

J. Warnatz, U. Maas, R.W. Dibble

Combustion

**Physical and Chemical Fundamentals,
Modeling and Simulation, Experiments,
Pollutant Formation**

4th Edition



Springer

J. Warnatz · U. Maas · R.W. Dibble

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Pollutant Formation

4th Edition

With 227 Figures and 22 Tables

 Springer

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Physical and Chemical Fundamentals,
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4th Edition
With 200 Illustrations

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Preface

This book has evolved from a lecture series (of *J. Wa.*) on combustion at Stuttgart University. The lectures were intended to provide first-year graduate students (and advanced undergraduates) with a basic background in combustion. Such a course was needed since students of combustion arrive with a wide variety of backgrounds, including physics, physical chemistry, mechanical engineering, computer science and mathematics, aerodynamics, and atmospheric science. After a few years of improving printed matter distributed to the students, the lecture notes have been organized into a book, first in German, and later translated and augmented in an English version.

We intend that the book provides a common basis from which research begins. Thus, the treatment of the many topics is compact with much citation to the research literature and presents numerous exercises. Beyond this, the book expects that combustion engineers and researchers will increasingly rely on mathematical modeling and numerical simulation for guidance toward greater understanding, in general, and, specifically, toward producing combustion devices with ever higher efficiencies and with lower pollutant emissions. Spatially homogeneous combustion and laminar flame computer codes and selected sample data to run them are available on the internet at <http://reaflow.iwr.uni-heidelberg.de/software/>.

The actual fourth edition presents a completely restructured book: Mathematical formulae and derivations and the space-consuming reaction mechanisms have been removed from the text to appendices, a new chapter has been added to discuss the impact of combustion processes on the earth atmosphere, the chapter on auto-ignition is moved and has been extended to deal with combustion in Otto and Diesel engines, and the chapters on heterogeneous combustion and on soot formation have been heavily revised. The rest of the chapters is polished and extended to account for recent developments and new results.

Because this book is a research launching point, we expect it to be updated in a timely fashion. For this reason, we invite the readers to contact our e-mail address (juergen@warnatz.de) for additional comments and constructive critical remarks that may be part of the next edition.

Heidelberg, Karlsruhe, Berkeley, in April 2006 *J. Warnatz, U. Maas, R. W. Dibble*

Table of Contents

1	Introduction, Fundamental Definitions and Phenomena	1
1.1	Introduction	1
1.2	Some Fundamental Definitions	1
1.3	Basic Flame Types	4
1.4	Exercises	8
2	Experimental Investigation of Flames	9
2.1	Velocity Measurements	10
2.2	Density Measurement	11
2.3	Concentration Measurements	13
2.4	Temperature Measurements	18
2.5	Pressure Measurements	20
2.6	Measurement of Particle Sizes	21
2.7	Simultaneous Diagnostics	22
2.8	Exercises	27
3	Mathematical Description of Premixed Laminar Flat Flames	29
3.1	Conservation Equations for Laminar Flat Premixed Flames	29
3.2	Heat and Mass Transport	33
3.3	The Description of a Laminar Premixed Flat Flame Front	33
3.4	Exercises	38
4	Thermodynamics of Combustion Processes	39
4.1	The First Law of Thermodynamics	39
4.2	Standard Enthalpies of Formation	41
4.3	Heat Capacities	43
4.4	The Second Law of Thermodynamics	44
4.5	The Third Law of Thermodynamics	45
4.6	Equilibrium Criteria and Thermodynamic Variables	46
4.7	Equilibrium in Gas Mixtures; Chemical Potential	47
4.8	Determination of Equilibrium Compositions in Gases	49
4.9	Determination of Adiabatic Flame Temperatures	51
4.10	Tabulation of Thermodynamic Data	52
4.11	Exercises	55

5	Transport Phenomena	57
5.1	A Simple Physical Model of Transport Processes	57
5.2	Heat Conduction in Gases	60
5.3	Viscosity of Gases	62
5.4	Diffusion in Gases	64
5.5	Thermal Diffusion, Dufour Effect, and Pressure Diffusion	66
5.6	Comparison with Experiments	67
5.7	Exercises	71
6	Chemical Kinetics	73
6.1	Rate Laws and Reaction Orders	73
6.2	Relation of Forward and Reverse Reactions	75
6.3	Elementary Reactions, Reaction Molecularity	75
6.4	Experimental Investigation of Elementary Reactions	77
6.5	Temperature Dependence of Rate Coefficients	79
6.6	Pressure Dependence of Rate Coefficients	81
6.7	Surface Reactions	84
6.8	Exercises	88
7.	Reaction Mechanisms	91
7.1	Characteristics of Reaction Mechanisms	91
7.1.1	Quasi-Steady States	92
7.1.2	Partial Equilibrium	94
7.2	Analysis of Reaction Mechanisms	97
7.2.1	Sensitivity Analysis	97
7.2.2	Reaction Flow Analysis	101
7.2.3	Eigenvalue Analyses of Chemical Reaction Systems	103
7.3	Stiffness of Ordinary Differential Equation Systems	107
7.4	Simplification of Reaction Mechanisms	107
7.5	Radical Chain Reactions	115
7.6	Exercises	117
8	Laminar Premixed Flames	119
8.1	Zeldovich's Analysis of Flame Propagation	119
8.2	Flame Structures	121
8.3	Flame Velocities	124
8.4	Sensitivity Analysis	127
8.5	Exercises	128
9	Laminar Nonpremixed Flames	129
9.1	Counterflow Nonpremixed Flames	129
9.2	Laminar Jet Nonpremixed Flames	133
9.3	Nonpremixed Flames With Fast Chemistry	135
9.4	Exercises	138

10	Ignition Processes	141
10.1	Semenov's Analysis of Thermal Explosions	142
10.2	Frank-Kamenetskii's Analysis of Thermal Explosions	143
10.3	Autoignition: Ignition Limits	145
10.4	Autoignition: Ignition-Delay Time	148
10.5	Induced Ignition, Minimum Ignition Energies	149
10.6	Spark Ignition	153
10.7	Detonations	157
10.8	Exercises	163
11	Low-Temperature Oxidation, Engine Knock	165
11.1	Fundamental Phenomena in Otto Engines	165
11.2	Oxidation at Intermediate Temperatures	168
11.3	Low-Temperature Oxidation	169
11.4	Ignition Processes in Reciprocating Engines	173
11.4.1	Knock Damages in Otto Engines	173
11.4.2	Ignition in Diesel Engines	174
11.4.3	The HCCI Concept	175
11.4.4	The DICI Concept	177
11.5	Exercises	178
12	The Navier-Stokes-Equations for Three-Dimensional Reacting Flow	179
12.1	The Conservation Equations	179
12.1.1	Overall Mass Conservation	180
12.1.2	Species Mass Conservation	181
12.1.3	Momentum Conservation	181
12.1.4	Energy Conservation	182
12.2	The Empirical Laws	183
12.2.1	Newton's Law	183
12.2.2	Fourier's Law	184
12.2.3	Fick's Law and Thermal Diffusion	184
12.2.4	Calculation of the Transport Coefficients from Molecular Parameters	185
12.3	Exercises	185
13	Turbulent Reacting Flows	187
13.1	Some Fundamental Phenomena	187
13.2	Direct Numerical Simulation	189
13.3	Concepts for Turbulence Modeling: Time- and Favre-Averaging	192
13.4	Reynolds-Averaged Navier-Stokes (RANS) Equations	194
13.5	Turbulence Models	196
13.6	Mean Reaction Rates	200
13.7	Concepts for Turbulence Modeling: Probability Density Functions	202
13.8	Eddy-Break-Up Models	206
13.9	Turbulent Scales	207
13.10	Large-Eddy Simulation (LES)	209
13.11	Exercises	211

14	Turbulent Nonpremixed Flames	213
14.1	Nonpremixed Flames with Equilibrium Chemistry	214
14.2	Finite-Rate Chemistry in Nonpremixed Flames	217
14.3	Flame Extinction	221
14.4	PDF-Simulations of Turbulent Non-Premixed Flames Using a Monte-Carlo Method	224
14.5	Exercises	226
15	Turbulent Premixed Flames	227
15.1	Classification of Turbulent Premixed Flames	227
15.2	Flamelet Models	230
15.2.1	Flamelet Modelling Using a Reaction Progress Variable	231
15.2.2	Flamelet Modelling Using a Level-Set Method	232
15.3	Turbulent Flame Velocity	233
15.4	Flame Extinction	235
15.5	Other Models of Turbulent Premixed Combustion	237
15.6	Exercises	238
16	Combustion of Liquid and Solid Fuels	239
16.1	Droplet Combustion	239
16.1.1	Combustion of Single Droplets	240
16.1.2	Combustion of Droplet Groups	244
16.2	Spray Combustion	246
16.2.1	Formation of Sprays	246
16.2.2	Spray Combustion Modes	247
16.2.3	Statistical Description of Sprays	249
16.2.4	Modeling of Turbulent Spray Combustion	252
16.2.5	Flamelet-Type Models for Spray Combustion	253
16.3	Coal Combustion	255
16.3.1	Pyrolysis of Coal	255
16.3.2	Burning of Volatile Compounds	256
16.3.3	Burning of the Coke	256
16.3.4	Coal Gasification	257
16.4	Exercises	258
17	Formation of Nitric Oxides	259
17.1	Thermal NO (Zeldovich NO)	259
17.2	Prompt NO (Fenimore NO)	262
17.3	NO Generated via Nitrous Oxide	265
17.4	Conversion of Fuel Nitrogen into NO	265
17.5	NO Reduction by Combustion Modifications	267
17.6	Catalytic Combustion	271
17.7	NO Reduction by Post-Combustion Processes	272
17.8	Exercises	275

18	Formation of Hydrocarbons and Soot	277
18.1	Unburnt Hydrocarbons	277
18.1.1	Flame Extinction Due to Strain	278
18.1.2	Flame Extinction at Walls and in Gaps	278
18.2	Formation of Polycyclic Aromatic Hydrocarbons (PAH)	280
18.3	The Phenomenology of Soot Formation	283
18.4	Modelling and Simulation of Soot Formation	287
18.5	Exercises	296
19	Effects of Combustion Processes on the Atmosphere	297
19.1	The Structure of the Atmosphere	297
19.1.1	Pressure in the Atmosphere	297
19.1.2	Temperature and Classification of Compartments in the Atmosphere	299
19.1.3	Composition of the Atmosphere	300
19.2.	The Atmosphere as a Photochemical System	300
19.2.1	Lambert-Beer Law	300
19.2.2	Stern-Vollmer Equation	301
19.2.3	Formation of Photochemical Layers	302
19.3	Incoming Sun Radiation, Photochemical Primary Processes	303
19.4.	Physical Processes in the Atmosphere	305
19.4.1	Conservation of the Mass of Species	305
19.4.2	Conservation of Energy	306
19.4.3	Solution of the Conservation Equations	307
19.5	Chemistry of the Unpolluted Atmosphere	307
19.5.1	Pure Oxygen Atmosphere	307
19.5.2	Oxygen-Nitrogen-Hydrogen-Carbon Atmosphere	308
19.6	Chemistry of the Polluted Atmosphere	310
19.6.1	Photochemical Smog	310
19.6.2	Supersonic Transports	314
19.6.3	Green-House Effect	315
19.6.4	Acid rain	316
19.7	The Role of Combustion Sources in Atmospheric Pollution	317
20	Appendix 1: Mathematics	319
20.1	Some Definitions and Laws for Vectors and Tensors	319
20.2.1	Formulation of the Problem	320
20.2.2	General Remarks on Solution Algorithms for ODE Systems	321
20.2.3	Euler Method	322
20.2.4	Extrapolation Method	324
20.3	Numerical Solution of Partial Differential Equation Systems	325
20.3.1	Spatial Discretization	326
20.3.2	Initial Values, Boundary Conditions, Stationary Solution	328
20.3.3	Explicit Solution Methods	329
20.3.4	Implicit Solution Methods	330
20.3.5	Semi-implicit Solution of Partial Differential Equations	330
20.3.6	Implicit Solution of Partial Differential Equations	331

21	Appendix 2: Reaction Mechanisms	333
21.1	Mechanism of the Oxidation of H_2 , CO, C_1 and C_2 Hydrocarbons	333
21.2	Reaction Mechanism of the Generation and Consumption of NO_x	340
22	References	345
23	Index	367

1 Introduction, Fundamental Definitions and Phenomena

1.1 Introduction

Combustion is the oldest technology of mankind; it has been used for more than one million years. At present, about 90% of our worldwide energy support (e. g., in traffic, electrical power generation, heating) is provided by combustion; therefore it is really worthwhile studying this process.

Combustion research in the past was directed to fluid mechanics that included global heat release by chemical reaction. This heat release was often described simply with the help of thermodynamics, which assumes infinitely fast chemical reaction. This approach was useful to some extent for designing stationary combustion processes; it is not sufficient for treating transient processes like ignition and quenching or if pollutant formation shall be treated. However, pollutant formation during combustion of fossil fuels is, and will continue to be, a central topic in the future.

The focus of this book is therefore to treat the coupling of chemical reaction and fluid flow; in addition, combustion-specific topics of chemistry (hydrocarbon oxidation, large reaction mechanisms, simplification of reaction mechanisms) and combustion-specific topics of fluid mechanics (turbulent flow with density change by heat release, potential generation of turbulence by heat release) shall be considered.

Thus, this book will not consider in great detail the theory of chemical reaction rates and experimental methods for the determination of reaction rate coefficients (this is the task of reaction kinetics). Nor will this book discuss the details of turbulence theory and the handling of complex geometries (this is the task of fluid mechanics), although all of these topics are needed in understanding combustion.

1.2 Some Fundamental Definitions

The quantitative treatment of combustion processes requires some understanding of fundamental concepts and definitions, which shall be described in this section.

A *chemical reaction* is the exchange and/or rearrangement of atoms between colliding molecules. In the course of a chemical reaction, e. g.,



the atoms (relevant in combustion: C, H, O, and N) are conserved; i. e., they are not created or destroyed. On the other hand, molecules (e. g., HCN, OH, CN, and H₂O) are not conserved. A partial list of molecules relevant in combustion is given in Table 1.1. Reactant molecules are rearranged to become product molecules, with simultaneous release of heat. A primary interest in the heat of reaction sets combustion engineering apart from chemical engineering.

Atoms and molecules are conveniently counted in terms of *amount of substance* or (worse, but used everywhere) *mole numbers* (unit: mol). 1 mol of a compound corresponds to $6.023 \cdot 10^{23}$ particles (atoms, molecules, etc.). Accordingly, the *Avogadro constant* (also called *Avogadro's constant*) is $N_A = 6.023 \cdot 10^{23} \text{ mol}^{-1}$. The *mole fraction* x_i of the species i denotes the ratio of the *mole number* n_i of species i to the total *mole number* $n = \sum n_i$ of the mixture ($x_i = n_i / n$).

The *mass* m is a fundamental property of matter (units of kg in the SI system). The *mass fraction* w_i is the ratio of the mass m_i of the species i and the total mass $m = \sum m_i$ of the mixture ($w_i = m_i / m$).

The *molar mass* (obsolete: *molecular weight*) M_i (units of, e. g., g/mol) of species i is the mass of 1 mol of this species. Some examples (for atomic carbon, molecular hydrogen, molecular oxygen, and methane) are $M_C = 12 \text{ g/mol}$, $M_{\text{H}_2} = 2 \text{ g/mol}$, $M_{\text{O}_2} = 32 \text{ g/mol}$, $M_{\text{CH}_4} = 16 \text{ g/mol}$. The mixture *mean molar mass* $\bar{M}$ (in g/mol, e. g.) denotes an average molar mass, using the mole fractions as weighting ($\bar{M} = \sum x_i M_i$).

Frequently mass fractions w_i and mole fractions x_i are expressed in terms of percentages (*mole-%* or *mass-%*). The following relations hold, which can be verified by simple calculations (S denotes the number of different compounds):

$$w_i = \frac{M_i n_i}{\sum_{j=1}^S M_j n_j} = \frac{M_i x_i}{\sum_{j=1}^S M_j x_j}, \quad (1.1)$$

$$x_i = \frac{w_i / M_i}{\sum_{j=1}^S w_j / M_j} = \frac{w_i / M_i}{\bar{M}}. \quad (1.2)$$

Densities do not depend on the size (extent) of a system. Such variables are called *intensive* properties, and are defined as the ratio of the corresponding *extensive* properties (which depend on the extent of the system) and the system volume V . Examples of intensive properties are

<i>mass density (density)</i>	$\rho = m / V$	(in, e. g., kg/m ³),
<i>molar density (called concentration)</i>	$c = n / V$	(in, e. g., mol/m ³).

It follows (very easy to verify) that the mean molar mass is given by the expression

$$\frac{\rho}{c} = \frac{m}{n} = \bar{M}. \quad (1.3)$$

Tab. 1.1. List of molecules relevant for combustion processes

	FAMILY										
	Alkane	Alkene	Alkyne	Arene	Haloalkane	Alcohol	Ether	Amine	Aldehyde	Ketone	Carboxylic Acid
Specific Example	$\text{CH}_3\text{-CH}_3$	$\text{CH}_2=\text{CH}_2$	$\text{HO}\equiv\text{CH}$		$\text{CH}_3\text{CH}_2\text{Cl}$	$\text{CH}_3\text{CH}_2\text{OH}$	CH_3OCH_3	CH_3NH_2	CH_3CHO	CH_3CCH_3 O	CH_3COOH O
IUPAC Name	Ethane	Ethene	Ethyne	Benzene	Chloroethane	Ethanol	Methoxy Methane	Methyl Amine	Ethanal	Propanone	Ethanoic Acid
Common Name	Ethane	Ethylene	Acetylene	Benzene	Ethyl Chloride	Ethyl Alcohol	Dimethyl Ether	Methyl Amine	Acetaldehyde	Acetone	Acetic Acid
General Formula	RH	$\text{H}_2\text{C}=\text{CH}_2$ $\text{RCH}=\text{CH}_2$ $\text{RCH}=\text{CHR}$ $\text{R}_2\text{C}=\text{CHR}$ $\text{R}_2\text{C}=\text{CR}_2$	$\text{RC}\equiv\text{CH}$ $\text{RC}\equiv\text{CR}$	Ar^nH , Ar^nR	RX	ROH	ROR	RNH_2 R_2NH R_3N	$\text{O}=\text{RCH}$	$\text{O}=\text{RCR}$	$\text{O}=\text{RCOH}$
Functional Group	C-H bonds C-C bonds	>C=C<	$\text{-C}\equiv\text{C-}$	Aromatic Ring	-C-X	-C-OH	-C-O-C-	-C-N-	$\text{O}=\text{C-H}$	$\text{O}=\text{C-C-}$	$\text{O}=\text{C-OH}$

In chemistry, concentrations c of chemical species defined in this way are usually denoted by species symbols in square brackets (e. g., $c_{\text{H}_2\text{O}} = [\text{H}_2\text{O}]$).

For the gases and gas mixtures in combustion processes, an equation of state relates temperature, pressure, and density of the gas. For many conditions it is satisfactory to use the *ideal gas equation of state*,

$$pV = nRT, \tag{1.4}$$

where p denotes the pressure (in units of Pa), V the volume (in m^3), n the mole number (in mol), T the absolute temperature (in K), and R the *universal gas constant* ($R = 8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$). It follows that

$$c = \frac{p}{RT} \quad \text{and} \quad \rho = \frac{p\overline{M}}{RT} = \frac{p}{RT} \sum_{i=1}^s \frac{w_i}{M_i}. \tag{1.5}$$

When temperatures are near or less than the critical temperature, or when pressures are near or above the critical pressures, the concentration or density is inadequately predicted using the ideal gas equation of state, i. e., (1.5). The system is better approximated as a *real gas*. One example of a real gas equation of state is that of *van der Waals*. Details of this and other equations of state for real gas conditions can be found in textbooks on physical chemistry (e. g., Atkins 1990).

1.3 Basic Flame Types

Tab. 1.2. Example of combustion systems ordered with respect to premixedness and flow type

Fuel/Oxidizer Mixing	Fluid Motion	Examples
premixed	turbulent	spark-ignited gasoline engine low NO_x stationary gas turbine
	laminar	flat flame Bunsen flame (followed by a nonpremixed candle for $\Phi > 1$)
nonpremixed	turbulent	pulverized coal combustion aircraft turbine Diesel engine H_2/O_2 rocket motor
	laminar	wood fire radiant burners for heating candle

In combustion processes, fuel and oxidizer (typically air) are mixed and burned. It is useful to identify several combustion categories based upon whether the fuel and oxidizer is mixed first and burned later (*premixed*) or whether combustion and mixing occur simultaneously (*nonpremixed*). Each of these categories is further subdivided based on whether the fluid flow is laminar or turbulent. Table 1.2 shows examples of combustion systems that belong to each of these categories, which will be discussed in the following sections.

Laminar Premixed Flames: In *laminar premixed flames*, fuel and oxidizer are premixed before combustion and the flow is laminar. Examples are laminar *flat flames* and (under fuel-lean conditions) *Bunsen flames* (see Fig. 1.1).

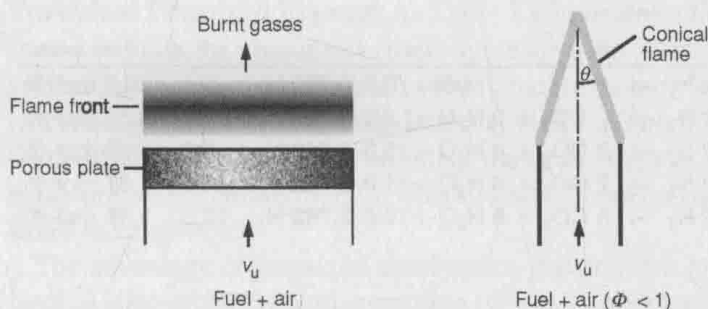
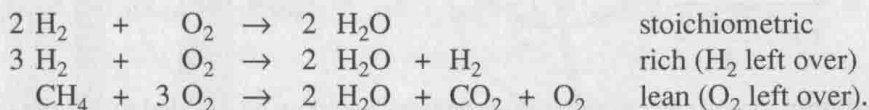


Fig. 1.1. Schematic illustration of a laminar flat flame (left) and of a Bunsen flame (right), both premixed

A premixed flame is said to be *stoichiometric*, if fuel (e. g., a hydrocarbon) and oxidizer (e. g., oxygen O_2) consume each other completely, forming only carbon dioxide (CO_2) and water (H_2O). If there is an excess of fuel, the system is called *fuel-rich*, and if there is an excess of oxygen, it is called *fuel-lean*. Examples are

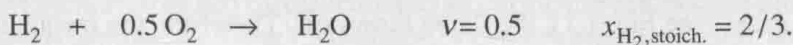


Each species symbol in such a chemical reaction equation represents 1 mol. Thus, the first equation means: 2 mol H_2 react with 1 mole O_2 to form 2 mole H_2O .

If the reaction equation is written such that it describes exactly the reaction of 1 mol fuel, the mole fraction of the fuel in a stoichiometric mixture can be calculated easily to be

$$x_{\text{fuel, stoich.}} = \frac{1}{1 + \nu} \quad (1.6)$$

Here ν denotes the number of moles of O_2 in the reaction equation for a complete reaction to CO_2 and H_2O . An example is



If air is used as an oxidizer, it has to be taken into account that dry air contains only about 21 % oxygen (78% nitrogen, 1% noble gases). Thus, for air $x_{N_2} = 3.762 x_{O_2}$. It follows that the mole fractions in a stoichiometric mixture with air are

$$x_{fuel,stoich.} = \frac{1}{1 + v \cdot 4.762}, \quad x_{O_2,stoich.} = v \cdot x_{fuel,stoich.}, \quad x_{N_2,stoich.} = 3.762 \cdot x_{O_2,stoich.} \quad (1.7)$$

v denotes, again, the mole number of O_2 in the reaction equation for a complete reaction of 1 mol of fuel to CO_2 and H_2O . Some examples are given in Table 1.3.

Tab. 1.3. Examples of stoichiometric numbers v and of fuel mole fractions at stoichiometric conditions $x_{fuel, stoich}$ in fuel/air mixtures

Reaction	v	$x_{fuel, stoich.}$
$H_2 + 0.5 O_2 + 0.5 \cdot 3.762 N_2 \rightarrow H_2O + 0.5 \cdot 3.762 N_2$	0.5	29.6 mol-%
$CH_4 + 2.0 O_2 + 2.0 \cdot 3.762 N_2 \rightarrow CO_2 + 2 H_2O + 2.0 \cdot 3.762 N_2$	2.0	9.50 mol-%
$C_3H_8 + 5.0 O_2 + 5.0 \cdot 3.762 N_2 \rightarrow 3 CO_2 + 4 H_2O + 5.0 \cdot 3.762 N_2$	5.0	4.03 mol-%
$C_7H_{16} + 11.0 O_2 + 11.0 \cdot 3.762 N_2 \rightarrow 7 CO_2 + 8 H_2O + 11.0 \cdot 3.762 N_2$	11.0	1.87 mol-%
$C_8H_{18} + 12.5 O_2 + 12.5 \cdot 3.762 N_2 \rightarrow 8 CO_2 + 9 H_2O + 12.5 \cdot 3.762 N_2$	12.5	1.65 mol-%

Premixtures of fuel and air (the proper amount of N_2 has to be added in this case on both sides of the reaction equation; see Table 1.3) are characterized by the *air equivalence ratio* (sometimes *air number*) or the reciprocal value, the *fuel equivalence ratio* $\Phi = 1/\lambda$ with

$$\lambda = (x_{air}/x_{fuel}) / (x_{air,stoich.}/x_{fuel, stoich.}) = (w_{air}/w_{fuel}) / (w_{air,stoich.}/w_{fuel, stoich.}) .$$

This formula can be rewritten to allow the evaluation of mole fractions in a mixture from Φ by

$$x_{fuel} = \frac{1}{1 + \frac{4.762 \cdot v}{\Phi}}, \quad x_{air} = 1 - x_{fuel}, \quad x_{O_2} = x_{air} / 4.762, \quad x_{N_2} = x_{O_2} \cdot 3.762 .$$

Accordingly, premixed combustion processes can now be divided into three groups,

rich combustion:	$\Phi > 1$	, $\lambda < 1$
stoichiometric combustion:	$\Phi = 1$	, $\lambda = 1$
lean combustion:	$\Phi < 1$	, $\lambda > 1$.

The burning of freely burning premixed laminar flat flames into the unburnt mixture can be characterized by the *laminar burning velocity* v_L (e. g., in m/s); other names in the literature are *flame velocity* or *flame speed*. It will be shown in Chapter 8 that the burning velocity depends only on the mixture composition (Φ or λ), the pressure p , and the initial temperature T_u .

If the laminar burning velocity of a flat flame is less than the velocity u_u of the unburnt gases (see Fig. 1.1), the flame blows off. Therefore, the inequality $v_L > u_u$