcher do not give the accuracy or range of validity of the data in Table 1. However, from the charts drawn by them, it is apparent that the data can at least be used in the range 200–2000 K.

There are other relations available in the literature; van

Table 1 Values of coefficients to be used with equation (1a)

	Dry air	O_2	N_2	CO_2	H_2O
A_0	0.992313	1.006450	1.075132	0.408089	1.937043
A_1	0.236688	−1.047869	−0.252297	2.027201	−0.967916
A_2	−1.852148	3.729558	0.341859	−2.405549	3.338905
A_3	6.083152	−4.934172	0.523944	2.039166	−3.652122
A_4	−8.893933	3.284147	−0.888984	−1.163088	2.332470
A_5	7.097112	−1.095203	0.442621	0.381364	−0.819451
A_6	−3.234725	0.145737	−0.074788	−0.052763	0.118783
A_7	0.794571				
A_8	−0.081873				

Wylen *et al.* (reference [5], p. 754), for example, provide accurate relations for a number of gases. Their relations employ fewer terms than equation (1a) but use non-integer indices. Their relations for specific heats at constant pressure have been given in units of kJ/kmol K. For consistency, these relations have been adapted here to express c_p in kJ/kg K.

For N_2:

$$c_p = 1.395 - 18.3139 \, (T/100)^{-1.5}$$
$$+ \, 38.311 \, (T/100)^{-2} - 29.3 \, (T/100)^{-3}$$

For O_2:

$$c_p = 1.16975 + 6.28187 \times 10^{-4} \, (T/100)^{1.5}$$
$$- \, 5.5803 \, (T/100)^{-1.5} + 7.4025 \, (T/100)^{-2}$$

For CO_2:

$$c_p = -0.0849 + 0.69384 \, (T/100)^{0.5}$$
$$- \, 0.09326 \, (T/100) + 5.49954 \times 10^{-4} \, (T/100)^{2}$$

For H_2O:

$$c_p = 7.9472 - 10.19667 \, (T/100)^{0.25}$$
$$+ \, 4.59728 \, (T/100)^{0.5} - 0.20549 \, (T/100)$$
$$\text{(1b)}$$

Van Wylen *et al.* [5] have given the accuracy and range of validity of equation (1b) which is reproduced in Table 2.

Table 2 Accuracy and range of validity of equation (1b)

Gas	Range (K)	Maximum error (%)
N_2	300–3500	0.43
O_2	300–3500	0.30
CO_2	300–3500	0.19
H_2O	300–3500	0.43

Whichever of equations (1a) and (1b) is used, determination of properties of combustion products by this method would be computationally demanding. This is because a typical turbomachinery CFD application or a gas turbine optimization process involves several of such calculations. The problem becomes magnified as the computer program sometimes has to perform the inverse task, for example, of determining the temperature through iterative procedures when, say, the enthalpy is known.

2.3 Method of using empirical relations

When an application uses the same fuel with fixed composition, it is possible to perform the combustion chemistry in advance. Various properties of the combustion products then can be expressed as functions of temperature and fuel–air ratios alone. As an example, Walsh and Fletcher (reference [1], p. 116) give the following formula for calculating the specific heat at constant pressure of combustion products, $c_{p,\text{combust}}$, when kerosene is used as the fuel:

$$c_{p,\text{combust}} = \sum_{i=0}^{8} A_i \left(\frac{T}{1000}\right)^i + \frac{r_{\text{fa}}}{1 + r_{\text{fa}}} \sum_{i=0}^{7} B_i \left(\frac{T}{1000}\right)^i$$
$$\text{(1c)}$$

where r_{fa} is the fuel–air ratio by mass. The values for A_i are those for air as given in Table 1. The coefficients, B_i, specific to kerosene are given by Walsh and Fletcher (reference [1], p. 116). For a different fuel, a different equation has to be developed. Moreover, although the computational cost is less than the method described in Section 2.2, it is still significant.

2.4 Method of using property tables

In this method, properties of combustion products are calculated *a priori* and are presented as tabular data sets. Values of various properties required for engine simulation are then calculated by interpolation from this supplied data.

This is the approach adopted in the latest version of GasTurb—a commercially available program to calculate design and off-design performance of gas turbines and to carry out optimization [6]. This method might reduce computational time for repetitive calculations. The accuracy, however, depends on the size of the data table. Moreover, for each fuel (and for each varying composition of the same fuel, e.g. natural gas) a separate data table has to be supplied.

2.5 The present approach, accurate but efficient

In the present approach generic equations have been devised that are applicable for any fuel, fuel–air ratio and temperature. The equations are very simple and yet the accuracy is comparable to the method described in Section 2.2. The equations would be useful both in hand calculations for thermodynamic cycle analysis as well as for the repetitive calculations necessary in computer applications.

3 THERMODYNAMIC ANALYSIS

3.1 The first step

The first step is to determine the equivalent chemical formula for the hydrocarbon fuel from volumetric or gravimetric analysis. Note that the fuel may be a mixture of many chemical compounds. For example, natural gas is a mixture of methane and small quantities of ethane, propane, butane, etc. For generality oxygen is also included as a possible constituent as car engines are sometimes run with alcohol. The method of analysis can easily be extended to include any other constituent element. The equivalent chemical formula of a hydro-carbon fuel is denoted by $C_{n_C} H_{n_H} O_{n_O}$; e.g. for methane, CH_4: $n_C = 1$, $n_H = 4$, $n_O = 0$.

3.2 Combustion equation

If complete combustion occurs, the overall stoichiometric combustion equation (without dissociation) takes the form

$$C_{n_C}H_{n_H}O_{n_O} + \left(n_C + \frac{n_H}{4} - \frac{n_O}{2}\right)O_2$$
$$= n_C CO_2 + \left(\frac{n_H}{2}\right)H_2O \tag{2}$$
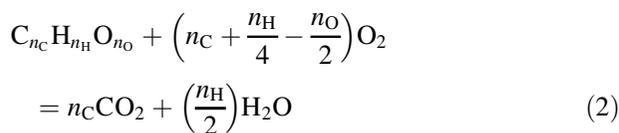
Consider the combustion of 1 kmol of fuel; if n_{air} is the number of kmol of air used, then equation (2) shows that there are $(n_{air} + n_H/4 + n_O/2)$ kmol of combustion products. Note that n_{air} includes the excess air and constituents other than oxygen, e.g. nitrogen and argon. Hence n_{air} is not the same as the coefficient of oxygen in equation (2). n_{air} can be calculated from the definition of the fuel–air ratio, r_{fa}, as

$$n_{air} = \frac{M_{fuel}}{r_{fa}M_{air}} \tag{3}$$

where M_{air} and M_{fuel} are the molecular weights of air and fuel respectively. Similarly the mass of combustion products per kmol of fuel is given by

$$m_{combust} = M_{fuel}\left(1 + \frac{1}{r_{fa}}\right) \tag{4}$$

3.3 The thermodynamic relation

The specific heat of the combustion products can be calculated by summing the contribution from each constituent. Thus

$$c_{p,combust} = \sum y_i c_{p,i} \tag{5}$$

where

$c_{p,combust}$ = specific heat at constant pressure of the combustion products

y_i and c_{pi} = mass fraction and specific heat at constant pressure of the ith constituent respectively

It can be shown from equations (2) to (5) that

$$\frac{c_{p,combust}}{c_{p,air}} = \frac{1 + S\,r_{fa}}{1 + r_{fa}} \tag{6}$$

where

$$S = n_C \frac{M_{CO_2}}{M_{fuel}} \frac{c_{p,CO_2}}{c_{p,air}} + \frac{n_H}{2} \frac{M_{H_2O}}{M_{fuel}} \frac{c_{p,H_2O}}{c_{p,air}}$$
$$- \left(n_C + \frac{n_H}{4} - \frac{n_O}{2}\right) \frac{M_{O_2}}{M_{fuel}} \frac{c_{p,O_2}}{c_{p,air}} \tag{7}$$

Equation (6) is exact and general. It applies to any fuel–air ratio and any hydrocarbon fuel.

The specific heat of combustion products can be calculated very accurately by substituting accurate expressions of the specific heat of the constituents in equation (7). For example, equation (1) could be employed, which expresses the specific heat of each constituent gas as an eighth-order polynomial. In a numerical calculation with no restriction on central processing unit (CPU) time (and storage), this can be done. However, the objective of the present article is to devise a simplified method with acceptable accuracy.

4 A SIMPLE, GENERIC METHOD FOR DETERMINING c_p, R AND γ

The simplification arises from a study of the variation of the specific heat of various gases. Figure 1 shows the variation with temperature of the specific heat of relevant
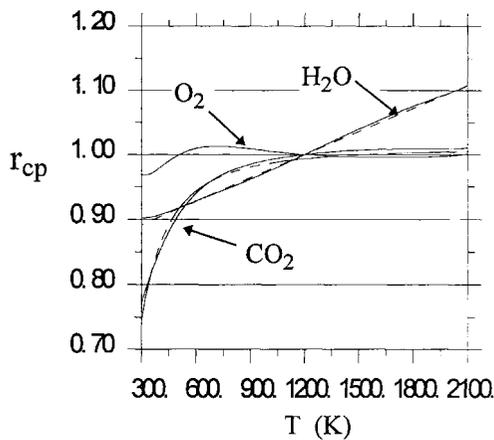
Fig. 1 Specific heat of various gases as a function of temperature. r_{cp} is calculated from equations (8) and (1) and is plotted as solid lines [– – – equation (9c); — – – equation (9b)]

gases calculated from equation (1). The specific heat of any particular gas has been expressed as a non-dimensional number, r_{c_p}, given by

$$r_{c_p} = \frac{c_{p,\mathrm{gas}}(T)/c_{p,\mathrm{air}}(T)}{(c_{p,\mathrm{gas}}/c_{p,\mathrm{air}})_{T=1200\mathrm{K}}} \tag{8}$$

It may be noted from Fig. 1 that r_{c_p} for oxygen is very nearly unity at all temperatures; the same is true for CO_2 at high temperatures. The variation of r_{c_p} for H_2O is almost linear with temperature.

Accordingly, the following simple equations are proposed:

$$r_{c_{p,O_2}} = 1 \tag{9a}$$

$$r_{c_{p,CO_2}} = 1.01 - \left(\frac{150}{T}\right)^2 \tag{9b}$$

$$r_{c_{p,H_2O}} = 1 + 0.00\,012(T - 1200) \tag{9c}$$

Equations (9b) and (9c) have also been plotted in Fig. 1 from which the agreement with accurate calculations may be judged.

Combining equations (6) to (9) gives

$$\frac{c_{p,\mathrm{combust}}}{c_{p,\mathrm{air}}} = \frac{1 + r_{\mathrm{fa}}(\mathfrak{I}_0 + \mathfrak{I}_1 T - \mathfrak{I}_2/T^2)}{1 + r_{\mathrm{fa}}} \tag{10}$$

where

$$\mathfrak{I}_0 = \frac{1}{M_{\mathrm{fuel}}}(18.0566 n_C + 8.3485 n_H + 15.1616 n_O) \tag{11a}$$

$$\mathfrak{I}_1 = 0.00\,223 n_H / M_{\mathrm{fuel}} \tag{11b}$$

$$\mathfrak{I}_2 = 1\,077\,768.4 n_C / M_{\mathrm{fuel}} \tag{11c}$$

Equation (10) is the new generalized equation which applies to any arbitrary hydrocarbon fuel, for any fuel–air ratio and at any temperature. $\mathfrak{I}_0$, $\mathfrak{I}_1$ and $\mathfrak{I}_2$ are three characteristic numbers which depend only on the fuel. When $T > 5300\,\sqrt{r_{\mathrm{fa}}}$, it is possible to neglect the term containing $\mathfrak{I}_2$ and still calculate c_p within 0.25 per cent accuracy. Equation (10) then becomes even simpler. The accuracy of equation (10) has been ascertained later.

Similar to the derivation of equation (6), the gas constant of the products of combustion can be calculated from

$$\frac{R_{\mathrm{combust}}}{R_{\mathrm{air}}} = \frac{1 + \Re r_{\mathrm{fa}}}{1 + r_{\mathrm{fa}}} \tag{12}$$

where

$R_{\mathrm{combust}} =$ specific gas constant of combustion products
$R_{\mathrm{air}} =$ specific gas constant of air

$\Re$, another characteristic number for the specific fuel, is calculated from

$$\Re = \left(\frac{M_{\mathrm{air}}}{M_{\mathrm{fuel}}}\right)\left(\frac{n_H}{4} + \frac{n_O}{2}\right) \tag{13}$$

Equation (12) is exact; some properties of equation (12) have been discussed in Appendix 2. The ratio of specific heats, $\gamma_{\mathrm{combust}}$, can be calculated from

$$\gamma_{\mathrm{combust}} = \frac{c_{p,\mathrm{combust}}}{c_{p,\mathrm{combust}} - R_{\mathrm{combust}}} \tag{14}$$

5 CHARACTERISTIC NUMBERS FOR VARIOUS FUELS

The characteristic numbers $\Re$, $\mathfrak{I}_0$, $\mathfrak{I}_1$ and $\mathfrak{I}_2$ for any fuel can be calculated from equations (13), (11a), (11b) and (11c) respectively. Table 3 lists these values for a few hydrocarbon fuels. The equivalent chemical formulae for natural fuels such as diesel, kerosene, natural gas or gasoline are not fixed but vary with the grade of fuel chosen. In Table 3 the chemical formulae for natural gas, diesel and kerosene have been estimated from the

Table 3 Characteristic numbers for various fuels

Fuel	Equivalent formula	$\mathfrak{R}$	$\mathfrak{I}_0$	$\mathfrak{I}_1/10^{-4}$ (K^{-1})	$\mathfrak{I}_2/10^4$ (K^2)
Methane	CH_4	1.811	3.216	5.575	6.736
Propane	C_3H_8	1.317	2.749	4.054	7.348
Octane	C_8H_{18}	1.144	2.585	3.521	7.563
Benzene	C_6H_6	0.557	2.031	1.715	8.291
Methyl alcohol	CH_4O	1.358	2.082	2.788	3.368
Ethyl alcohol	C_2H_6O	1.260	2.204	2.909	4.686
Gasoline	C_7H_{17}	1.219	2.657	3.753	7.470
Diesel	$C_{12.9}H_{23.9}$	0.969	2.420	2.982	7.780
Kerosene	$C_{12}H_{23.5}$	1.016	2.465	3.129	7.721
Carbon monoxide	CO	0.517	1.186	0.000	3.849
Sample natural gas	$C_{1.07}H_{4.1}$	1.753	3.161	5.397	6.808
Pure carbon	C	0.000	1.505	0.000	8.981
Hydrogen	H_2	7.243	8.349	22.30	0.000

compositions given by Walsh and Fletcher [1] so that a direct comparison can be made of the present analysis with their predictions. The chemical formula of gasoline is taken from reference [5] (p. 578). The variation of chemical composition of commercial fuels does not pose any problem to the present theory. The values of $\mathfrak{R}$, $\mathfrak{I}_0$, $\mathfrak{I}_1$, and $\mathfrak{I}_2$ can always be calculated from known composition; equations (10) to (12) remain unchanged.

6 COMPARISON OF PRESENT ANALYSIS WITH ACCURATE CALCULATIONS

Figures 2 to 7 show the comparison of the present analysis with accurate calculations. It should be noted that in these figures the lines corresponding to $r_{fa} = 0$ represent the data for dry air. In Figs 2, 4, 6 and 7 the continuous lines involve accurate determination of
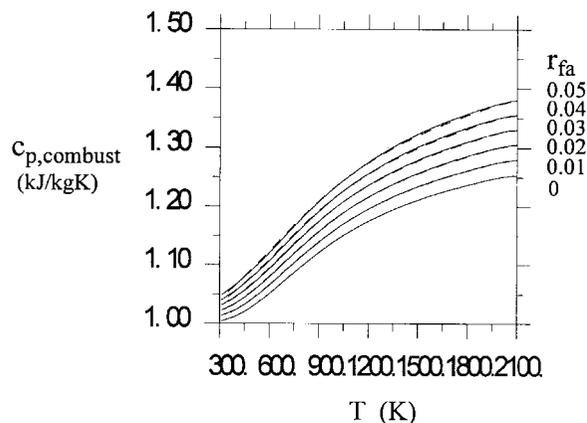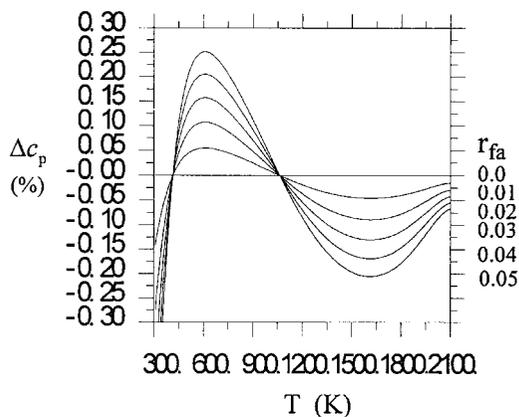
Fig. 3 Differences between the present analysis [equation (10)] and elaborate relations [equations (6), (7) and (1)] in determining c_p value of the combustion products of kerosene ($C_{12}H_{23.5}$) as a function of temperature. Fuel–air ratio is used as a parameter

$c_{p,\text{combust}}$, calculated from equations (6), (7) and (1). The dashed lines employ equation (10) for calculating $c_{p,\text{combust}}$. γ_{combust} is calculated from equation (14) where R_{combust} is given by equation (12). Figures 3 and 5 show explicitly the differences in values calculated by the elaborate methods and the present methods (these can be studied in conjunction with Table 2 that shows the accuracy of the primary equations themselves giving the specific heats of the constituent gases).

It may be seen from the above figures that the present analysis, equation (10), performs well at all temperatures and all fuel–air ratios. The comparison is illustrated here for two fuels, i.e. kerosene and methane, but similar results are obtained for other fuels.

Fig. 2 Specific heat at constant pressure of combustion products of kerosene ($C_{12}H_{23.5}$) as a function of temperature. Fuel–air ratio is used as a parameter. The solid lines represent accurate calculation based on equations (6), (7) and (1). The dashed lines are the predictions of the present analysis, equation (10)
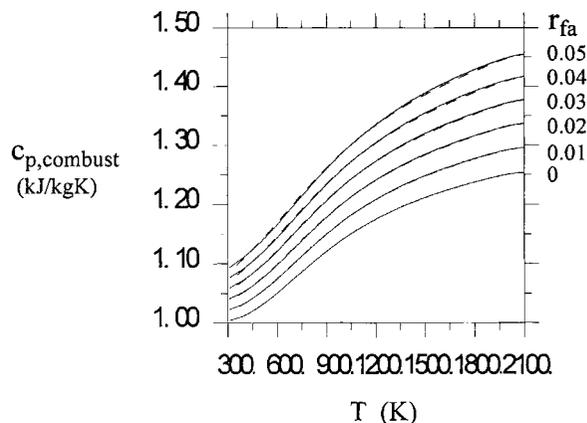
Fig. 4 Specific heat at constant pressure of combustion products of methane (CH_4) as a function of temperature. Fuel–air ratio is used as a parameter. The solid lines represent accurate calculation based on equations (6), (7) and (1). The dashed lines are the predictions of the present analysis, equation (10)
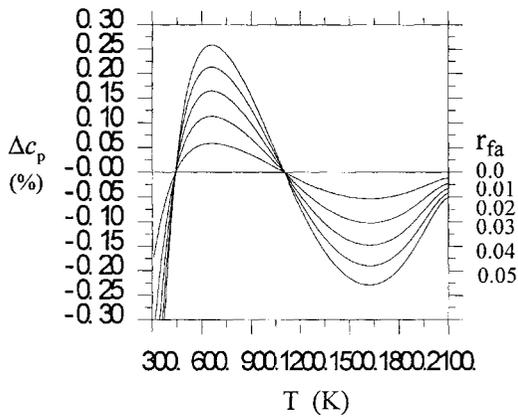
Fig. 5 Differences between the present analysis [equation (10)] and elaborate relations [equations (6), (7) and (1)] in determining c_p values of the combustion products of methane (CH_4) as a function of temperature. Fuel–air ratio is used as a parameter

As for other methods quoted in the references, the calculations presented here assume that the gases are semi-perfect and that the combustion is complete. The present method can, however, be extended to include incomplete combustion. (See Appendix 1 for the effects of dissociation.)

7 CALCULATION OF ENTHALPY

The enthalpy of combustion products can be calculated, once $c_{p,\text{combust}}(T)$ is known, from the thermodynamic
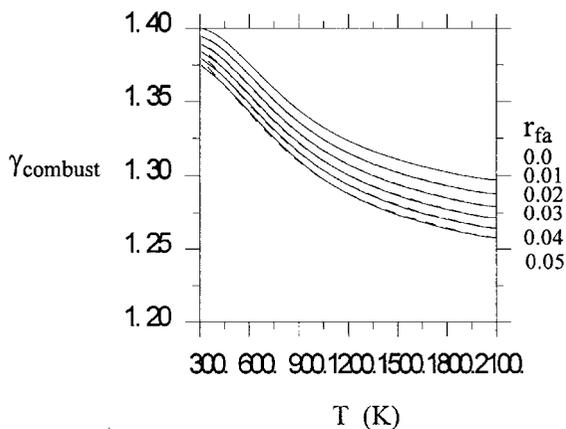
Fig. 6 Specific heat ratio of combustion products of kerosene ($C_{12}H_{23.5}$) as a function of temperature. Fuel–air ratio is used as a parameter. The solid lines represent accurate calculation of c_p based on equations (6), (7) and (1). The dashed lines use equation (10) for the determination of c_p
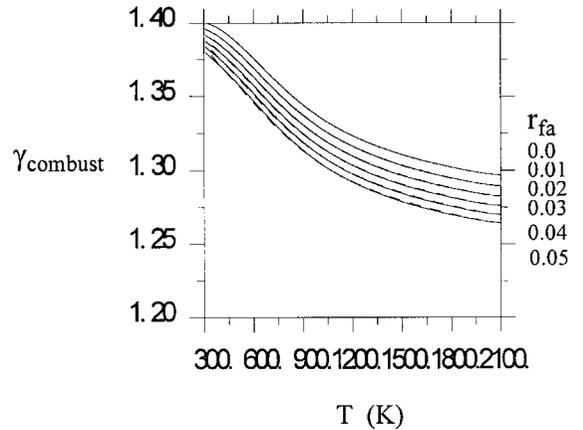
Fig. 7 Specific heat ratio of combustion products of methane (CH_4) as a function of temperature. Fuel–air ratio is used as a parameter. The solid lines represent accurate calculation of c_p based on equations (6), (7) and (1). The dashed lines use equation (10) for the determination of c_p

relation

$$h_{2,\text{combust}} - h_{1,\text{combust}} = \int_{T_1}^{T_2} c_{p,\text{combust}} \, \mathrm{d}T \qquad (15)$$

Equation (15) assumes that the constituent gases are semi-perfect. The change of enthalpy can be calculated at various levels of accuracy and computational effort as were involved in determining $c_{p,\text{combust}}(T)$ described in Section 2.

7.1 The method of accurate integration

For this, equation (6) is substituted in equation (15) to give

$$h_{2,\text{combust}} - h_{1,\text{combust}} = \int_{T_1}^{T_2} c_{p,\text{air}} \left\{ \frac{1 + S r_{\text{fa}}}{1 + r_{\text{fa}}} \right\} \mathrm{d}T \qquad (16)$$

where S is calculated from equation (7) and the specific heats of various gases are given by equation (1). Equation (16) can then be integrated analytically, the computational cost is high.

7.2 A method of intermediate complexity

This results when equation (10) is substituted in equation (15) and the resulting equation is integrated analytically. The accuracy of this method would be comparable with that provided by equation (16) but the computational cost would be lower.

7.3 The recommended method

A closer examination of the present analysis suggests that a similar level of accuracy can be obtained at a significantly reduced computational cost. The reduction is achieved by appreciating that although $c_{p,\text{combust}}$ shows strong variation with temperature (Figs 2 and 4), the ratio $c_{p,\text{combust}}/c_{p,\text{air}}$ shows much smaller variation with temperature and, moreover, this variation is almost linear. Therefore, it is suggested that the enthalpy change of combustion products can be calculated from

$$\frac{h_{2,\text{combust}} - h_{1,\text{combust}}}{h_{2,\text{air}} - h_{1,\text{air}}} = \chi \qquad (17)$$

where

$$\chi = \frac{1 + r_{\text{fa}}\left[\Im_0 + 0.5\Im_1(T_2 + T_1) - 0.5\Im_2(1/T_2^2 + 1/T_1^2)\right]}{1 + r_{\text{fa}}} \qquad (18)$$

The change of enthalpy for air can either be calculated by integrating the expression for specific heat given by equation (1) or it can be supplied in tabular form.

It should be appreciated that equation (17) is *not* equivalent to assuming an average $c_{p,\text{combust}}$ over the temperature range T_1–T_2 in equation (15). The latter method avoids the integration altogether. The recommended method only exploits an advantage offered by the behaviour of the ratio $c_{p,\text{combust}}/c_{p,\text{air}}$. The performance of equation (17) compared with that of equation (16) is examined in Table 4.

Table 4 shows that, in general, the error grows with increasing fuel–air ratio and increasing temperature differential. Here, the results for only two fuels, i.e. kerosene and methane, are presented, but the trend is similar for other fuels. The present theory, equation (17), has been subjected to a very severe test by applying it over a temperature differential of 800 K. Yet the maximum error is within an acceptable limit because, as Table 2 shows, the error with which the specific heats of individual components can be estimated is comparable with, or higher than, the difference between the predictions of equations (16) and (17). Equation (17), therefore, can be used for all practical calculations.

8 CALCULATION OF ENTROPY

Entropy changes can be calculated from the general thermodynamic relation

$$T\,ds = dh - v\,dp \qquad (19)$$

The change in entropy of combustion products is,

therefore, given by

$$s_{2,\text{combust}} - s_{1,\text{combust}} = \int_{T_1}^{T_2} c_{p,\text{combust}} \frac{dT}{T}$$
$$- R_{\text{combust}} \ln\left(\frac{p_2}{p_1}\right) \qquad (20)$$

Equation (20) can be evaluated accurately by substituting equations (6), (7) and (1) in it. A more efficient method would be to substitute equation (10) instead.

However, in the same spirit of Section 7.3, the recommended simple method is to use the following equation:

$$S_{2,\text{combust}} - S_{1,\text{combust}} = \chi \int_{T_1}^{T_2} c_{p,\text{air}} \frac{dT}{T}$$
$$- R_{\text{combust}} \ln\left(\frac{p_2}{p_1}\right) \qquad (21)$$

The first term on the right-hand side of equation (21) can

Table 4 Accuracy of the recommended method for calculating enthalpy changes of combustion products

	Fuel–air ratio	Enthalpy change calculated from equation (16) Δh_1 (MJ/kg)	Enthalpy change calculated from equation (17) Δh_2 (MJ/kg)	Relative difference $\left\|\dfrac{\Delta h_1 - \Delta h_2}{\Delta h_1}\right\|$
Kerosene, $C_{12}H_{23.5}$				
($T_1 = 600$ K,	0.00	0.4390	0.4390	0.0000
$T_2 = 1000$ K,	0.01	0.4457	0.4458	0.2162×10^{-3}
$\Delta T = 400$ K)	0.02	0.4523	0.4525	0.4219×10^{-3}
	0.03	0.4588	0.4591	0.6175×10^{-3}
	0.04	0.4651	0.4655	0.8046×10^{-3}
	0.05	0.4714	0.4718	0.9828×10^{-3}
Kerosene, $C_{12}H_{23.5}$				
($T_1 = 1200$ K,	0.00	0.9743	0.9743	0.0000
$T_2 = 2000$ K,	0.01	0.9934	0.9929	0.4687×10^{-3}
$\Delta T = 800$ K)	0.02	1.0121	1.0111	0.9109×10^{-3}
	0.03	1.0304	1.0290	0.1329×10^{-2}
	0.04	1.0484	1.0466	0.1725×10^{-2}
	0.05	1.0660	1.0638	0.2100×10^{-2}
Methane, CH_4				
($T_1 = 600$ K,	0.00	0.4390	0.4390	0.0000
$T_2 = 1000$ K,	0.01	0.4498	0.4500	0.4001×10^{-3}
$\Delta T = 400$ K)	0.02	0.4605	0.4608	0.7740×10^{-3}
	0.03	0.4709	0.4714	0.1124×10^{-2}
	0.04	0.4811	0.4818	0.1453×10^{-2}
	0.05	0.4911	0.4920	0.1762×10^{-2}
Methane, CH_4				
($T_1 = 1200$ K,	0.00	0.9743	0.9743	0.0000
$T_2 = 2000$ K,	0.01	1.0045	1.0040	0.5544×10^{-3}
$\Delta T = 800$ K)	0.02	1.0342	1.0331	0.1066×10^{-2}
	0.03	1.0632	1.0616	0.1541×10^{-2}
	0.04	1.0918	1.0896	0.1981×10^{-2}
	0.05	1.1197	1.1170	0.2391×10^{-2}

Table 5 Summary of the proposed relations for combustion products

Property	Proposed equation	Comment
Gas constant	$\dfrac{R_{\text{combust}}}{R_{\text{air}}} = \dfrac{1 + \Re r_{\text{fa}}}{1 + r_{\text{fa}}}$	Exact relation. $\Re$ is given by equation (13) and depends only on the fuel (Table 3).
Specific heat at constant pressure	$\dfrac{c_{p,\text{combust}}}{c_{p,\text{air}}} = \dfrac{1 + r_{\text{fa}}(\mathfrak{I}_0 + \mathfrak{I}_1 T - \mathfrak{I}_2/T^2)}{1 + r_{\text{fa}}}$	$\mathfrak{I}_0, \mathfrak{I}_1, \mathfrak{I}_2$ are given by equations (11) and depend only on the fuel (Table 3). The term containing $\mathfrak{I}_2$ can be dropped at higher temperatures (at $T > 5300 \sqrt{r_{\text{fa}}}$ to calculate c_p within 0.25% accuracy; for less than 1% error, drop at $T > 2600 \sqrt{r_{\text{fa}}}$). See Figs 2 and 4.
Specific heat ratio	$\gamma_{\text{combust}} = \dfrac{c_{p,\text{combust}}}{c_{p,\text{combust}} - R_{\text{combust}}}$	See Figs 6 and 7.
Change in specific enthalpy	$\dfrac{h_{2,\text{combust}} - h_{1,\text{combust}}}{h_{2,\text{air}} - h_{1,\text{air}}} = \chi$	χ is given by equation (18). Accuracy comparable with exact calculation, equation (16). See Tables 4 and 2.
Change in specific entropy	$S_{2,\text{combust}} - S_{1,\text{combust}} = \chi \Delta\psi_{\text{air}} - R_{\text{combust}} \ln(p_2/p_1)$	χ is again given by equation (18). $$\Delta\psi_{\text{air}} = \int_{T_1}^{T_2} c_{p,\text{air}} \frac{\mathrm{d}T}{T}$$ and depends only on the *air* properties.

be evaluated either by substituting the expression of $c_{p,\text{air}}$ from equation (1) or by interpolation from a tabular data file. The ratio χ is still given by equation (18). Thus equation (21) is not only very simple and accurate, but also offers a bonus in terms of computational efficiency in that χ would already be known from the calculation of enthalpy changes.

9 CONCLUSION

A theory is presented for calculating the properties of combustion products. The main results are summarized in Table 5. The theory is generic and the same equations apply to any fuel, fuel–air ratio and temperature. Yet the equations are simple and suitable both for hand calculations and computer applications requiring repetitive property evaluations.

The accuracy of the present equations given in Table 5 is comparable with exact calculations which use equations (1), (6), (7), (16) and (20). The latter method, in some form or other, is the industry standard [1]. Implementation of the present method would therefore offer considerable savings in computational time with no significant loss of accuracy. The saving would be particularly important as many computations do not just involve the determination of enthalpy, entropy, etc., at a given temperature but involve the inverse task of determining temperature through iterative procedures when, say, the enthalpy is known.

The only inputs needed for the present theory are the properties of air, in particular $c_{p,\text{air}}$, h_{air} and ψ_{air}. The

present theory is, however, flexible and does not depend on the form in which this information is provided. One method would be to use a polynomial-type expression for $c_{p,\text{air}}$, such as equation (1), and to calculate h_{air} and ψ_{air} by performing the relevant integrations. For this, depending on the temperature range involved, a simpler polynomial than equation (1) could be used.

Another method would be to supply property tables for air, which are readily available. Note that the present method needs the table only for *air*, and for only three properties $c_{p,\text{air}}$, h_{air} and ψ_{air}. This is very different from the approach taken in the leading computer program GasTurb [6], where the properties of the *combustion products* are calculated *a priori* and used as tabular data sets. There are five entries at each temperature and each fuel–air ratio. Thus the data set is necessarily large to cover representative ranges in temperature and fuel–air ratio, making the interpolation process difficult. Moreover, each data set is specific to a particular fuel. The versatility of a computer application would then depend on the number of available data sets. In fact, even for the same fuel, variation in its chemical composition might restrict the value of a supplied data set. For example, in GasTurb, a data file is supplied for natural gas. However, Walsh and Fletcher (reference [1], p. 106) state that the compositions of natural gas vary significantly so that the use of any one particular data set may give errors of up to 3 per cent in leading performance parameters. In contrast to this difficulty in using tabular data sets for combustion products (which are precalculated with a fixed composition of the fuel), the present method only takes the air data as input and accurately calculates the properties of combustion products through very simple equations

which are valid for any fuel, fuel–air ratio and temperature.

Three-dimensional flowfields both within one blade row and in a complete multistage turbine (a component of a gas turbine power plant which is physically located after the combustion chamber) are now routinely calculated by time-marching methods (see, for example, references [7] and [8]). Despite the tremendous improvement in computing power, at present only some average constant values of c_p, etc., for the combustion products are used in such calculations. The restrictions originate from the fact that time-marching calculations might involve many millions of property evaluations. For example, Denton and Dawes [8] state that a three-dimensional viscous calculation with shock waves and tip leakage requires about 300 000 grid points for a single-blade row to achieve a grid-independent solution. According to these authors, a steady, multistage solution would typically require about 70 000 grid points per blade row—a turbine with six stages would therefore need about 1×10^6 grid points. These many property evaluations have to be carried out for each time step of the time-marching calculation. It is thus not feasible to couple these CFD codes with numerical programs such as those in references [9] and [10] for property evaluation, and the current practice is to use constant values of thermodynamic properties even though the change in temperature through the turbine is significant. The present theory offers an inexpensive method of incorporating accurate values of properties in all such computations of turbomachinery flowfield. The method being generic, it is ready to deal with future developments in technology, for example, the analysis of coal-fired gas turbines in a combined power plant.

A new methodology for the thermodynamic optimization of bypass engines—turbofan or advanced propulsors—has been developed recently [11, 12]. The process starts with establishing an optimum specific thrust for the engine based on an economic analysis (range, payload, installation constraints, noise regulations, etc., are to be considered). The task of the optimization process is then to find the combination of optimum variables (e.g. overall pressure ratio, bypass ratio, fan pressure ratio and turbine entry temperature) that *concurrently* minimizes specific fuel consumption at the fixed specific thrust. This method is quite different from the usual parametric studies where the effects of a single variable are calculated numerically while all other variables are kept fixed and therefore at their non-optimum levels. The present method of calculating properties of combustion products can be used for such optimization studies.

The present method can also be used for realistic hand calculations. Walsh and Fletcher [1] comment that constant, standard values for properties of combustion products ($c_p = 1156.9$ J/kg K, $\gamma = 1.33$) 'should only be used in illustrative calculations for teaching purposes'. The proposed method, with its inherent simplicity,

might reconcile the academic efforts with industry standards.

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APPENDIX 1

Effects of dissociation

The analysis presented in the main body of the paper has not included dissociation; this is also the method adopted by other workers. Even the detailed in-house computer softwares of aero-engine manufacturers seem to follow the method described in Section 2.2 [1]. Kurzke [6] used one of the most sophisticated NASA computer programs [9] to calculate the property tables of combustion products provided as a data set to the program GasTurb [6], but chose to include only N_2, O_2, CO_2, H_2O and Ar in the combustion products as has been done here. (The calculation of the temperature increase due to combustion

in reference [**6**], however, takes dissociation into account.)

At high temperatures dissociation may become significant and the combustion products might include, in addition to the five gases mentioned earlier, varying quantities of CO, OH, H_2, NO_x, C, H, O and others. It is possible to determine the equilibrium concentration of each species at a given temperature and pressure by applying computer programs such as that in reference [**9**]. Computational time, however, becomes a severe constraint especially for iterative solutions. Another difficulty is that pressure becomes another independent variable.

In reciprocating internal combustion engines and rocket engines dissociation should be taken into account because of the very high temperatures involved. However, in rocket engines, the problem becomes compounded as, during the rapid expansion through the nozzle, the flow may not pass through equilibrium states which are calculated by programs like that in reference [**9**]. Non-equilibrium analysis might have to be invoked in this case [**13**]. Non-equilibrium analysis may also be required for high-speed reciprocating engines.

In gas turbines, the trend of using ever-increasing temperatures in modern aircraft engines might make the neglect of dissociation unacceptable by the industry standard. Dissociation also plays a role in afterburners which operate at lower pressure and high fuel–air ratios. At any rate, the properties calculated by neglecting dissociation may be taken as a starting point on which some correction is to be applied to include the effect of dissociation.

The present method can easily be extended to include other constituents in the products of combustion. Considering N_2, O_2, CO_2, H_2O, Ar, CO, OH and H_2, the combustion equation may be rewritten as

$$C_{n_C}H_{n_H}O_{n_O} + \frac{M_{fuel}}{M_{air}r_{fa}}\text{air}$$

$$= \frac{M_{fuel}}{M_{air}r_{fa}}\text{air} - \left(n_C + \frac{n_H}{4} - \frac{n_O}{2} - \frac{a}{2} + \frac{b}{4} - \frac{c}{2}\right)O_2$$

$$+ (n_C - a)CO_2 + aCO$$

$$+ \left(\frac{n_H}{2} - \frac{b}{2} - c\right)H_2O + bOH + cH_2 \quad (22)$$

where *a, b* and *c* are to be determined either from the three relevant equilibrium constants (corresponding to reactions $CO_2 \Leftrightarrow CO + \frac{1}{2}O_2$, $H_2O \Leftrightarrow OH + \frac{1}{2}H_2$ and $H_2O \Leftrightarrow H_2 + \frac{1}{2}O_2$) or by computer programs such as in reference [**9**]. The equilibrium constants can either be read from tabular data or expressed as polynomials in temperature.

Following the methods of Section 4, the specific heats
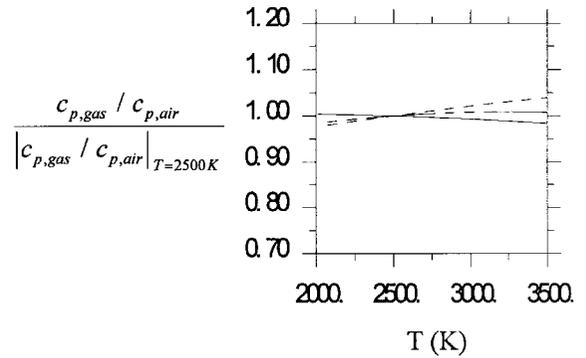
Fig. 8 Variation with temperature of specific heat at constant pressure of various products of dissociation. (—— CO; $- - - -$ H_2; —– – OH)

of the three dissociated products have been plotted in Fig. 8, the basic data being taken from reference [**5**]. The variations of the non-dimensional ratios in Fig. 8 are quite small. For this reason and also due to the fact that the concentration of these gases would usually be small, it is proposed that the ratio $c_{p,gas}/c_{p,air}$ for each of the constituents CO, OH and H_2 is taken as constant at their respective values at 2500 K. Following the procedure of Section 4 the following equation is obtained:

$$\frac{c_{p,combust}}{c_{p,air}} = \frac{1 + r_{fa}(\mathfrak{I}'_0 + \mathfrak{I}'_1 T - \mathfrak{I}'_2/T^2)}{1 + r_{fa}} \quad (23)$$

where, for $T \leqslant 2250$ K,

$$\mathfrak{I}'_0 = \frac{1}{M_{fuel}}(18.0566\,n_C + 8.3485\,n_H + 15.1616\,n_O$$

$$- 4.2927a + 4.6367b + 11.321c) \quad (24a)$$

$$\mathfrak{I}'_1 = \frac{0.002\,23\,(n_H - b - 2c)}{M_{fuel}} \quad (24b)$$

$$\mathfrak{I}'_2 = \frac{1\,077\,768.4\,(n_C - a)}{M_{fuel}} \quad (24c)$$

and, for $2250\,\text{K} \leqslant T < 3500$ K,

$$\mathfrak{I}'_0 = \frac{1}{M_{fuel}}(18.0566\,n_C + 12.234\,n_H + 15.1616\,n_O$$

$$- 4.2927a + 0.7511b + 3.5497c) \quad (25a)$$

$$\mathfrak{I}'_1 = \frac{5.0616 \times 10^{-4}\,(n_H - b - 2c)}{M_{fuel}} \quad (25b)$$

$$\mathfrak{I}'_2 = \frac{1\,077\,768.4\,(n_C - a)}{M_{fuel}} \quad (25c)$$

The two slightly variant equation sets result from the fact

that in the temperature range $2250\,\mathrm{K} \leqslant T < 3500\,\mathrm{K}$, the right-hand side of equation (9c) should be replaced with $1.0648 + 2.72 \times 10^{-5}\,T$. Equations (9a) and (9b) can be used in the temperature range $300\,\mathrm{K} < T < 3500\,\mathrm{K}$. At $T = 2250\,\mathrm{K}$ both sets of equations will give identical results. The term containing $\mathfrak{J}_2'$ can always be neglected at temperatures at which dissociation becomes relevant.

Substitution of equations (24) or (25) into equation (23) results in the general form

$$\frac{c_{p,\mathrm{combust}}}{c_{p,\mathrm{air}}} = \frac{1 + r_{\mathrm{fa}}(k_{\mathrm{fuel}} + C_a a + C_b b + C_c c)/M_{\mathrm{fuel}}}{1 + r_{\mathrm{fa}}}$$

(26)

where k_{fuel} depends on the composition of the fuel, and C_a, C_b, C_c are the coefficients of a, b and c respectively. Each of C_a, C_b, C_c depends on the temperature and has been plotted in Fig. 9.

Figure 9 shows that C_a is always negative and hence equation (26) shows that the dissociation of CO_2 into CO decreases $c_{p,\mathrm{combust}}$ compared with its non-dissociated value at all temperatures. The term containing b would increase $c_{p,\mathrm{combust}}$ up to about $2080\,\mathrm{K}$ and decrease it above this temperature. The term containing c would increase $c_{p,\mathrm{combust}}$ up to about $3500\,\mathrm{K}$ although the rate of increase decreases with temperature. At high temperatures other dissociation reactions forming elemental H and O might become relevant. It may be recalled that the equilibrium values of a, b and c themselves are functions of temperature and pressure (but are always positive).

Equation (23) is similar in form to equation (10). The term containing $\mathfrak{J}_2'$ can always be neglected at temperatures at which dissociation becomes relevant. However, unlike $\mathfrak{J}_0$, $\mathfrak{J}_1$ and $\mathfrak{J}_2$ given by equations (11), $\mathfrak{J}_0'$, $\mathfrak{J}_1'$ and $\mathfrak{J}_2'$ do not depend only on the composition of the fuel.

Once a, b and c are determined, equation (23) maintains the simple but accurate nature of the present analysis. It would be compatible with the present analysis
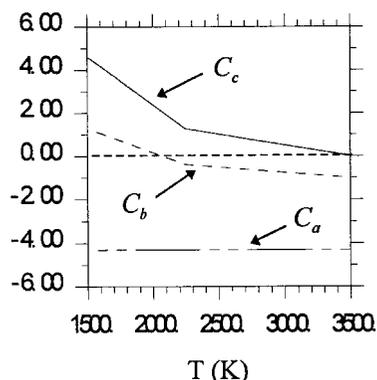
if some simple means could be found to determine a, b and c.

APPENDIX 2

Gas constant of combustion products

Such calculations are usually performed either by detailed combustion analysis as a part of specialized computational tools or by in-house empirical formulae [1]. As an example, Walsh and Fletcher [1] suggest the use of the following equations (their equations F3.22, p. 115):

$$R_{\mathrm{combust}} = 287.05 - 0.009\,90 r_{\mathrm{fa}} + 1 \times 10^{-7} r_{\mathrm{fa}}^2$$
$$\text{kerosene}$$

$$R_{\mathrm{combust}} = 287.05 - 8.0262 r_{\mathrm{fa}} + 3 \times 10^{-7} r_{\mathrm{fa}}^2$$
$$\text{diesel}$$

$$R_{\mathrm{combust}} = 287.05 + 212.85 r_{\mathrm{fa}} - 197.89 r_{\mathrm{fa}}^2$$
$$\text{sample natural gas}$$

(27)

Walsh and Fletcher have also plotted equations (27) (their Chart 3.1, p. 126) which show that the gas constant increases with increasing fuel–air ratio for natural gas, decreases for diesel and is almost constant for kerosene. Empirical relations like equations (27) are obviously very convenient to use. However, there are a number of difficulties:

1. The relations are specific to a particular composition. Hence for every fuel and for varying compositions of the same fuel a separate equation needs to be developed.
2. The relations are dimensional. The coefficients will change depending on the system of units used.
3. The relations are empirical, obtained by curve fitting and hence physically not satisfying. The equations do not offer any physical explanation, for example, as to why the variation of the gas constant with fuel–air ratio is qualitatively different for natural gas, diesel and kerosene as noted above.

Generalization about qualitative variation

Equation (12) given in the main text, on the other hand, shows that the variation of the gas constant of combustion products depends on the characteristic number of the fuel, $\mathfrak{R}$:

$$R_{\mathrm{combust}} > R_{\mathrm{air}}, \qquad \text{if } \mathfrak{R} > 1$$

Fig. 9 Variation with temperature of the coefficients of a, b and c in equation (26)

$$R_{\text{combust}} = R_{\text{air}}, \qquad \text{if } \Re = 1$$
$$R_{\text{combust}} < R_{\text{air}}, \qquad \text{if } \Re < 1$$

Examples are:

Methane CH_4:
$$\Re = \frac{28.97}{16} \frac{4}{4} = 1.811,$$
$$\text{hence } R_{\text{combust}} > R_{\text{air}}$$

Diesel $C_{12.9}H_{23.9}$:
$$\Re = \frac{28.97}{178.7} \frac{23.9}{4} = 0.969,$$
$$\text{hence, } R_{\text{combust}} < R_{\text{air}}$$

Kerosene $C_{12}H_{23.5}$:
$$\Re = \frac{28.97}{167.7} \frac{23.5}{4} = 1.015,$$
$$\text{hence } R_{\text{combust}} \approx R_{\text{air}}$$

This provides the physical basis of the observed behaviour as noted above. This also explains why for the simulation of gas turbines using kerosene it may be acceptable to use the same gas constant for combustion products as that for air.

(a) *The limit of vanishingly small fuel–air ratio*

$$\mathop{\text{Lt}}_{r_{\text{fa}} \to 0} \{R_{\text{combust}}\} = R_{\text{air}}$$

hence equation (12) behaves consistently in this limit.

(b) *Approximation for low fuel–air ratio*

Equation (12) is exact. However, when the fuel–air ratio is low, it can be expressed as a polynomial, if that is more convenient for certain applications. Binomial expansion is used for the term $(1 + r_{\text{fa}})^{-1}$. For low fuel–air ratios, the first three terms in the expansion are sufficient.
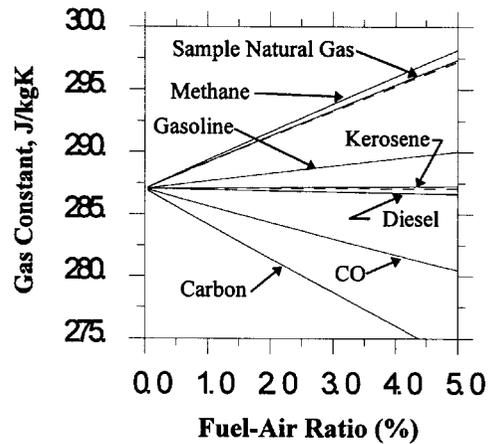
Fig. 10 Gas constant of combustion products: comparison of present analysis, equation (12), with empirical data of Walsh and Fletcher [1], equations (27). [—— equation (12); – – – equations (27)]

Equation (12) then takes the form

$$\frac{R_{\text{combust}}}{R_{\text{air}}} \approx 1 + (\Re - 1)r_{\text{fa}} + (1 - \Re)r_{\text{fa}}^2 \qquad (28)$$

where, as before, $\Re$ is the characteristic fuel number, and depends on the particular fuel chosen.

Equation (28) gives the physical basis for the polynomial-type empirical relations such as equations (27). However, in contrast to equation (27) given by Walsh and Fletcher [1], equation (28) is general, applies to any hydrocarbon fuel, is non-dimensional and has a thermodynamic foundation. Figure 10 shows the predictions of equation (12) for various fuels. The data of Walsh and Fletcher [1] obtained from equations (27) for sample natural gas, diesel and kerosene are superposed in this figure.