COMBUSTION CALCULATIONS

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Theory, worked examples and problems

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PREFACE

Examination syllabuses concerned with combustion reactions and their products tend to draw on material appearing in texts on chemistry, physics, thermodynamics, fuel science and the few publications devoted to combustion itself. Furthermore, some aspects of the subject tend to be handled in a 'case law' manner by depending solely on worked examples to illustrate the techniques of solution, whereas a prior general statement of the relevant theory permits much wider application.

The objectives of this present book, therefore, are threefold.

- (1) To assemble in one small volume the key relationships of stoichiometry, thermochemistry and kinetics that apply to the calculation of combustion quantities.
- (2) To unify these relationships by starting with a general combustion equation, in simple terms of molecular products only, and adapting this systematically to each aspect in turn.
- (3) To provide solutions in general terms before illustrating their use in examples typical of examination questions met in combustion and allied fields.

The motivation for a work of this kind stemmed from experience with examination marking at H.N.C., H.N.D. and first- and higher-degree levels in various branches of engineering and fuel technology, where it has become apparent that questions of this type present difficulties to some candidates. This approach can also serve in professional practice as a reminder of the basic principles involved before turning to the more sophisticated instrumentation and computational techniques available in industry and research.

The book opens with a brief review of the main features of atmospheric air and conventional fuels, together with those of the most common combustion products and their methods of measurement. The following chapter deals with the determination of the proportions of reactants, and of the cooled, stable products of combustion. Chapter 5 is concerned with the determination of proportions of hot products that are still reacting but have reached some condition of dynamic equilibrium. Chapter 6 deals with the quantities of energy involved in combustion reactions, and chapter 7 with the temperatures reached under adiabatic, or some other specified, conditions. The efficiency of combustion is covered in chapter 8, whereas chapter 9 indicates the enhanced efficiency realised by electrochemical oxidation in the absence of substantial heat release. All key equations are numbered in sequence, and listed in a final summary. As a general rule, decimal fractions are used, but it has occasionally proved more convenient to include such a term as $(x + y/4)$ rather than $(x + 0.25y)$. Worked examples are included at the

ends of chapters, and a number of problems provided, with answers. SI units are used throughout, and extracts from the wealth of thermochemical data published in kcal/mol have been converted by the relationship

$$(X) \text{ kcal/mol} = 4.184(X) \text{ kJ/mol}$$

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UNITS

In any system of units, certain quantities are defined as basic to the system, and all further quantities derived from them. If the system is coherent, the products and quotients of any two or more unit quantities themselves become the units of the derived quantities. Thus, in the case of Newton's second law, $F = ma$, 1 derived unit of force is equal to

$$(1 \text{ unit of mass}) \times (1 \text{ unit of length}) / (1 \text{ unit of time})^2$$

One of the most significant developments in this area is the adoption of a rationalised system of metric units known as SI (Système International d'Unités), which is coherent, with a derived unit of energy common to the mechanical, electrical and most other forms. SI includes the following base units

length	metre (m)
mass	kilogram (kg)
time	second (s)
electric current	ampere (A)
thermodynamic temperature	kelvin (K)
amount of substance	mole (mol)

It should be noted that the kelvin is also used for temperature intervals, and that the mole relates to what was formerly called the 'gram-mole' and not the 'kilogram-mole' (kmol).

SI includes the following derived units

force	newton (N) = kg m/s^2
pressure	pascal (Pa) = $\text{N/m}^2 = \text{kg/m s}^2$
energy	joule (J) = $\text{N m} = \text{kg m}^2/\text{s}^2$
power	watt (W) = $\text{J/s} = \text{kg m}^2/\text{s}^3$

No change is made to any symbol to indicate the plural.

SI has been adopted by various industries (for example, *Recommended SI Units*, Institute of Petroleum, London, 1970), some of which also use earlier metric units such as the litre and the bar, which are not part of SI but are considered acceptable. Since the adoption of SI is not yet worldwide, the following conversion factors and other metric relationships are given.

length	1 ft = 0.3048 m
volume	1 ft ³ = 0.028 32 m ³
	1 U.K. gal = 1.201 U.S. gal = 4.546 litre
mass	1 lb = 0.4536 kg
	1 tonne = 1000 kg
density	1 lb/ft ³ = 16.0185 kg/m ³

force	1 lbf = 4.4482 N
pressure	1 lbf/in. ² = 6.894 76 kPa
	1 mm Hg = 133.322 Pa
	1 atm = 101.325 kPa = 1.01325 bar
	1 bar = 100 kPa = 10 ⁵ Pa
energy	1 Btu = 1.0551 kJ
	1 Chu = 1.8991 kJ
	1 kcal (international table) = 4.1868 kJ
	1 kcal (thermochemical) = 4.184 kJ
	1 kWh = 3.6 MJ
	1 hp h = 2.6845 MJ
	1 therm = 10 ⁵ Btu = 105.51 MJ
specific energy	1 Btu/lb = 2.326 kJ/kg
specific energy	1 Btu/lb °R = 1 Chu/lb K = 4.1868 kJ/kg K
capacity	
volumetric energy	1 Btu/ft ³ = 0.0373 kJ/litre (or MJ/m ³)
	1 Btu/U.K. gal = 0.232 kJ/litre (or MJ/m ³)
power	1 hp = 745.7 W

NOTATION

When two symbols are given for one item, upper case represents an extensive property (dependent on mass) and lower case a specific property (per unit mass). When one symbol is used for more than one item, the particular meaning in any instance will be apparent from the context.

A	air mass
A, a	non-flow availability function
A	air mass flow rate
A/F	air/fuel ratio by mass or by volume
B, b	steady-flow availability function
C	molar heat capacity
c	specific heat capacity
C/H	carbon/hydrogen mass ratio
CV	calorific value
E	electrical potential
e	charge/electron
F	fuel mass
F	fuel mass flow rate
G, g	Gibbs free-energy function
(g)	gas
GCV	gross calorific value
(gr)	graphite
H, h	enthalpy
i	electrical current
ip	indicated power
K	equilibrium constant
k	rate constant

(l)	liquid
M	number of moles of oxygen/gram of fuel
m	number of moles of oxygen/mole of fuel
$\dot{m}$	mass consumption rate
NCV	net calorific value
n	number of moles of a combustion product/mole of fuel
n-f	non-flow
p	pressure
Q, q	heat transfer (note: not a property)
R_0	universal gas constant
RAM	relative atomic mass (formerly atomic weight)
RMM	relative molecular mass (formerly molecular weight)
r	ratio
S, s	entropy
(s)	solid
s-f	steady-flow
T	absolute thermodynamic temperature (K)
t	empirical temperature ($^{\circ}\text{C}$); time
U, u	internal energy
V, v	volume
W, w	work transfer (note: not a property)
X	any oxygen-consuming component of a fuel
x	number of atoms of carbon/molecule fuel
y	number of atoms of hydrogen/molecule fuel
z	number of atoms of oxygen/molecule fuel
α	cut-off ratio in diesel cycle
γ	ratio of specific heat capacities
Δ	finite change

η	efficiency
ϕ	equivalence ratio

Superscripts

$^{\circ}$	standard state of 25 $^{\circ}\text{C}$ (298.15 K) and 1 atm
'	concentration basis; theoretical; molar basis
*	algebraic sum of sensible and standard formation

Subscripts

A	air
a	atomisation
ad	adiabatic
C	change
c	combustion; corrected
cc	combustion chamber
F	fuel
f	formation
fg	saturated vapour - saturated liquid
I	initial
i	any arbitrary reactant component
j	any arbitrary product component
max	maximum
max useful	maximum useful
min	minimum
0	absolute zero temperature; environment
o	observed
P	products
p	pressure (constant)
R	reactants; reverse
r	reaction

s	stoichiometric
T	temperature (either constant, or equal initial and final); total
t	total head
V, v	volume (constant)
V	volumetric
WG	water gas