physical properties of natural gases

N.V. Nederlandse Gasunie

© 1980 N.V. Nederlandse Gasunie

This book, or parts thereof, may not be reproduced in any form without written permission of N.V. Nederlandse Gasunie.

Preface

The considerable response to the earlier Dutch-language editions of this reference work on physical and thermodynamic material constants and properties of pure gases and mixtures thereof, namely "Basisgegevens over Gronings aardgas", published 1968 (2200 copies), and "Basisgegevens Aardgassen", published 1980 (15,000 copies), has prompted N.V. Nederlandse Gasunie to publish a third reference work of this kind.
On this occasion, in view of the interest from outside the Netherlands, it was decided that the work should be in English. SI units have been used throughout, although conversion factors are given in the various tables.
As indicated by the large number of literature references, much of the data has been derived from an extensive literature search, with every effort being taken to make an intelligent selection from the large amount of information published on the various subjects. A number of formulas have also been refined to take account of non-ideal gases.
Section 3.15 gives test data on the flammability limits of Groningen natural gas and Ekofisk gas. The tests were carried out on Gasunie's behalf by the Environmental Research Department of DSM.
The calculation procedures in Sections 2 and 3 are fitted into an user friendly computer program FYSCAL (= fysical calculations). The basic information for these calculation procedures (databank) is completely taken from this handbook.
The advantages of this reference work for the user are that a selection has already been made from the large amount of basic data available from different sources and that this information has been collected in one volume. This has also enabled a large degree of uniformity to be achieved. N.V. Nederlandse Gasunie can, however, accept no liability whatsoever in respect of data derived from the literature.
In a number of instances, the literature references cite reports published by N.V. Nederlandse Gasunie. These reports are available free of charge from the company.

Theo M. Geerssen

Groningen, June 1988

Contents

Section 1

General data

Section 2

Properties of gases and gas mixtures

Section 3

Combustion and flue gas properties

Section 4

General information

Section 5

Index

Section 6

References

Section 1

General data

1.1 Fundamental constants

1.2 SI base units

1.3 SI units and commonly used prefixes

1.4 Definitions

1.5 Classification of various hydrocarbons

1.6 Conversion tables

1.7 Properties of 52 pure gases

1.8 Conversion of molar percentage, percentage by volume and percentage by mass

1.9 Properties of Groningen natural gas

1.10 Properties of liquid Groningen natural gas and liquid nitrogen

Section 1 General data

1.1 Fundamental constants (lit. 1)

1.1.1 Thermochemical calorie: 1 cal_{tc} = 4.184 0 joule (exactly)
International calorie: 1 cal_{IT} = 4.186 8 joule (exactly)
1 cal_{tc} = 0.999 331 cal_{IT}

N.B. Wherever the term "cal" is used in this reference work without an index, it will refer to the cal_{IT} (IT = International Steam Tables).

1.1.2 Speed of light in vacuum (see definition of meter):
$c = 299.792\,458 \times 10^6$ m/s

1.1.3 Normal molar volume of an ideal gas:
$V_m = 22.413\,83 \times 10^{-3} \pm 0.000\,69 \times 10^{-3}$ m^3/mol

1.1.4 Normal temperature and pressure (NTP):
absolute temperature (freezing point of water in air at 101 325 Pa):
$T = 273.15$ K (0 °C)
absolute pressure:
$p = 101\,325$ Pa (exactly) (1 atm)

1.1.5 Universal gas constant ($R_a = \frac{p \cdot V}{T}$) [1.1]:
$R_a = 8.314\,41 \pm 0.000\,26$ J/(mol · K)

1.1.6 Standard acceleration due to gravity:
$g = 9.806\,65$ m/s^2 (exactly)

1.1.7 Atomic mass (based on ^{12}C):

argon	Ar	39.948
carbon	C	12.011
hydrogen	H	1.0079
helium	He	4.0026
nitrogen	N	14.0067
oxygen	O	15.9994
sulphur	S	32.06

1.1.8 Definition of the m^3: Except where otherwise stated, the measure of 1 m^3 as used in this reference work means 1 m^3 of the product or substance concerned at an absolute pressure of 101.325 kPa (1.01325 bar) and an absolute temperature of 273.15 K (0 °C).

1.2 **SI base units**
As adopted by the Conférence Générale des Poids et Mesures (General Conference on Weights and Measures) (CGPM, Paris, 1960).

1.2.1 Metre (m): The distance travelled by light in vacuum during a period of time of 299 792 458 s^{-1} (CGPM, Paris, October 1983).

1.2.2 Kilogram (kg): The unit of mass equal to the mass of the platinum-iridium alloy protoype adopted as the unit of mass by the third General Conference on Weights and Measures (kept by the International Bureau of Weights and Measures at Sèvres, near Paris).

1.2.3 Second (s): The duration of 9 192 631 770 periods of the radiation associated with a specified transition, between two hyperfine energy levels, of the cesium-133 atom (Cs).

1.2.4 Ampere (A): The constant magnitude of the electric current that, when flowing through each of two parallel, straight and infinitely long conductors of negligible circular cross section separated by one metre in vacuum, results in a force between the two conductors of 2×10^{-7} newton (N) per metre of length.

1.2.5 Kelvin (K): The unit of thermodynamic temperature equal to 1/273.16 of the thermodynamic temperature of the triple point of water.

1.2.6 Mole (mol): The quantity of matter in a system that contains as many elementary entities as there are atoms in 0.012 kg of carbon-12 (^{12}C). The elementary entities must be specified: they may be atoms, molecules, ions, electrons, other particles or specific groups of like particles.

1.2.7 Candela (cd): The luminous intensity (normal to the surface) of an area equal to 1/600 000 of a square having sides of one metre of an integral radiating cavity at the temperature of freezing platinum at a pressure of 101.325 kPa.

Supplementary SI units

1.2.8 Radian (rad): The plane angle at the centre of a circle subtended by an arc of the circle equal in length to its radius.

1.2.9 Steradian (sr): The solid angle subtended at the centre of a sphere by an area of its surface equal to the square of the radius of the sphere.

1.3 SI units and commonly used prefixes

1.3.1 Multiples of SI units

exa	E	10^{18}	atto	a	10^{-18}
peta	P	10^{15}	femto	f	10^{-15}
tera	T	10^{12}	pico	p	10^{-12}
giga	G	10^{9}	nano	n	10^{-9}
mega	M	10^{6}	micro	μ	10^{-6}
kilo	k	10^{3}	milli	m	10^{-3}
hecto	h	10^{2}	centi	c	10^{-2}
deca	da	10	deci	d	10^{-1}

1.3.2 Time: symbol *t*

second	s = 1 s
kilosecond	ks = 10^{3} s
millisecond	ms = 10^{-3} s
microsecond	μs = 10^{-6} s
nanosecond	ns = 10^{-9} s

1.3.3 Length: symbols *l, b, h, r, d, s, λ*

metre	m = 1 m
kilometre	km = 10^{3} m
decimetre	dm = 10^{-1} m
centimetre	cm = 10^{-2} m
millimetre	mm = 10^{-3} m
micrometre	μm = 10^{-6} m
nanometre	nm = 10^{-9} m

Area: symbol *A*

square metre	m^2 = 1 m^2
square kilometre	km^2 = 10^{6} m^2
square decimetre	dm^2 = 10^{-2} m^2
square centimetre	cm^2 = 10^{-4} m^2
square millimetre	mm^2 = 10^{-6} m^2

Volume: symbol *V*

cubic metre	m^3 = 1 m^3
cubic decimetre	dm^3 = 10^{-3} m^3
cubic centimetre	cm^3 = 10^{-6} m^3
cubic millimetre	mm^3 = 10^{-9} m^3

1.3.4 Thermodynamic temperature: symbol T

kelvin	K	= 1 K
celsius temperature: symbol t		
degree Celsius, difference	°C	= 1 K
degree Celsius, absolute	t°C	= $(t+273.15)$ K

1.3.5 Mass: symbol m

kilogram	kg	= 1 kg
megagram	Mg	= 10^3 kg
gram	g	= 10^{-3} kg
milligram	mg	= 10^{-6} kg
microgram	μg	= 10^{-9} kg

1.3.6 Amount of substance: symbol n

mole	mol	= 1 mol
kilomole	kmol	= 10^3 mol
millimole	mmol	= 10^{-3} mol
micromole	μmol	= 10^{-6} mol

1.3.7 Force: symbol F

newton	N	= 1 N
meganewton	MN	= 10^6 N
kilonewton	kN	= 10^3 N
decanewton	daN	= 10 N

1.3.8 Pressure: symbol p

pascal	Pa	= 1 Pa
megapascal	MPa	= 10^6 Pa
kilopascal	kPa	= 10^3 Pa
millipascal	mPa	= 10^{-3} Pa
micropascal	μPa	= 10^{-6} Pa

1.3.9 Energy: symbols E, U, Q, W

joule	J	= 1 J
exajoule	EJ	= 10^{18} J
petajoule	PJ	= 10^{15} J
terajoule	TJ	= 10^{12} J
gigajoule	GJ	= 10^9 J
megajoule	MJ	= 10^6 J
kilojoule	kJ	= 10^3 J
millijoule	mJ	= 10^{-3} J

1.3.10 Power: symbol P

watt	W	= 1	W
gigawatt	GW	= 10^9	W
megawatt	MW	= 10^6	W
kilowatt	kW	= 10^3	W
milliwatt	mW	= 10^{-3}	W
microwatt	μW	= 10^{-6}	W

1.3.11 Dynamic viscosity: symbol μ

pascal-second	Pa · s	= 1	Pa · s
millipascal-second	mPa · s	= 10^{-3}	Pa · s

kinematic viscosity: symbol ν

square metre per second	m^2/s	= 1	m^2/s
square millimetre per second	mm^2/s	= 10^{-6}	m^2/s

1.3.12 Electricity

current: symbol I

ampère	A	= 1	A
kiloampère	kA	= 10^3	A
milliampère	mA	= 10^{-3}	A
microampère	μA	= 10^{-6}	A
nanoampère	nA	= 10^{-9}	A
picoampère	pA	= 10^{-12}	A

voltage: symbol V

volt	V	= 1	V
megavolt	MV	= 10^6	V
kilovolt	kV	= 10^3	V
millivolt	mV	= 10^{-3}	V
microvolt	μV	= 10^{-6}	V

resistance: symbol R

ohm	Ω	= 1	Ω
gigaohm	GΩ	= 10^9	Ω
megaohm	MΩ	= 10^6	Ω
kilo-ohm	kΩ	= 10^3	Ω
milliohm	mΩ	= 10^{-3}	Ω
micro-ohm	μΩ	= 10^{-6}	Ω

1.3.13 Units associated with the SI system

time:

day	d	= 24 h	= 86 400 s
hour	h	= 60 min	= 3 600 s
minute	min	= 60 s	

area:

are	a	= 10^2 m^2
hectare	ha	= 10^4 m^2

volume:

litre	L	= 1 dm^3	= 10^{-3} m^3
hectolitre	hL	= 100 dm^3	= 10^{-1} m^3
decilitre	dL	= 0.1 dm^3	= 10^{-4} m^3
centilitre	cL	= 10 cm^3	= 10^{-5} m^3
millilitre	mL	= 1 cm^3	= 10^{-6} m^3

mass:

tonne t = 1 Mg = 10^3 kg = 10^6 g

pressure:

bar	bar	= 10^2 kPa = 10^5 Pa*)
millibar (hectopascal)	mbar	= 10^{-1} kPa = 10^2 Pa

*) 1 Pa = 1 N/m^2

energy:

kilowatt-hour 1 kWh = 3.6 MJ = 3.6 x 10^3 kJ = 3.6 x 10^6 J

1.3.14 Some obsolete units and usages

length:

ångström	$1\ \text{Å} = 10^{-1}\ \text{nm} = 10^{-10}\ \text{m}$

volume:

cubic centimetre	$1\ \text{cc} = 1\ \text{mL} = 10^{-6}\ \text{m}^3$

viscosity:

Poise	$1\ \text{P} = 10^{-1}\ \text{Pa} \cdot \text{s}$
Stokes	$1\ \text{St} = 10^{-4}\ \text{m}^2/\text{s}$

energy:

calorie	$1\ \text{cal}_{\text{tc}} = 4.1840\ \text{J}$ (exactly)
	$1\ \text{cal}_{\text{IT}} = 4.1868\ \text{J}$ (exactly)

1.4 Definitions

1.4.1 Natural gas: A naturally occurring complex mixture of hydrocarbons and non-hydrocarbons that at room temperature and under atmospheric pressure is entirely in the gaseous phase.

1.4.2 Gross calorific value H_s: The amount of heat evolved by the complete combustion of a unit volume of gas $V(T_v; p_v)$ with air at a constant pressure of 101.325 kPa and a constant temperature T_H when the combustion products have once more cooled to the starting conditions and whereby the water produced by the combustion is assumed to be completely condensed.
Net calorific value H_i: The amount of heat evolved by the complete combustion of a unit volume of gas $V(T_v; p_v)$ with air at a constant pressure of 101.325 kPa and a constant temperature T_H when the combustion products have once more cooled to the starting conditions and whereby the water produced by the combustion is assumed to remain as vapour.
The internationally applicable starting conditions are:
an absolute pressure of 101.325 kPa;
a temperature T_H of 298.15 K (25 °C).
The difference between the gross calorific value and the net calorific value is the latent heat of vaporisation of the water produced by the chemical reaction: at 298.15 K (25 °C) this amounts to 2442.5 kJ/kg (583.38 kcal/kg).
Only with gases and gas mixtures in which free or chemically bonded hydrogen occurs is it possible to differentiate between gross and net calorific values.

N.B.
a. The internationally applied starting conditions refer only to the method of determining the calorific value and therefore do not relate to the gas medium,
b. The definitions of gross calorific value and net calorific value are covered by an international standard, ISO 6976 – 1983 (E) (lit. 2).

1.4.3 Relative density d: The ratio of the mass of a unit volume of a gas (ϱ_g) to that of the same unit volume of dry air (ϱ_a) at an absolute pressure of 101.325 kPa and a temperature of 273.15 K (0 °C):
$d = \varrho_g/\varrho_a$ [1.2]

1.4.4 Wobbe index W: The ratio of the gross calorific value H_s to the square root of the relative density d of a gas:
$W = H_s/\sqrt{d}$ [1.3]
The Wobbe index is a measure of the amount of energy delivered to a burner via an injector. The energy input is a linear function of W. Two gases of differing

composition but having the same Wobbe index will deliver the same amount of energy for any given injector under the same injector pressure.

Extended Wobbe index W_e: In addition to the Wobbe index W, an extended Wobbe index W_e is used which takes into account the injector pressure Δp:
$W_e = W\sqrt{\Delta p}$ [1.4]

1.4.5 Gas modulus m: The gas modulus $m = \sqrt{\Delta p/W}$ [1.5] is a measure of the primary aeration obtained via an injector. It is a comparative measure and is used as such in considering the effect of changing gas compositions.

1.4.6 SRG method: Application of the SRG method (Sommers-Ruhrgas method) involves adjusting all gas appliances such that the rated input is achieved with a gas having the maximum admissible or occurring Wobbe index. Gases having a lower Wobbe index can be supplied to the appliances without modification but the heat input will be reduced.

1.4.7 Theoretical air requirement a: The calculated volume of air required for complete combustion of a unit volume of gas, i.e. that required to produce a stoichiometric mixture.

1.4.8 Air factor a_f: The ratio of the volume of air employed per unit mass or volume of fuel to the volume of air theoretically required for complete combustion:
stoichiometric mixture: $a_f = 1$
excess air*): $a_f > 1$
air deficiency: $a_f < 1$

*) Example: $a_f = 1.2$ means 0.2 (20 %) excess air.

1.4.9 Delbourg's combustion potential C: A dimensionless variable calculated from the gas composition. The combustion potential C is a measure of the laminar burning velocity w of a gas.

1.4.10 Sooting number I: A dimensionless number providing a measure of the propensity of a gas to sooting when burnt. The sooting number I can be calculated from the gas composition.

1.4.11 Laminar burning velocity w: The velocity, relative to the unburnt gas, with which a plane, one-dimensional flame front travels along the normal to its surface.

1.4.12 Flammability limits: The concentrations of a gas in air or oxygen above and below which the mixture will not support combustion. The lower flammability limit *LL* is the minimum concentration of a gas in air or oxygen at which the mixture will just support combustion. The upper flammability limit *UL* is the maximum concentration of a gas in air or oxygen at which the mixture will just support combustion. The flammability limits of a natural gas/air or a natural gas/oxygen mixture can be calculated with reasonable accuracy from the gas composition using Le Chatelier's Rule (3.15.3).

1.4.13 Deflagration: Rapid combustion of a gas/air mixture in the range between the upper and lower flammability limits. The burning velocity is several tens of metres per second.

1.4.14 Detonation: Combustion of a gas/air mixture that is in the range between the upper and lower flammability limits, characterised by supersonic burning velocities producing shock waves and violent pressure rise.

1.4.15 Critical temperature T_k: The highest temperature at which gas and liquid phases can coexist. Along with the critical pressure and the critical density, the critical temperature defines the critical point at which the distinction between the fluid phases is eliminated.

1.4.16 Retrograde condensation: Where the critical point of multicomponent liquid-vapour equilibrium occurs below the maxima in temperature and pressure of the two phase region, a sequence of increasing pressure change, at a temperature between the temperature maximum and the critical point, will cause a partial condensation of the vapour to liquid and then a full return to the vapour state, called retrograde condensation. (ASTM Standard Definition)

1.4.17 Gas hydrates: The light hydrocarbons ($C_1 - C_4$) present in a natural gas combined with free water produce hydrate, the form of which can vary from wet snow to ice. Hydrate formation depends on pressure, temperature and composition of the natural gas.

1.4.18 Flue losses: The amount of energy lost in the combustion products exhausted through the flue of an appliance or other gas-fired equipment.

Radiation and convection losses: The amount of energy which is given off to the surroundings by heat radiation and convection and which cannot be utilised.

Standing losses: The amount of energy that has to be supplied to an installation in order to hold it on standby, without supplying any useful energy.

Useful energy: The difference between the amount of energy supplied and the sum of the energy losses of all kinds (flue losses, radiation and convection losses and standing losses). In other words, the amount of energy transferred to the medium of a heating installation.

Efficiency: The ratio of the amount of useful energy produced to the amount of energy supplied. Efficiency can be expressed in terms of gross calorific value or net calorific value. Commonly employed efficiencies are:
a. indirect efficiency η_{ind} (flue efficiency): the ratio of the amount of energy supplied less flue losses to the total amount of energy supplied;
b. direct efficiency η_{dir} (heating efficiency): the ratio of the amount of energy supplied less the sum of radiation and convection losses and flue losses to the total amount of energy supplied;
c. average overall efficiency η_{av} (annual efficiency): the ratio of the energy supplied less the sum of radiation and convection losses, flue losses and standing losses to the total amount of energy supplied, taken over a specified period of time.

1.4.19 Gas constant: The Universal gas constant R_a (1.1.5) is a constant of proportionality which is independent of pressure and temperature:
$R_a = 8.314\,41 \pm 0.000\,26$ J/(mol · K)

1.4.20 Critical flow: Critical flow conditions will occur for a particular ratio of gas pressure to backpressure (i.e. downstream pressure – generally atmospheric pressure) at which sonic velocity is reached at the point of minimum section of the orifice. Reduction of the backpressure will then not increase the rate of flow. To describe the condition where the flow is increased by an increase in upstream pressure, the term supercritical flow is used.

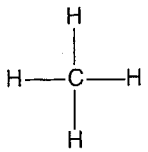
1.4.21 Autoignition temperature: The autoignition temperature is the temperature at which a gas/air mixture will spontaneously ignite, i.e. without an external source of ignition. The autoignition temperature is a function of the pressure and composition of the gas.

1.5 Classification of various hydrocarbons

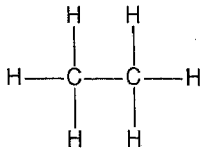
1.5.1 Paraffins: C_nH_{2n+2}

CH_4 methane
C_2H_6 ethane
C_3H_8 propane
C_4H_{10} 2-methylpropane
C_4H_{10} butane
etc.

CH_4 – methane

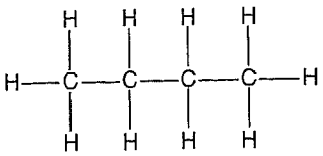


C_2H_6 – ethane

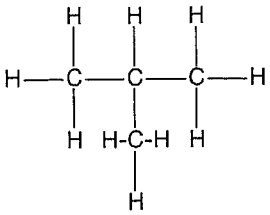


Butane is the first component that has an isomer. Isomers have the same chemical composition and the same molar mass as the normal molecule, differing only in certain properties.

C_4H_{10} – butane



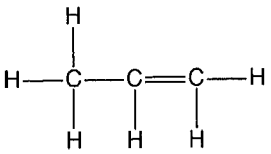
C_4H_{10} – 2-methylpropane



1.5.2 Olefins: C_nH_{2n}

C_2H_4 ethene
C_3H_6 propene
C_4H_8 butene
etc.

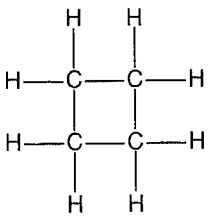
C_3H_6 – propene



1.5.3 Naphtenes (cycloalkanes): C_nH_{2n}

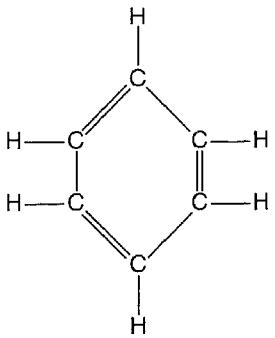
C_3H_6 cyclopropane
C_4H_8 cyclobutane
C_5H_{10} cyclopentane
C_6H_{12} cyclohexane
etc.

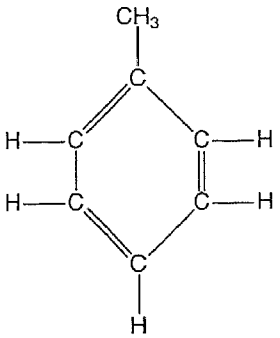
C_4H_8 – cyclobutane



1.5.4 **Aromatics:** C_6H_6 – benzene C_7H_8 – toluene

C_6H_6 benzene
C_7H_8 toluene
C_8H_{10} o-xylene

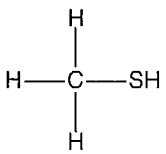


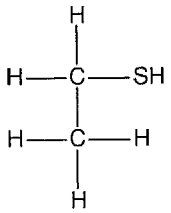


1.5.5 **Mercaptans:** RSH

R = alkyl group CH_3SH – methyl mercaptan C_2H_5SH – ethyl mercaptan

CH_3SH methyl mercaptan
C_2H_5SH ethyl mercaptan
C_3H_7SH n-propyl mercaptan
C_3H_7SH i-propyl mercaptan

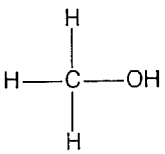


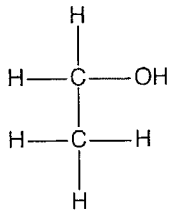


1.5.6 **Alcohols:** ROH CH_3OH – methyl alcohol C_2H_5OH – ethyl alcohol

R = alkyl group

CH_3OH methyl alcohol (methanol)
C_2H_5OH ethyl alcohol
C_3H_7OH n-propyl alcohol
C_3H_7OH i-propyl alcohol





1.6 Conversion tables

1.6.1 Imperial weights and measures and US variants:

1 inch (in)	=	0.025 4	m
1 foot (ft)	=	0.304 8	m
1 yard (yd)	=	0.914 4	m
1 mile	=	1609.344	m
1 square inch (sq in)	=	$6.451\,6 \times 10^{-4}$	m^2
1 square foot (sq ft)	=	0.092 903	m^2
1 square yard (sq yd)	=	0.836 127	m^2
1 cubic inch (cu in)	=	$16.387\,064 \times 10^{-6}$	m^3
1 cubic foot (cu ft)	=	$28.316\,847 \times 10^{-3}$	m^3
1 Imperial gallon (UK)	=	4.546×10^{-3}	m^3
1 US gallon	=	3.785×10^{-3}	m^3
1 barrel (US)	=	0.158 988	m^3
1 grain (gr)	=	64.8×10^{-6}	kg
1 ounce (oz)	=	28.35×10^{-3}	kg
1 pound (lb)	=	0.453 592 37	kg
1 long ton (UK) (2240 lbs)	=	1016.05	kg
1 short ton (US) (2000 lbs)	=	907.185	kg

1.6.2 Force:

1 kilogram force (kgf)	=	9.806 65	N
1 pound force (lbf)	=	4.448 22	N

1.6.3 Pressure:

1 bar	=	10^5	Pa**)
1 atm	=	101 325	Pa
1 kgf/cm² (at)	=	98 066.5	Pa
1 lbf/sq in (psi)	=	6 894.757 293	Pa
1 mmwc (water)	=	9.806 65	Pa
1 mmHg (mercury) *)	=	133.322	Pa

*) ϱ = 13.595 08 kg/dm³ (lit. 3)
**) 1 Pa = 1 N/m²

1.6.4 Quantity of heat:

1 cal (1.1.1)	=	4.1868	J
1 therm (10^5 Btu)	=	105.506×10^6	J
1 thermie (1 $Mcal_{15}$*))	=	4.1858×10^6	J
1 kWh**))	=	3.6×10^6	J
1 Btu_{IT}	=	1055.056	J

1.6.5 Heat flow:

1 W	=	1	J/s
1 cal/h (1.1.1)	=	1.163×10^{-3}	J/s
1 PS (Pferdestärke) (hp DIN)	=	735.499	J/s
1 hp (horsepower)	=	745.700	J/s
1 Btu/h	=	0.293 071	J/s

1.6.6 Calorific values:

1 cal/m^3 (1.1.1)	=	4.1868	J/m^3
1 Btu/ft^3 (ISC) dry	=	39 361.916	J/m^3
1 Btu/ft^3 (Int) dry	=	39 277.838	J/m^3
1 Btu/ft^3 (ISC) sat.	=	40 059.783	J/m^3
1 Btu/ft^3 (Int) sat.	=	39 972.701	J/m^3

ft^3 (ISC = Imperial Standard Conditions): 60 °F, 30 inches Hg = 101 374 Pa (g at 53 °N)
ft^3 (Int = international cubic foot); 60 °F, 30 inches Hg = 101 591 Pa ($g = 9.806\,65\ m/s^2$)

N.B.: in the conversion of 60 °F to 0 °C no account is taken of compressibility.

*) 1 $Mcal_{15}$ (c_p of water at 15 °C) = 0.99976 Mcal (lit. 4)
**) 1 W = 1 J/s = 1 N · m/s

1.6.7	**Thermal conductivity:**	
	1 kcal/(m · h · K) (1.1.1)	= 1.163 W/(m · K)
	1 Btu/(ft · h · °F)	= 1.732 W/(m · K)
1.6.8	**Heat transfer:**	
	1 kcal/(m^2 · h · K) (1.1.1)	= 1.163 W/(m^2 · K)
	1 Btu/(ft^2 · h · °F)	= 5.679 W/(m^2 · K)
1.6.9	**Viscosity:**	
	Kinematic viscosity ν	
	1 St (Stokes)	= 10^{-4} m^2/s
	1 ft^2/s	= 0,0929 m^2/s
	Dynamic viscosity μ	
	1 P (Poise)	= 0.1 N · s/m^2 = 0.1 Pa · s
	1 lb/(ft · s)	= 1.488 N · s/m^2 = 1.488 Pa · s

Table 1.7 Properties of 52 gaseous components

1. Molar mass M kg/kmol:
   The molar mass M of each of the 52 components of table 1.7 is calculated using the atomic masses from 1.1.7. The molar mass M of a gas mixture is calculated using:

   $$M = \sum_{i=1}^{n} n_i \cdot M_i / 100 \qquad [1.6]$$

   where:

M	= the molar mass of gas mixture	kg/kmol
n_i	= the concentration of component i	% (mol)
M_i	= the molar mass of component i (table 1.7)	kg/kmol
n	= the number of components in the gas mixture	–

2. Real molar volume V m^3/kmol:
   $V = z \cdot V_m$ [1.7]
   – V_m = 22.413 83 m^3/kmol (1.1.3);
   – z = compressibility according to API (lit. 5) (table 2.2.5)
   except for z_{H_2O} = 0.9650 (lit. 6)

   In the case of components 10–27 the molar volume has been taken to be 20.5 m^3/kmol. This assumption is not based on any theoretical consideration and is therefore completely arbitrary.

3. Density ϱ kg/m^3:
   calculated from M kg/kmol and V m^3/kmol

4. Relative density d:
   calculated from $\varrho_{component}$ and ϱ_{air} (no. 52 in table 1.7)

5. Critical constants (lit. 5)
   Critical temperature T_c K
   Critical pressure p_c kPa
   Critical volume V_c m^3/kmol

6. Boiling point at 101.325 kPa T_b K (lit. 5)

Table 1.7 Properties of 52 pure gases

No.	Component	Formula	Molar mass M kg/kmol	Real molar volume V m³/kmol	Density ϱ kg/m³
1	methane	CH_4	16.043	22.360 0	0.717
2	ethane	C_2H_6	30.069	22.187 5	1.355
3	propane	C_3H_8	44.096	21.929 7	2.011
4	2-methylpropane (isobutane)	C_4H_{10}	58.123	21.615 9	2.689
5	butane	C_4H_{10}	58.123	21.519 5	2.701
6	2,2-dimethylpropane	C_5H_{12}	72.150	21.284 2	3.390
7	2-methylbutane (isopentane)	C_5H_{12}	72.150	21.055 6	3.427
8	pentane	C_5H_{12}	72.150	20.887 4	3.454
9	2,2-dimethylbutane	C_6H_{14}	86.177	20.515 4	4.201
10	2,3-dimethylbutane	C_6H_{14}	86.177	20.5	4.204
11	3-methylpentane	C_6H_{14}	86.177	20.5	4.204
12	2-methylpentane (isohexane)	C_6H_{14}	86.177	20.5	4.204
13	hexane	C_6H_{14}	86.177	20.5	4.204
14	2-methylhexane (isoheptane)	C_7H_{16}	100.203	20.5	4.888
15	heptane	C_7H_{16}	100.203	20.5	4.888
16	octane	C_8H_{18}	114.230	20.5	5.572
17	nonane	C_9H_{20}	128.257	20.5	6.256
18	decane	$C_{10}H_{22}$	142.284	20.5	6.941
19	undecane	$C_{11}H_{24}$	156.311	20.5	7.625
20	dodecane	$C_{12}H_{26}$	170.337	20.5	8.309
21	tridecane	$C_{13}H_{28}$	184.364	20.5	8.993
22	tetradecane	$C_{14}H_{30}$	198.391	20.5	9.678
23	cyclohexane	C_6H_{12}	84.161	20.5	4.105
24	methylcyclohexane	C_7H_{14}	98.188	20.5	4.790
25	benzene	C_6H_6	78.113	20.5	3.810
26	toluene	C_7H_8	92.140	20.5	4.495
27	xylene (o)	C_8H_{10}	106.167	20.5	5.179

	Relative density d	Critical constants			Boiling point (101.325 kPa) T_b K
		Temperature T_c K	Pressure p_c kPa	Volume V_c m³/kmol	
	0.555	190.58	4 604	0.099	111.66
	1.048	305.42	4 880	0.148	184.55
	1.555	369.82	4 250	0.203	231.11
	2.080	408.14	3 648	0.263	261.43
	2.089	425.18	3 797	0.255	272.65
	2.622	433.78	3 199	0.303	282.65
	2.650	460.43	3 381	0.306	301.00
	2.671	469.7	3 369	0.304	309.21
	3.249	488.78	3 080	0.359	322.88
	3.251	499.98	3 127	0.358	331.13
	3.251	504.5	3 124	0.367	336.42
	3.251	497.50	3 010	0.367	333.41
	3.251	507.5	3 012	0.370	341.88
	3.780	530.37	2 734	0.421	363.20
	3.780	540.3	2 736	0.432	371.58
	4.309	568.83	2 487	0.492	398.83
	4.838	594.64	2 290	0.548	423.97
	5.368	617.7	2 100	0.603	447.30
	5.897	638.73	1 965	0.660	469.04
	6.426	658.3	1 820	0.712	489.43
	6.955	675.8	1 724	0.774	508.58
	7.485	691.9	1 620	0.833	526.67
	3.175	553.6	4 070	0.308	353.87
	3.705	572.19	3 471	0.368	374.08
	2.947	562.16	4 898	0.259	353.24
	3.476	591.79	4 109	0.316	383.78
	4.005	630.4	3 733	0.369	417.58

No.	Component	Formula	Molar mass M kg/kmol	Real molar volume V m³/kmol	Density ϱ kg/m³
28	methyl mercaptan	CH_3SH	48.10	21.7907	2.208
29	ethyl mercaptan	C_2H_5SH	62.13	21.3402	2.911
30	propyl mercaptan	C_3H_7SH	76.16	20.5647	3.703
31	carbonyl sulphide	COS	60.07	22.0642	2.723
32	hydrogen sulphide	H_2S	34.08	22.1875	1.536
33	sulphur dioxide	SO_2	64.06	21.9431	2.919
34	ethene	C_2H_4	28.054	22.2435	1.261
35	propene	C_3H_6	42.080	21.9902	1.914
36	1-butene	C_4H_8	56.107	21.6159	2.596
37	1-pentene	C_5H_{10}	70.134	21.0443	3.333
38	1,2-butadiene	C_4H_6	54.091	21.4904	2.517
39	1-butyne	C_4H_6	54.091	21.3402	2.535
40	methanol	CH_3OH	32.042	21.4523	1.494
41	ethanol	C_2H_5OH	46.069	20.5557	2.241
42	argon	Ar	39.948	22.3937	1.784
43	helium	He	4.0026	22.4340	0.178
44	carbon dioxide	CO_2	44.010	22.2569	1.977
45	carbon monoxide	CO	28.010	22.4026	1.250
46	hydrogen	H_2	2.0158	22.4362	0.090
47	nitrogen	N_2	28.0134	22.4049	1.250
48	oxygen	O_2	31.9988	22.3914	1.429
49	nitric oxide	NO	30.0061	22.4004	1.340
50	nitrogen dioxide	NO_2	46.0055	21.8019	2.110
51	water vapour	H_2O	18.0152	21.629	0.833
52	air (dry)	–	28.964	22.4004	1.293

Relative density d	Critical constants			Boiling point (101.325 kPa) T_b K
	Temperature T_c K	Pressure p_c kPa	Volume V_c m^3/kmol	
1.708	470.0	7 233	0.145	279.11
2.251	499	5 495	0.207	308.15
2.864	533	4 256	–	339.8
2.105	375	5 877	0.140	222.9
1.188	373.6	9 005	0.098	211.4
2.258	430.7	7 895	0.122	263.2
0.975	282.36	5 032	0.129	169.47
1.480	364.8	4 610	0.181	225.43
2.008	419.6	4 020	0.240	266.90
2.578	464.78	3 550	0.305	303.11
1.947	444	4 500	0.219	284.00
1.961	463.7	4 712	0.221	281.22
1.155	512.6	8 094	0.118	337.85
1.733	516.3	6 380	0.167	351.44
1.380	150.8	4 865	0.076	87.3
0.138	5.3	229	0.058	4.3
1.529	304.3	7 382	0.094	194.65
0.967	133.0	3 499	0.093	81.2
0.070	33.3	1 298	0.065	20.4
0.967	126.3	3 399	0.090	77.4
1.105	154.8	5 081	0.076	90.3
1.036	180.26	6 547	0.060	121.4
1.632	431.4	10 133	0.170	294.3
0.644	647.4	22 120	0.057	373.0
1.000	132.45	3 771	–	81.8

1.8 Conversion of molar percentage, percentage by volume and percentage by mass

1.8.1 Conversion of percentage by volume – molar percentage % (vol.) – % (mol)

$$n_i = \frac{x_i/V_i}{\sum_{i=1}^{n} x_i/V_i} \times 100\ \%\ (\text{mol}) = \frac{x_i/z_i}{\sum_{i=1}^{n} x_i/z_i} \times 100\ \%\ (\text{mol}) \qquad [1.8]$$

$$x_i = \frac{n_i \cdot V_i}{\sum_{i=1}^{n} n_i \cdot V_i} \times 100\ \%\ (\text{vol.}) = \frac{n_i \cdot z_i}{\sum_{i=1}^{n} n_i \cdot z_i} \times 100\ \%\ (\text{vol.}) \qquad [1.9]$$

where:

x_i = the concentration of component i	% (vol.)
V_i = the real molar volume of component i (table 1.7)	m^3/kmol
n_i = the concentration of component i	% (mol)
z_i = the compressibility factor of component i (273.15 K; 101.325 kPa)	
n = the number of components in the gas mixture	

In the case of natural gas mixtures, the use of x_i instead of n_i has little effect on the final result.

1.8.2 Conversion of molar percentage – percentage by mass % (mol) – % (mass)

$$g_i = \frac{n_i \cdot M_i}{\sum_{i=1}^{n} n_i \cdot M_i} \times 100\ \%\ (\text{mass}) \qquad [1.10]$$

$$n_i = \frac{g_i/M_i}{\sum_{i=1}^{n} g_i/M_i} \times 100\ \%\ (\text{mol}) \qquad [1.11]$$

where:

g_i = the concentration of component i	% (mass)
M_i = the molar mass of component i (table 1.7)	kg/kmol
n_i = the concentration of component i	% (mol)

The conversion of percentage by volume – percentage by mass is performed in the same way.

1.9 *Table 1.9 Properties of Groningen natural gas (average composition).*

Component	Formula	x_i % (vol.)	n_i % (mol)	g_i % (mass)
methane	CH_4	81.30	81.29	69.97
ethane	C_2H_6	2.85	2.87	4.63
propane	C_3H_8	0.37	0.38	0.90
butane	C_4H_{10}	0.14	0.15	0.47
pentane	C_5H_{12}	0.04	0.04	0.16
hexane	C_6H_{14}	0.05	0.05	0.23
nitrogen	N_2	14.35	14.32	21.52
oxygen	O_2	0.01	0.01	0.02
carbon-dioxide	CO_2	0.89	0.89	2.10
		100	100	100

Molar mass	[1.6]	18.637 kg/kmol
Real molar volume	[1.7]	22.363 m^3/kmol
Compressibility factor	(2.2.1.1, table 2.2.1)	0.9977 (44)
Pseudo critical pressure	(table 2.1.1)	4460 kPa
Pseudo critical temperature	(table 2.1.1)	187.0 K
Density	[2.69]	0.833 kg/m^3
Relative density	[1.2]	0.645
Acentric factor	[2.63]	0.0209
Gross calorific value	[3.3]	35.096 MJ/m^3
Net calorific value	[3.4]	31.669 MJ/m^3
Wobbe index	[1.3]	43.700 MJ/m^3
Air requirement: wet	[3.7]	8.528 m^3/m^3
dry	[3.7]	8.430 m^3/m^3
Flammability limits in air	(101.325 kPa; 20 °C)	
(fig. 3.15.4): upper limit		16.6 % (mol)
lower limit		4.7 % (mol)
Autoignition temperature	(101.325 kPa)	
(fig. 3.15.4)		890 K

1.10 Properties of liquid Groningen natural gas and liquid nitrogen

1.10.1 If Groningen natural gas (table 1.9) is liquefied, the LNG produced may be assumed to possess approximately the following composition and properties:

– composition of liquefied gas in % (mol):	CH_4	91.6
	C_2H_6	6.7
	C_3H_8	1.0
	C_4H_{10}	0.3
	N_2	0.4
– density of gas at 273.15 K (0 °C) and 101.325 kPa	0.781 kg/m^3	
– density of liquefied gas at 112 K (–161 °C) and 101.325 kPa	453 kg/m^3	
– boiling point of liquid T_b at 101.325 kPa	112 K (–161 °C)	
– latent heat of vaporisation (CH_4) at T_b and 101.325 kPa (lit. 3,4)	509.90 kJ/kg	
– liquid/gas volume ratio	1:580*)	

1.10.2 The liquefied nitrogen (N_2) from the Groningen natural gas is stored separately:

– density of N_2 at 273.15 K (0 °C) and 101.325 kPa (table 1.7)	1.250 kg/m^3
– density of liquefied N_2 at 77.4 K (–195.8 °C) and 101.325 kPa	795 kg/m^3
– boiling point of liquid T_b at 101.325 kPa	77.4 K (–195.8 °C)
– latent heat of vaporisation at T_b and 101.325 kPa (lit. 4)	199.1 kJ/kg
– liquid/gas volume ratio	1:636*)

*) – 1 m^3 of LNG evaporates to produce 580 m^3 of natural gas (see gas composition) at 273.15 K and 101.325 kPa.
– 1 m^3 of liquid N_2 evaporates to produce 636 m^3 of nitrogen gas at 273.15 K and 101.325 kPa.

Section 2

Properties of gases and gas mixtures

2.1 Critical pressure and critical temperature
2.1.1 Weighted average method (Kay's rule)
2.1.2 EMR method

2.2 Compressibility and supercompressibility
2.2.1 Compressibility of gas mixtures
2.2.1.1 Research project NX-19
2.2.1.2 BWR
2.2.1.3 ISO
2.2.1.4 GERG
2.2.1.5 Edmister
2.2.2 Compressibility of pure gases
2.2.2.1 API
2.2.2.2 DIN

2.3 Thermal conductivity

2.4 Density

2.5 Viscosity
2.5.1 Dynamic (absolute) viscosity
2.5.1.1 Herning-Zipperer
2.5.1.2 Carr, Kobayashi and Burrows
2.5.1.3 Chapman and Cowling
2.5.1.4 Dynamic viscosity at p and T
2.5.2 Kinematic viscosity

2.6 Heat capacity
2.6.1 Isobaric heat capacity
2.6.2 Isochoric heat capacity

2.7 **Isentropic exponents**
2.7.1 Ideal gases
2.7.2 Non-ideal gases
2.7.2.1 Volume change with pressure
2.7.2.2 Temperature change with pressure
2.7.3 Velocity of sound

2.8 **H-S-diagram**
2.8.1 Enthalpy
2.8.2 Entropy
2.8.3 H-S-diagram
2.8.4 Isentropic expansion
2.8.5 Isenthalpic expansion
2.8.6 Enthalpy change with pressure and temperature
2.8.6.1 Isothermal change
2.8.6.2 Isobaric change
2.8.7 Isentropic compression

2.9 **Reynolds number**

2.10 **Pressure loss in pipes and bends**
2.10.1 Pressure loss in pipes
2.10.2 Pressure loss in bends

2.11 **Water content of natural gases**

2.1 Critical pressure and critical temperature

A number of variables relating to a gas mixture can only be calculated if the critical pressure and critical temperature of the mixture are known. Although the precise critical pressure and temperature are known for the individual components of the gas mixture, it is not possible to calculate the real critical pressure and temperature of the mixture from this data. The commonly applied calculation methods give only approximate values. The critical variables calculated by these methods are therefore referred to as pseudo-critical.

2.1.1 Weighted average method (Kay's rule)

Pseudo-critical pressure p_c:

$$p_c = \frac{\sum_{i=1}^{n} n_i \cdot p_{c,i}}{100} \qquad [2.1]$$

Pseudo-critical temperature T_c:

$$T_c = \frac{\sum_{i=1}^{n} n_i \cdot T_{c,i}}{100} \qquad [2.2]$$

where:

p_c	=	pseudo-critical pressure of the gas mixture	kPa
n	=	number of components	–
n_i	=	concentration of component i	% (mol)
$p_{c,i}$	=	critical pressure of component i (table 1.7)	kPa
T_c	=	pseudo-critical temperature of the gas mixture	K
$T_{c,i}$	=	critical temperature of component i (table 1.7)	K

Table 2.1.1 Pseudo-critical pressure and temperature of Groningen natural gas

Component	Formula	n_i*) % (mol)	$p_{c,i}$ kPa	$T_{c,i}$ K
methane	CH_4	81.29	4604	190.58
ethane	C_2H_6	2.87	4880	305.42
propane	C_3H_8	0.38	4250	369.82
butane	C_4H_{10}	0.15	3797	425.18
pentane	C_5H_{12}	0.04	3369	469.7
hexane	C_6H_{14}	0.05	3012	507.5
nitrogen	N_2	14.32	3399	126.3
oxygen	O_2	0.01	5081	154.8
carbon dioxide	CO_2	0.89	7382	304.3
Groningen gas		100	4460	187.0

*) Table 1.9

Groningen natural gas:
pseudo-critical pressure = 4460 kPa (44.60 bar)
pseudo-critical temperature = 187.0 K (–86.2 °C)

In order to arrive at numerical values which approximate the real values, i.e. the measured values, N.V. Nederlandse Gasunie employs, among other methods, special computer programs which use convergence techniques to work out the phase diagram of a gas mixture, including its critical pressure and temperature. The critical pressure and temperature arrived at in this way are generally taken as being the real critical pressure and temperature.

A formula given in publications by Campbell (lit. 8), derived from measurements involving 25 different natural gases with molar masses $M < 30$ also enables the rapid calculation of the critical temperature with an accuracy equal to that of the above-mentioned computer programs:

$T_c^l = T_c\,[1 + 0.03\,(M - 16)]$ [2.3] K

where:

T_c^l	=	real critical temperature	K
T_c	=	pseudo-critical temperature according to the weighted average method	K
M	=	molar mass of the gas mixture	kg/kmol

For Groningen natural gas ($M = 18.637$ kg/kmol):
$T_c^l = 201.8$ K (–71.4 °C)

From the aforementioned measured data it is not possible to derive a sufficiently accurate correlation for the critical pressure p_c.

2.1.2 EMR method

The EMR method (Eykman Molecular Refraction) (lit. 8, 9) also essentially computes pseudo-critical values which, as with the weighted average method described under 2.1.1, again closely approximate the real values.

Method (table 2.1.2):
- Divide the gas mixture into two groups:
  group 1 – CH_4, CO_2, H_2S, N_2, H_2 and O_2
  group 2 – C_2H_6 and the remaining hydrocarbons
- express the composition of the two groups in terms of 100 % for each (n^*_i)
- for each group calculate the EMR values on the basis of this composition, using the EMR values for the individual components (table 2.1.4)

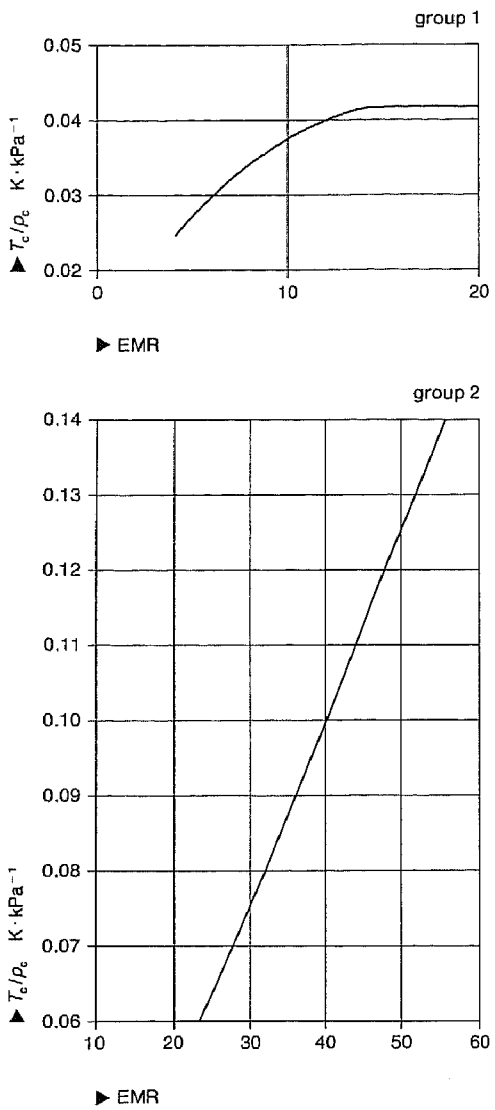
$$\mathrm{EMR}_{1/2} = \sum_{i=1}^{n} n^*_i \cdot \mathrm{EMR}_i / 100 \qquad [2.4]$$

- from fig. 2.1.1 determine the values of $\left(\frac{T_c}{p_c}\right)_1$ and $\left(\frac{T_c}{p_c}\right)_2$

and from this calculate the average value for the gas mixture using the formula:

$$\left(\frac{T_c}{p_c}\right)_m = n_1 \left(\frac{T_c}{p_c}\right)_1 + n_2 \left(\frac{T_c}{p_c}\right)_2 \qquad [2.5]$$

Fig. 2.1.1 EMR values for group 1 and group 2 as a function of critical pressure p_c and critical temperature T_c



$$n_1 = \sum_{i=1}^{n} n_i/100 \qquad \text{group 1} \qquad [2.6]$$

$$n_2 = \sum_{i=1}^{n} n_i/100 \qquad \text{group 2} \qquad [2.7]$$

– calculate the EMR value for the gas mixture using:

$$EMR_m = n_1 \cdot EMR_1 + n_2 \cdot EMR_2 \qquad [2.8]$$

and from fig. 2.1.2 determine the value of $\left(\frac{T_c}{\sqrt{p_c}}\right)_m$

– from $\left(\frac{T_c}{p_c}\right)_m$ and $\left(\frac{T_c}{\sqrt{p_c}}\right)_m$ the critical pressure p_c and critical temperature T_c for the gas mixture can now be calculated.

Table 2.1.2 EMR values for group 1 and group 2 for Groningen natural gas

Group 1				Group 2			
Component	n_i*) % (mol)	n^*_i	EMR	Component	n_i*) % (mol)	n^*_i	EMR
CH_4	81.29	84.23	14.084	C_2H_6	2.87	82.23	24.279
N_2	14.32	14.84	9.546	C_3H_8	0.38	10.89	34.343
O_2	0.01	0.01	9.469	C_4H_{10}	0.15	4.30	43.478
CO_2	0.89	0.92	14.647	C_5H_{12}	0.04	1.15	55.278
				C_6H_{14}	0.05	1.43	65.575
	$n_1 = 96.51$	$\Sigma = 100$			$n_2 = 3.49$	$\Sigma = 100$	

*) Table 1.9

n_i^* = pseudo-concentration of component i in % (mol) with the sum of the components in the part mixture taken as 100 %

Group 1 – $EMR_1 = 13.415$
Group 2 – $EMR_2 = 27.148$

From fig. 2.1.1:

for $EMR_1 = 13.415 \rightarrow \left(\frac{T_c}{p_c}\right)_1 = 0.041\,0$

for $EMR_2 = 27.148 \rightarrow \left(\frac{T_c}{p_c}\right)_2 = 0.069\,0$

$\left(\frac{T_c}{p_c}\right)_1$ and $\left(\frac{T_c}{p_c}\right)_2$ can also be calculated as follows:

$$\left(\frac{T_c}{p_c}\right)_1 = 0.01204 + 3.5983 \times 10^{-3} \times EMR_1 - 1.0762 \times 10^{-4} \times EMR_1^2 \quad (=0.0409) \qquad [2.9]$$

$$\left(\frac{T_c}{p_c}\right)_2 = 0.01406 + 1.7781 \times 10^{-3} \times EMR_2 + EMR_2 + 9.9172 \times 10^{-6} \times EMR_2^2 + -2.0102 \times 10^{-8} \times EMR_2^3 \quad (= 0.0692) \qquad [2.10]$$

For the gas mixture:

$$EMR_m = 13.894 \qquad [2.8]$$

$$\left(\frac{T_c}{p_c}\right)_m = 0.042\,0 \qquad [2.5]$$

From fig. 2.1.2

for $EMR_m = 13.894 \rightarrow \left(\frac{T_c}{\sqrt{p_c}}\right)_m = 2.85$

$\left(\frac{T_c}{\sqrt{p_c}}\right)_m$ may also be calculated from:

$$\left(\frac{T_c}{\sqrt{p_c}}\right)_m = 0.89246 + 1.43757 \times 10^{-1} \times EMR_m - 2.4271 \times 10^{-4} \times EMR_m^2 \quad (=2.843) \qquad [2.11]$$

Fig. 2.1.2 EMR values for gas mixtures as a function of the critical pressure p_c and critical temperature T_c

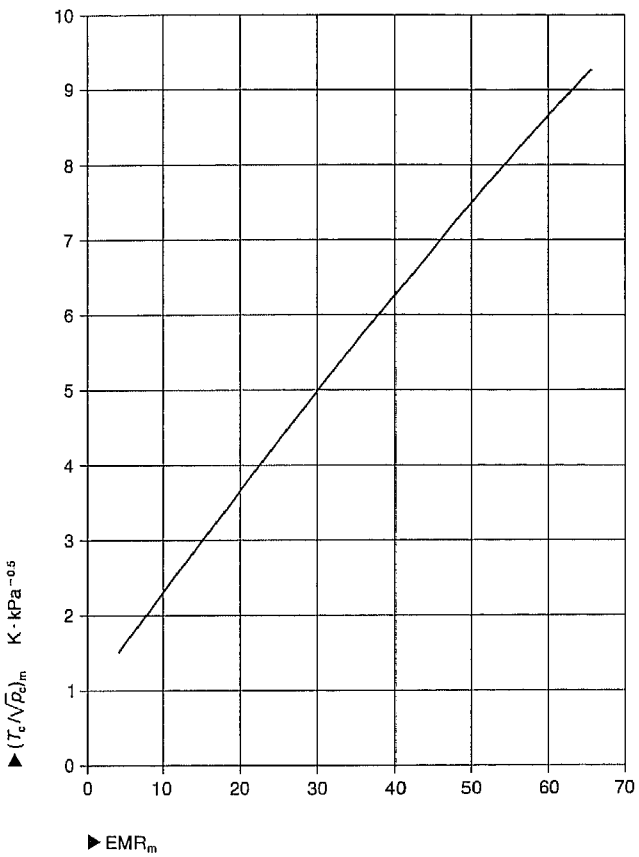


Table 2.1.4 Refractive index, density and EMR values for pure gases

No.	Component	Formula	Refractive index (101.325 kPa, 298.15 K) n	Density (101.325 kPa, 298.15 K) ϱ kg/L	EMR	Lit.
1	methane	CH_4	1.000 404 4	0.000 658	14.084	(3)
2	ethane	C_2H_6	1.000 700	0.001 238 3	24.279	(3)
3	propane	C_3H_8	1.001 000	0.001 833 9	34.343	(3)
4	2-methylpropane (isobutane)	C_4H_{10}	–	–	–	
5	butane	C_4H_{10}	1.001 286	0.002 455 3	43.478	(3)
6	2.2-dimethylpropane	C_5H_{12}	1.339	0.585 1	56.226	(3)
7	2-methylbutane (isopentane)	C_5H_{12}	1.350 88	0.614 62	55.305	(3)
8	pentane	C_5H_{12}	1.354 72	0.621 3	55.278	(3)
9	2.2-dimethylbutane	C_6H_{14}	1.365 95	0.644 46	65.561	(3)
10	2.3-dimethylbutane	C_6H_{14}	1.372 31	0.657 02	65.366	(3)
11	3-methylpentane	C_6H_{14}	1.373 86	0.659 76	65.351	(3)
12	2-methylpentane (isohexane)	C_6H_{14}	1.368 73	0.648 52	65.619	(3)
13	hexane	C_6H_{14}	1.372 26	0.654 84	65.575	(3)
14	2-methylhexane (isoheptane)	C_7H_{16}	1.382 27	0.674 39	75.920	(3)
15	heptane	C_7H_{16}	1.385 11	0.679 46	75.883	(3)
16	octane	C_8H_{18}	1.395 05	0.698 62	86.185	(3)
17	nonane	C_9H_{20}	1.403 11	0.713 75	96.541	(3)
18	decane	$C_{10}H_{22}$	1.409 67	0.726 35	106.857	(3)
19	undecane	$C_{11}H_{24}$	1.415 07	0.736 5	117.213	(3)
20	dodecane	$C_{12}H_{26}$	1.419 52	0.745 18	127.518	(3)
21	tridecane	$C_{13}H_{28}$	1.423 46	0.752 71	137.848	(3)
22	tetradecane	$C_{14}H_{30}$	1.426.85	0.759 20	148.177	(3)

23	cyclohexane	C_6H_{12}	1.423 54	0.773 89	61.215	(3)
24	methylcyclohexane	C_7H_{14}	1.420 58	0.765 06	71.767	(3)
25	benzene	C_6H_6	1.497 92	0.873 70	58.590	(3)
26	toluene	C_7H_8	1.494 13	0.862 31	69.524	(3)
27	xylene (o)	C_8H_{10}	1.502 95	0.875 96	80.178	(3)
28	methyl mercaptan	CH_3SH	1.435 3	0.857 0	32.421	(1, 4, 5)
29	ethyl mercaptan	C_2H_5SH	1.427 77	0.831 7	42.445	(1, 4, 5)
30	propyl mercaptan	C_3H_7SH	1.435 33	0.835 0	52.684	(1, 4, 5)
31	carbonyl sulphide	COS	1.340 5	0.998 0	27.560	(4, 5)
32	hydrogen sulphide	H_2S	1.000 584 5	0.001 407	20.220	(1)
33	sulphur dioxide	SO_2	1.456 9	1.367	28.329	(4, 5)
34	ethene	C_2H_4	1.209 8	0.404 1	19.994	(4, 5)
35	propene	C_3H_6	1.268 0	0.505 3	30.346	(3, 4, 5)
36	1-butene	C_4H_8	1.313 8	0.588 8	40.371	(3, 4, 5)
37	1-pentene	C_5H_{10}	1.368 35	0.635 33	54.459	(3, 4, 5)
38	1.2-butadiene	C_4H_6	1.318 2	0.646	35.948	(3, 4, 5)
39	1-butyne	C_4H_6	1.321 2	0.65	36.047	(3, 4, 5)
40	methanol	CH_3OH	1.326 52	0.784 4	17.973	(1)
41	ethanol	C_2H_5OH	1.359 41	0.783 7	28.333	(1)
42	argon	Ar	1.000 258 7	0.001 634 4	9.033	(3, 4, 5)
43	helium	He	1.000 031 97	0.000 163 5	1.118	(3, 4, 5)
44	carbon dioxide	CO_2	1.000 422	0.001 811 2	14.647	(4, 5)
45	carbon monoxide	CO	1.000 311	0.001 452	10.866	(4, 5)
46	hydrogen	H_2	1.000 127 5	0.000 082 5	4.451	(1)
47	nitrogen	N_2	1.000 273 2	0.001 145 2	9.546	(1)
48	oxygen	O_2	1.000 271 2	0.001 309 2	9.469	(1)
49	nitric oxide	NO	1.000 269 7	0.001 227 6	9.417	(1)
50	nitrogen dioxide	NO_2	1.000 491	0.001 933 1	16.692	(4, 5)
51	water vapour	H_2O	1.000 234	0.000 763 2	7.890	(4, 5)
52	air (dry)	–	1.000 268	0.001 184 6	9.360	(4, 5)

Then from $\left(\frac{T_c}{p_c}\right)_m = 0.042\,0$ and $\left(\frac{T_c}{\sqrt{p_c}}\right)_m = 2.85$:

T_c = 193.4 K (–97.8 °C)
p_c = 4605 kPa (46.05 bar)

where:

EMR	=	Eykman Molecular Refraction
n_i^*	=	pseudo-concentration of component i with the sum of the components in the part mixture taken as 100 %
n_i	=	concentration of component i in (mol) %
m	=	mixture

The EMR value for the individual components of a gas mixture can be calculated according to lit. 3,8,9 using:

$$\text{EMR} = [(n^2-1)/(n+0.4)]\,\frac{M}{\varrho} \qquad [2.12]$$

where:

n	=	refractive index of the gas or liquid (table 2.1.4)	–
M	=	molar mass (table 1.7)	kg/kmol
ϱ	=	density of the gas or liquid (table 2.1.4)	kg/L

For paraffins (C_nH_{2n+2}) the formula below gives good results:

$$\text{EMR} = 2.6495 + 7.0338 \times 10^{-1} \times M + 3.6153 \times 10^{-4} \times M^2 - 1.074 \times 10^{-6} \times M^3 \qquad [2.13]$$

Table 2.1.3 Critical pressure and critical temperature of Groningen natural gas as calculated by the different methods

Method	p_c kPa	T_c K
Kay's Rule	4460	187.0
Formula from lit. 8		201.8
EMR method (lit. 3, 8, 9)	4605	193.4

2.2 Compressibility and supercompressibility

Ideal gases obey the ideal gas law (Boyle's Law and Charles' Law):

$$p \cdot V = n \cdot R_a \cdot T \qquad [2.14]$$

where:

p	= absolute pressure	N/m^2 (= Pa)
V	= volume at p and T	m^3
R_a	= universal gas constant (1.1.5)	J/(mol · K)
T	= absolute gas temperature	K
n	= number of moles	mol

For non-ideal gases, which includes all natural gases, a dimensionless factor z is added to the gas law:

$$p \cdot V = z \cdot n \cdot R_a \cdot T \qquad [2.15]$$

where z is the compressibility factor at p and T

The term "compressibility factor" for the factor z is confusing since z has little to do with compressing a gas. The factor z in fact makes allowances for the deviation from the ideal gas law. The German term "Realgasfaktor" for z is a more appropriate name.

The supercompressibility factor (2.2.1.1) is defined as:

$$F_{pv} = \frac{1}{\sqrt{z}} \qquad [2.16]$$

2.2.1 Compressibility of gas mixtures

In literature, various methods are given for calculating the compressibility factor of a gas mixture. As far as we are aware, there is no one method that can be put forward as being equally accurate for all the different natural gases (lit. 13,30)

Table 2.2.1 lists several frequently applied calculation methods, of which AGA NX–19 is probably the most common, showing the results for Groningen natural gas.

Table 2.2.1 Compressibility factor z for Groningen natural gas (table 1.9) as determined by various methods

Method		101.325 kPa 273.15 K	5000 kPa 288.15 K
NX–19	(2.2.1.1)	0.9977 (44)	0.9117 (83)
BWR	(2.2.1.2)	0.9976 (45)	0.9076 (72)
ISO*	(2.2.1.3)	0.9977 (23)	–
GERG–86	(2.2.1.4)	0.9977 (44)	0.9122 (16)
Edmister	(2.2.1.5)	0.9977 (64)	0.9122 (63)

* Only suitable for an absolute gas pressure of 101.325 kPa

2.2.1.1 PAR Research project NX–19:
Method for calculating z and/or F_{pv} for pure methane and natural gases (lit. 10, 31). This method is not really suitable for users who do not have access to computer facilities. To obviate this problem, the NX–19 formulas are given in graphic form in figs. 2.2.1 to 2.2.3. The results derived from the graphs differ only slightly from the computed results.

Applicable range:
pressure – 100 to 35 000 kPa (1 to 350 bar)
temperature – 233 to 388 K (–40 to 115 °C)
relative density – 0.554 to 1.000
CO_2 content – 0 to 15 % (mol)
N_2 content – 0 to 15 % (mol)

Calculation method:

$$F_p = \frac{156.47}{160.8 - 7.22 \cdot d + n_{CO_2} - 0.392 \cdot n_{N_2}} \text{ (fig. 2.2.1)} \qquad [2.17]$$

$$F_t = \frac{226.29}{99.15 + 211.9 \cdot d - n_{CO_2} - 1.681 \cdot n_{N_2}} \text{ (fig. 2.2.2)} \qquad [2.18]$$

($F_p = F_t = 1$ for $n_{CO_2} = n_{N_2} = 0$ and $d = 0.6$)

$$p_{adj} = \frac{14.503\,76 \cdot p \cdot F_p}{100} \quad (p = \text{absolute pressure in kPa}) \qquad [2.19]$$

$$t_{adj} = 1.8 \cdot T \cdot F_t - 459.67 \quad (T = \text{absolute temperature in K}) \qquad [2.20]$$

$$\pi = \frac{p_{adj} + 14{,}7}{1000} \quad \text{(figs. 2.2.1 and 2.2.3)} \qquad [2.21]$$

$$\tau = \frac{t_{adj} + 459.67}{500} \quad \text{(figs. 2.2.2 and 2.2.3)} \qquad [2.22]$$

$$m = 0.033\,037\,8 \cdot \tau^{-2} - 0.022\,132\,3 \cdot \tau^{-3} + 0.016\,135\,3 \cdot \tau^{-5} \qquad [2.23]$$

$$n = \frac{0.265\,827 \cdot \tau^{-2} + 0.045\,769\,7 \cdot \tau^{-4} - 0.133\,185 \cdot \tau^{-1}}{m} \qquad [2.24]$$

$$B = \frac{3 - m \cdot n^2}{9 \cdot m \cdot \pi^2} \qquad [2.25]$$

$$b = \frac{9 \cdot n - 2 \cdot m \cdot n^3}{54 \cdot m \cdot \pi^3} - \frac{E^{*)}}{2 \cdot m \cdot \pi^2} \qquad [2.26]$$

$$D = \left(b + \sqrt{b^2 + B^3}\right)^{1/3} \qquad [2.27]$$

$$F_{pv} = \frac{\sqrt{\frac{B}{D} - D + \frac{n}{3 \cdot \pi}}}{1 + \frac{0{,}00132}{\tau^{3.25}}} \qquad [2.28]$$

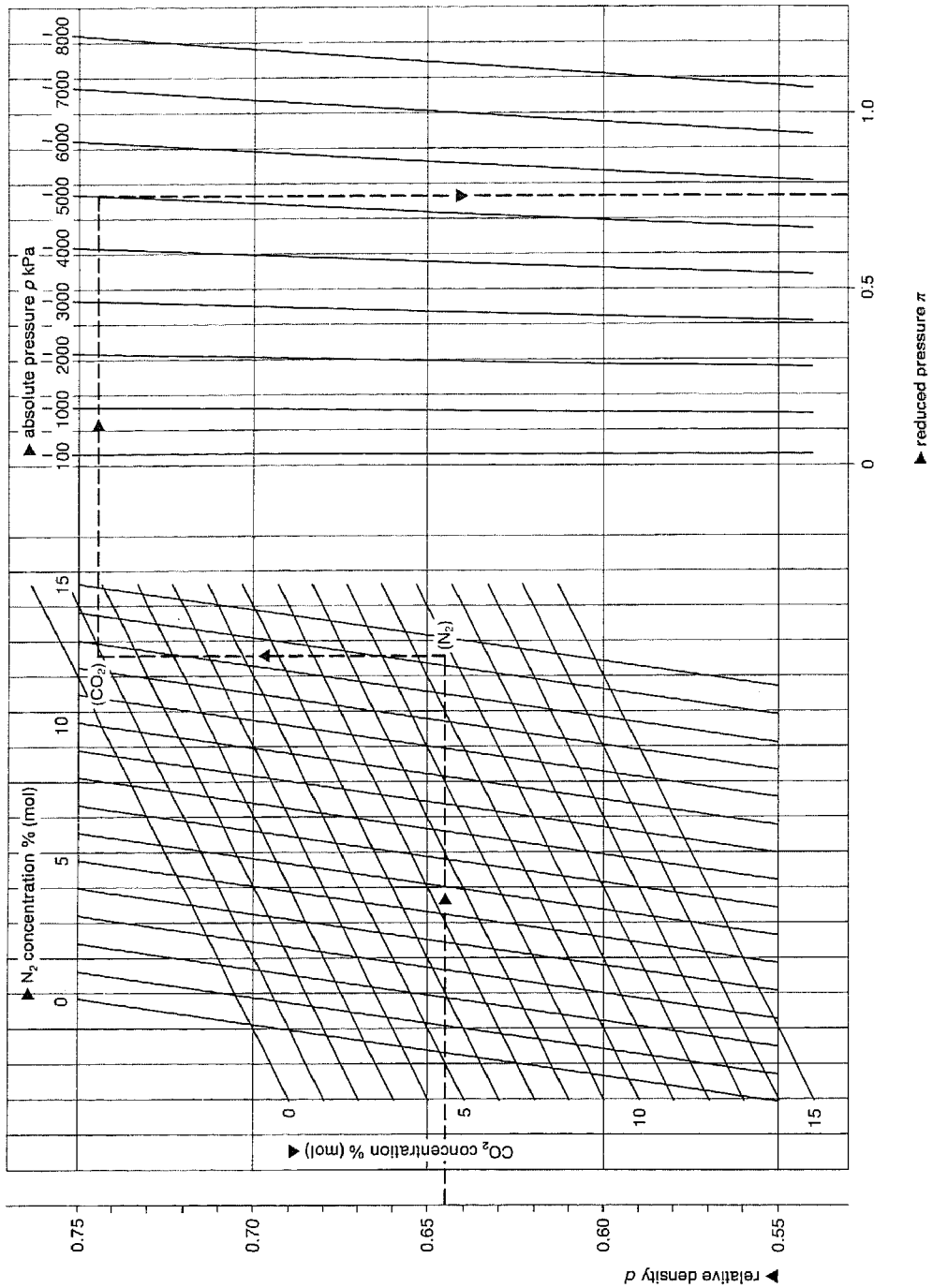
$$z = \frac{1}{F_{pv}^2} \quad \text{(fig. 2.2.3)} \qquad [2.29]$$

*) E is a function of π and τ

where:

d	= relative density	–
n_{CO_2}	= CO_2 concentration in the natural gas	% (mol)
n_{N_2}	= N_2 concentration in the natural gas	% (mol)
p	= absolute pressure (see note below)	kPa
T	= absolute temperature	K

N. B.: According to the AGA NX-19 manual, gauge pressure should be entered in formula [2.19]. In this case however, a modification according to Herning and Wolowsky (lit. 10) is applied, which allows for absolute pressure input in aforesaid formula.


▶ absolute pressure p kPa
100
1000
2000
3000
4000
5000
6000
7000
8000
▶ N2 concentration % (mol)
0
5
10
15
(CO2)
(N2)
CO2 concentration % (mol) ◀
0
5
10
15
0
0.5
1.0
▶ reduced pressure π
0.75
0.70
0.65
0.60
0.55
▶ relative density d

Example: Groningen natural gas (table 1.9)
$T = 288.15$ K (15 °C)
$p = 5000$ kPa (50 bar)
(figs. 2.2.1, 2.2.2 and 2.2.3)
$z = 0.9115$ (calculated value (table 2.2.1): 0.9118)
E for the various ranges of validity:

$1.09 < \tau < 1.4$
$0 < \pi < 2$

$$E_1 = 1 - 0.00075\,\pi^{2.3}\,e^{-20(\tau - 1.09)} - 0.0011\,(\tau - 1.09)^{0.5} \times \pi^2\,[2.17 + 1.4\,(\tau - 1.09)^{0.5} - \pi]^2 \qquad [2.30]$$

$0.84 < \tau < 1.09$
$0 < \pi < 1.3$

$$E_2 = 1 - 0.00075\,\pi^{2.3}\,[2 - e^{-20(1.09 - \tau)}] + - 1.317\,(1.09 - \tau)^4\,\pi\,(1.69 - \pi^2) \qquad [2.31]$$

$0.88 < \tau < 1.09$
$1.3 < \pi < 2.0$

$$E_3 = 1 - 0.00075\,\pi^{2.3}\,[2 - e^{-20(1.09 - \tau)}] + + 0.455\,[200\,(1.09 - \tau)^6 - 0.03249\,(1.09 - \tau) + 2.0167\,(1.09 - \tau)^2 + - 18.028\,(1.09 - \tau)^3 + 42.844\,(1.09 - \tau)^4]\,(\pi - 1.3)\,(1.69 \cdot 2^{1.25} - \pi^2) \qquad [2.32]$$

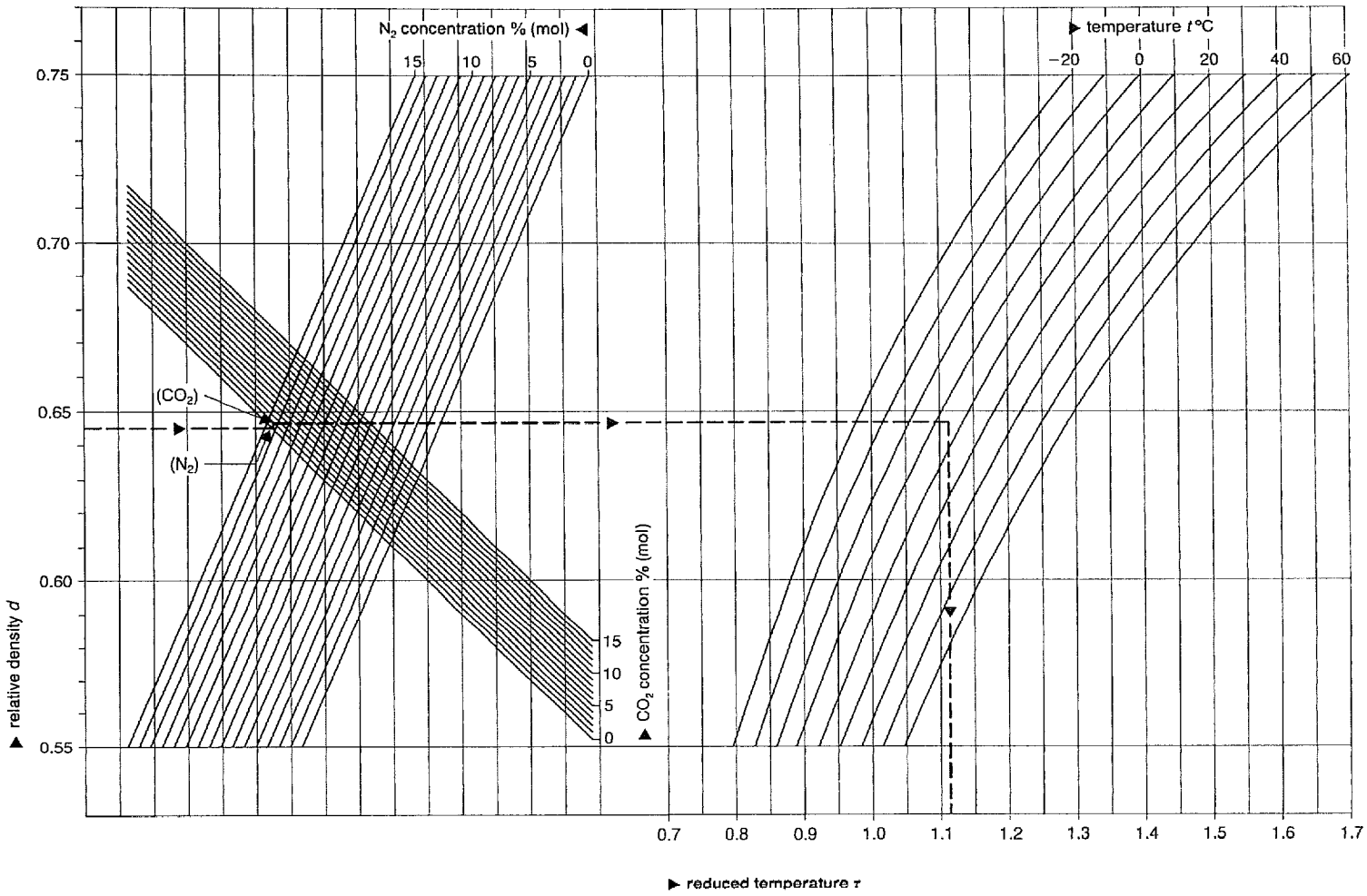
$0.84 < \tau < 0.88$
$1.3 < \pi < 2.0$

E_4 is the same as E_3, except for the last term:

$$(1.69 \cdot 2^{1.25} - \pi^2) \text{ becomes } (1.69 \cdot 2^{[1.25 + 80(0.88 - \tau)^2]} - \pi^2) \qquad [2.33]$$

Fig. 2.2.1 Reduced pressure π for natural gases as a function of the relative density d, the N_2 concentration n_{N_2}, the CO_2 concentration n_{CO_2} and the absolute pressure p

Example: Groningen natural gas (table 1.9)	
$d = 0.645$ $n_{N_2} = 14.32$ % (mol) $n_{CO_2} = 0.89$ % (mol) $p = 5000$ kPa	$\pi = 0.763$ (fig. 2.2.1) $\pi = 0.764$ [2.21]


N2 concentration % (mol)
15
10
5
0
temperature t °C
−20
0
20
40
60
0.75
0.70
0.65
0.60
0.55
(CO2)
(N2)
CO2 concentration % (mol)
15
10
5
0
relative density d
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
reduced temperature τ

$0.84 < \tau < 0.88$
$2.0 < \pi < 5.0$
$E_{5a} = E_4^{*)} - Y$ [2.34]

$0.88 < \tau < 1.09$
$2.0 < \pi < 5.0$
$E_{5b} = E_3^{*)} - Y$ [2.35]

$1.09 < \tau < 1.32$
$2.0 < \pi < 5.0$
$E_{5c} = E_1^{*)} - Y$ [2.36]

*) In this case, calculate E_1, E_3 and E_4 using $\pi = 2$

$1.32 < \tau < 1.40$
$2.0 < \pi < 5.0$
$E_6 = E_{5c} - U$ [2.37]

For E_{5a} to E_{5c} inclusive:

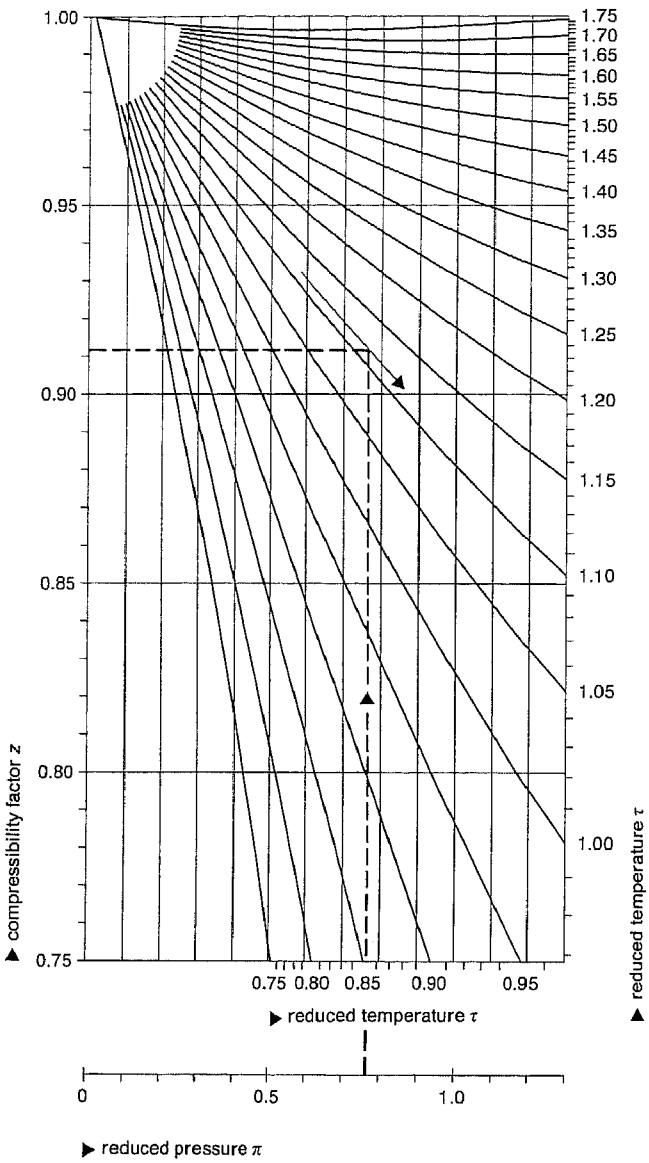
$A = 1.71720 - 2.33123 \cdot \tau - 1.56796 \cdot \tau^2 + 3.47644 \cdot \tau^3 - 1.28603 \cdot \tau^4$ [2.38]
$A_1 = 0.016299 - 0.028094 \cdot \tau + 0.48782 \cdot \tau^2 - 0.728221 \cdot \tau^3 + 0.27839 \cdot \tau^4$ [2.39]
$A_2 = -0.35978 + 0.51419 \cdot \tau + 0.16453 \cdot \tau^2 - 0.52216 \cdot \tau^3 + 0.19687 \cdot \tau^4$ [2.40]
$A_3 = 0.075255 - 0.10573 \cdot \tau - 0.058598 \cdot \tau^2 + 0.14416 \cdot \tau^3 - 0.054533 \cdot \tau^4$ [2.41]
$Y = A(\pi - 2) + A_1(\pi - 2)^2 + A_2(\pi - 2)^3 + A_3(\pi - 2)^4$ [2.42]

For E_6:

$U = (\tau - 1.32)^2 (\pi - 2) [3 - 1.483 (\pi - 2) - 0.10 (\pi - 2)^2 + 0.0833 (\pi - 2)^3]$ [2.43]

Fig. 2.2.2 Reduced temperature τ for natural gases as a function of the relative density d, the N_2 concentration n_{N_2}, the CO_2 concentration n_{CO_2} and the temperature τ

Example: Groningen natural gas (table 1.9)	
$d = 0.645$ $n_{N_2} = 14.32$ % (mol) $n_{CO_2} = 0.89$ % (mol) $T = 288.15$ K (0 °C)	$\tau = 1.113$ (fig. 2.2.2) $\tau = 1.113$ [2.22]


1.00
0.95
0.90
0.85
0.80
0.75
▲ compressibility factor z
1.75
1.70
1.65
1.60
1.55
1.50
1.45
1.40
1.35
1.30
1.25
1.20
1.15
1.10
1.05
1.00
▲ reduced temperature τ
0.75 0.80 0.85 0.90 0.95
▶ reduced temperature τ
0
0.5
1.0
▶ reduced pressure π

Tests have shown that this method produces a "very good" result for pure methane (CH_4) and natural gases with a high N_2 content (up to 18 % (mol)); for natural gases with a high CO_2 content (up to 28 % (mol)) it is "reasonably good" and for natural gases with a high C_2H_6 content (up to 10 % (mol)) and with a high C_3H_8 content (up to 5 % (mol)) it is "not very satisfactory".

Jaeschke and Harbrink (lit. 28) give a method for calculating a correction factor f to NX-19 for high calorific natural gases, the real compressibility factor z_{corr} being given by:

$$z_{corr} = z_{NX\text{-}19} \cdot f \qquad [2.44]$$

where for f they give:

$$\begin{aligned} f = 1 &- 1.233\,507 \times 10^{-8} \cdot p \cdot H_s^3 \cdot d^2 \\ &+ 9.584\,050 \times 10^{-7} \cdot p \cdot T \\ &- 9.218\,982 \times 10^{-10} \cdot p \cdot T \cdot H_s^2 \cdot d^2 \cdot n_{CO_2}^2 \\ &- 1.764\,190 \times 10^{-12} \cdot p \cdot T^2 \cdot H_s^2 \cdot n_{CO_2}^2 \\ &+ 5.449\,614 \times 10^{-12} \cdot p \cdot T^2 \cdot H_s^2 \cdot d \cdot n_{CO_2}^2 \\ &- 1.350\,988 \times 10^{-14} \cdot p \cdot T^2 \cdot H_s^3 \cdot n_{CO_2} \\ &- 7.622\,085 \times 10^{-12} \cdot p^2 \cdot H_s^3 \cdot n_{CO_2} \\ &- 5.433\,670 \times 10^{-9} \cdot p^2 \cdot T \cdot d^2 \\ &+ 1.479\,580 \times 10^{-11} \cdot p^2 \cdot d^2 \cdot n_{CO_2} \cdot T^2 \end{aligned} \qquad [2.45]$$

Fig. 2.2.3 Compressibility factor z for natural gases as a function of the reduced pressure π and the reduced temperature τ

Example: Groningen natural gas (table 1.9)
$\pi = 0.763$ (fig. 2.2.1) $\tau = 1.113$ (fig. 2.2.2) $z = 0.9115$ (fig. 2.2.3) $z = 0.9118$ [2.29]

where:

f	= correction factor		–
p	= absolute pressure		bar
T	= absolute temperature		K
H_s	= gross calorific value (1.4.2)	[3.3]	MJ/m^3
d	= relative density (1.4.3)		–
n_{CO_2}	= CO_2 concentration in the gas		% (mol)

Valid range:

$0 \leq p \leq 90$ bar $0 \leq n_{CO_2} \leq 2.5$ % (mol)
$-10 \leq T \leq 30$ °C $0 \leq n_{N_2} \leq 7$ % (mol)
$39 \leq H_s \leq 47$ MJ/m^3 $0 \leq n_{H_2} \leq 4$ % (mol)
$0.55 \leq d \leq 0.70$

2.2.1.2 BWR

The Benedict-Webb-Rubin equation of state can be used to calculate z for natural gases and for pure gases. This method is only suitable for users having access to computer facilities. Table 2.2.1 gives z values for Groningen natural gas (table 1.9) computed by this method.

Calculation method:

$$p = R_a \cdot T \cdot \varrho + (B_0 \cdot R_a \cdot T - A_0 - C_0 / T^2)\,\varrho^2 + (b \cdot R_a \cdot T - a)\,\varrho^3 + a \cdot \alpha \cdot \varrho^6 + \frac{c \cdot \varrho^3}{T^2}\,(1 + \gamma \cdot \varrho^2)\,e^{-\gamma \cdot \varrho^2} \qquad [2.46]$$

where:

p	= absolute pressure	atm
T	= absolute temperature	K
R_a	= universal gas constant (0.082 06)	atm · L/(mol · K)
ϱ	= density	mol/L

Mixing rules:

$$B_{0,m} = \frac{1}{4}\sum_{i=1}^{n} n_i \cdot B_{0,i} + \frac{3}{4}\sum_{i=1}^{n} n_i \cdot B_{0,i}^{1/3} \times \sum_{i=1}^{n} n_i \cdot B_{0,i}^{2/3} \qquad [2.47]$$

$$A_{0,m} = \left[\sum_{i=1}^{n} n_i \cdot A_{0,i}^{1/2}\right]^2 \qquad [2.48]$$

$$C_{0,m} = \left[\sum_{i=1}^{n} n_i \cdot C_{0,i}^{1/2}\right]^2 \qquad [2.49]$$

$$a_m = \left[\sum_{i=1}^{n} n_i \cdot a_i^{1/3}\right]^3 \qquad [2.50]$$

$$b_m = \left[\sum_{i=1}^{n} n_i \cdot b_i^{1/3}\right]^3 \qquad [2.51]$$

$$c_m = \left[\sum_{i=1}^{n} n_i \cdot c_i^{1/3}\right]^3 \qquad [2.52]$$

$$\alpha_m \quad \left[\sum_{i=1}^{n} n_i \cdot \alpha_i^{1/3}\right]^3 \qquad [2.53]$$

$$\gamma_m = \left[\sum_{i=1}^{n} n_i \cdot \gamma_i^{1/2}\right]^2 \qquad [2.54]$$

where:
n_i = molar fraction of component i
n = number of components
m = mixture.

Table 2.2.2 lists the coefficients for the various components for the BWR equation (lit. 11, 12).

Table 2.2.2 Coefficients for the BWR equation for pure gases

No.	Component	Formula	$A_0 \times 10^{-1}$ *)	$B_0 \times 10$	$C_0 \times 10^{-5}$
1	methane	CH_4	0.18712416	0.43203053	0.23500139
2	ethane	C_2H_6	0.33694517	0.47836255	2.1242566
3	propane	C_3H_8	0.59995798	0.73771408	5.0824370
4	2-methylpropane (isobutane)	C_4H_{10}	0.99391990	1.3149901	9.0456865
5	butane	C_4H_{10}	1.0196945	1.2786628	9.9892910
6	2.2-dimethylpropane	C_5H_{12}	1.29635	1.70530	12.73
7	2-methylbutane (isopentane)	C_5H_{12}	1.3850687	1.7226312	16.060581
8	pentane	C_5H_{12}	1.1961292	1.2292766	17.211571
9	2.2-dimethylbutane	C_6H_{14}	1.1842	1.9214	33.595
10	2.3-dimethylbutane	C_6H_{14}	1.3828	0.9209	18.670
11	3-methylpentane	C_6H_{14}	1.7973	1.7900	18.861
12	2-methylpentane (isohexane)	C_6H_{14}	1.4930	1.729	28.500
13	hexane	C_6H_{14}	1.7242174	2.1381624	32.118381
14	2-methylhexane (isoheptane)	C_7H_{16}	1.5799	1.856	49.530
15	heptane	C_7H_{16}	1.7400941	2.1174513	51.337115
16	octane	C_8H_{18}	2.5770533	3.9840039	75.734303
17	nonane	C_9H_{20}	3.4572536	5.5673163	107.48997
18	decane	$C_{10}H_{22}$	3.9375142	6.1734390	133.85286
19	undecane	$C_{11}H_{24}$			
20	dodecane	$C_{12}H_{26}$			
21	tridecane	$C_{13}H_{28}$			
22	tetradecane	$C_{14}H_{30}$			
23	cyclohexane	C_6H_{12}			
24	methylcyclohexane	C_7H_{14}			
25	benzene	C_6H_6	0.651013	0.503020	34.3016
26	toluene	C_7H_8			
27	xylene (o)	C_8H_{10}			

*) N. B.: the notation $A_0 \times 10^{-1}$ means that the numerical value for A_0 has been multiplied by 10^{-1}, i. e. the r
E. g.: for CH_4, $A_0 = 1.871\ 241\ 6$.

$a \times 10$	$b \times 10^2$	$c \times 10^{-4}$	$\alpha \times 10^4$	$\gamma \times 10^2$	Applicable range	
					Maximum pressure bar	Temperature K
0.69197996	0.39787382	0.30179295	0.96835765	0.57118125	689	165–623
4.3040066	1.2548604	3.6099896	2.1688803	1.0970452	709	264–548
9.3265688	2.4228587	11.187364	4.8673088	1.8911758	689	273–510
23.336257	4.8755556	33.096106	9.9851955	3.4889348	345	244–573
19.385909	4.0737290	32.335018	10.442644	3.3385434	689	310–573
34.905	6.68120	54.6	20	5	320	433–548
31.995467	5.9691011	63.969012	19.622886	5.0483466	213	294–573
47.865495	9.2539518	69.983519	13.043829	4.3925926	689	294–573
101.08	14.000	174.83	21.890	5.6500	–	–
55.238	10.994	85.505	22.759	6.5044	–	–
43.546	8.637	89.829	30.450	7.2131	–	–
74.286	12.15	140	23.5	6.20	400	250–275
72.566978	11.287862	160.71350	26.553281	6.6797489	674	310–573
92.778	16.43	203.14	31.4	7.76	–	–
122.92505	17.644551	277.93572	33.896262	7.9043803	689	311–623
148.23592	16.594366	450.73712	61.241114	10.301145	304	294–569
192.71408	21.684926	657.78328	75.142491	10.770395	689	293–511
244.35467	26.569730	883.88508	101.13456	13.081063	689	311–511
557.047	7.66343	117.652	7.00159	2.93016	–	–

ıe value for A_0 is 10 × as great.

No.	Component	Formula	$A_0 \times 10^{-1}$ *)	$B_0 \times 10$	$C_0 \times 10^{-5}$	a
28	methyl mercaptan	CH_3SH				
29	ethyl mercaptan	C_2H_5SH				
30	propyl mercaptan	C_3H_7SH				
31	carbonyl sulphide	COS				
32	hydrogen sulphide	H_2S	0.37652960	0.52078546	2.0278814	
33	sulphur dioxide	SO_2	0.212054	0.261827	7.93879	
34	ethene	C_2H_4	0.333958	0.556833	1.31140	
35	propene	C_3H_6	0.611220	0.850647	4.39182	
36	1-butene	C_4H_8	0.895325	1.16025	9.27280	
37	1-pentene	C_5H_{10}	1.105967	1.279227	13.88744	
38	1,2-butadiene	C_4H_6				
39	1-butyne	C_4H_6				
40	methanol	CH_3OH				
41	ethanol	C_2H_5OH				
42	argon	Ar	0.0823417	0.22282597	0.1314125	
43	helium	He	0.0040962	0.23661	0.00000162	
44	carbon dioxide	CO_2	0.18367101	0.32014927	1.7602805	
45	carbon monoxide	CO	0.12211169	0.45809483	0.07683175	
46	hydrogen	H_2	0.02099032	0.2361049	0.00051116	
47	nitrogen	N_2	0.12654834	0.47170114	0.04836143	
48	oxygen	O_2	0.09508520	0.00000035	0.32643518	
49	nitric oxide	NO	0.25441140	0.39458452	1.4794968	
50	nitrogen dioxide	NO_2				
51	water vapour	H_2O				
52	air (dry)	–				

*) N. B.: the notation $A_0 \times 10^{-1}$ means that the numerical value for A_0 has been multiplied by 10^{-1}, i. e. the real value
E. g.: for CH_4, $A_0 = 1.871\ 241\ 6$.

$a \times 10$	$b \times 10^2$	$c \times 10^{-4}$	$\alpha \times 10^4$	$\gamma \times 10^2$	Applicable range	
					Maximum pressure bar	Temperature K
2.5665687	0.63514110	2.9086082	0.52722820	0.45739050	689	277–411
84.4395	1.46542	11.3362	0.719604	0.592390	–	–
2.59000	0.8600	2.1120	1.78000	0.923000	–	–
7.74056	1.87059	10.2611	4.55696	1.82900	–	–
16.9270	3.48156	27.4920	9.10889	2.95945	–	–
22.62858	4.228689	45.37675	12.19270	3.594533	–	–
0.288558	0.215269	0.07982437	0.5558895	0.23382711	500	160–600
–0.0057339	–0.00001973	–0.00000055	–0.072673	0.077942	–	–
2.4204855	0.62536078	1.9008120	0.48784066	0.42808218	608	273–523
0.23439776	0.21683496	0.073332301	2.0968189	0.67019093	785	273–473
0.00502886	0.05531	281.1889	2.113289	0.3507597	–	–
0.23094543	0.25483185	0.05775574	0.98032114	0.52104571	689	77–423
1.62689940	0.358834736	1.28273741	–39270.58894	3.01	71	300–1000
1.6774177	0.51001644	1.5946	0.25559433	0.48129414	–	–

ue for A_0 is 10 × as great.

2.2.1.3 ISO

According to ISO 6976 – 1983 (E) (lit. 2), the compressibility factor z for gas mixtures can be calculated for an absolute pressure of 101.325 kPa and T K by the formula:

$$z = 1 - \left[\sum_{i=1}^{n} \frac{n_i\sqrt{b_i}}{100}\right]^2 + 0.0005\left[\frac{2 \cdot n_{H_2}}{100} - \left(\frac{n_{H_2}}{100}\right)^2\right] \qquad [2.55]$$

where:

n	=	number of components	–
n_i	=	concentration of component i	% (mol)
n_{H_2}	=	concentration of H_2	% (mol)
$\sqrt{b_i}$	=	summation factor ($=\sqrt{(1-z_i)}$)*) [2.56] for component i (table 2.2.5)	–
z_i	=	compressibility factor z for component i at temperature T K (table 2.2.5), z_i being calculated using the API formula [2.64]	–

*) With the exception of CO_2 and He, for which pseudo-values are given.

Table 2.2.3 Compressibility factor z of Groningen natural gas (table 1.9) according to ISO 6976

Component	Formula	n_i % (mol)	$\sqrt{b_i}$ (table 2.2.5)	$n_i\sqrt{b_i}$
methane	CH_4	81.29	0.049 0	3.983 210
ethane	C_2H_6	2.87	0.101 5	0.291 305
propane	C_3H_8	0.38	0.153 0	0.058 140
butane	C_4H_{10}	0.15	0.211 2	0.031 680
pentane	C_5H_{12}	0.04	0.261 0	0.010 440
hexane	C_6H_{14}	0.05	0.331 7	0.016 585
nitrogen	N_2	14.32	0.022 4	0.320 768
oxygen	O_2	0.01	0.031 6	0.000 316
carbon dioxide	CO_2	0.89	0.067 0	0.059 630
		100.00		4.772 074

$z = 1 - (4.772\,074/100)^2 = 0.997\,723$ (table 2.2.1)

2.2.1.4 GERG

Amsterdam University's Van der Waals Laboratory was commissioned by GERG (4.2) to develop an equation of state from literature data and test data of member countries, which will enable the compressibility factor z of gas mixtures to be accurately calculated from pressure, temperature and composition (report 8410–3; October 1984):

$$z = 1 + \frac{1}{V} \sum_{i=j=1}^{13} B_{ij} \cdot n_i \cdot n_j + \frac{1}{V^2} \sum_{i=j=k=1}^{13} C_{ijk} \cdot n_i \cdot n_j \cdot n_k \qquad [2.56a]$$

where:

V	= molar volume	L/mol
n_i	= mole fraction of component i	–
n_j	= mole fraction of component j	–
n_k	= mole fraction of component k	–

Valid range:

temperature:	0 – 40 °C
absolute pressure:	≤ 80 bar

The virial coefficients B_{ij} and C_{ijk} are a function of temperature only and are calculated from:

B_{ij}	= $A + B \cdot T + C \cdot T^2$	L/mol
C_{ijk}	= $A + B \cdot T + C \cdot T^2$	L^2/mol^2

where:

T	= temperature of gas mixture	K

Table 2.2.3.1 Constants for the virial coefficient $B_{ij} = A + B \cdot T + C \cdot T^2$

i, j	A	B	C
1.1	−.305530 E+0	.138050 E−2	−.167430 E−5
1.2	−.162897 E+0	.723055 E−3	−.796055 E−6
1.3	−.377721 E+0	.161771 E−2	−.190044 E−5
1.4	−.534311 E+0	.228510 E−2	−.270302 E−5
1.5	−.144562 E+0	.921030 E−3	−.135212 E−5
1.6	−.808030 E+0	.362500 E−2	−.455555 E−5
1.8	−.133598 E+1	.650241 E−2	−.857077 E−5
1.10	−.148583 E+1	.694054 E−2	−.866938 E−5
1.11	−.775140 E+0	.184050 E−2	−.400000 E−6
1.12	−.209989 E+1	.979707 E−2	−.125373 E−4
1.13	−.239409 E+1	.112199 E−1	−.143976 E−4
2.2	−.144600 E+0	.740910 E−3	−.911950 E−6
2.3	−.191944 E+0	.666407 E−3	−.537698 E−6
2.4	−.412214 E+0	.203558 E−2	−.270693 E−5
2.5	−.237582 E−1	.179302 E−3	−.194991 E−6
2.6	−.442660 E−0	.204986 E−2	−.261400 E−5
3.3	−.868340 E−0	.403760 E−2	−.516570 E−5
3.4	−.901431 E−0	.431802 E−2	−.577366 E−5
3.6	−.126372 E+1	.584661 E−2	−.747500 E−5
3.8	−.188108 E+1	.926431 E−2	−.124525 E−4
3.10	−.202135 E+1	.954081 E−2	−.121639 E−4
4.4	−.107320 E+1	.464810 E−2	−.560520 E−5
4.5	+.266450 E−2	−.102765 E−3	+.374149 E−6
4.6	−.142020 E+1	.575230 E−2	−.640000 E−5
4.8	−.283644 E+1	.136800 E−1	−.181244 E−4
4.10	−.331426 E+1	.152019 E−1	−.189007 E−4
5.5	−.175160 E−2	.849590 E−4	−.103660 E−6
6.6	−.259920 E+1	.119650 E−1	−.152910 E−4
6.8	−.435393 E+1	.213786 E−1	−.287483 E−4
7.7	−.130820 E+0	.602540 E−3	−.644300 E−6
8.8	−.708016 E+1	.363100 E−1	−.503829 E−4
9.9	+.206740 E−1	−.513060 E−4	+.724000 E−7
10.10	−.111580 E+2	.535740 E−1	−.684970 E−4

Table 2.2.3.2 Constants for the virial coefficient $C_{ijk} = A + B \cdot T + C \cdot T^2$

i, j, k	A	B	C
1.1.1	.110140 E−1	−.492640 E−4	.683960 E−7
1.1.2	.950336 E−2	−.446604 E−4	.646311 E−7
1.1.3	.921537 E−2	−.326297 E−4	.384277 E−7
1.1.4	.471391 E−2	.131521 E−4	−.450064 E−7
1.1.5	.252725 E−2	−.904332 E−5	.115616 E−7
1.1.6	.145768 E−1	−.278502 E−4	0
1.1.8	.692768 E−1	−.214852 E−3	0
1.1.10	.892362 E−1	−.272925 E−3	0
1.2.2	.866892 E−2	−.424907 E−4	.635102 E−7
1.2.3	.900338 E−2	−.355487 E−4	.467680 E−7
1.2.4	.449508 E−2	.530233 E−6	−.152576 E−7
1.2.5	.360589 E−2	−.145437 E−4	.204722 E−7
1.2.6	−.187767 E−1	.142145 E−3	−.221855 E−6
1.3.3	.637108 E−2	−.747903 E−5	−.643736 E−8
1.3.4	−.176574 E−2	.597684 E−4	−.123785 E−6
1.3.6	−.623055 E−1	.459485 E−3	−.733765 E−6
1.4.4	−.180009 E−1	.187768 E−3	−.344478 E−6
1.4.5	−.116095 E−2	.263812 E−4	−.512600 E−7
1.4.6	−.992498 E−1	.713458 E−3	−.114420 E−5
1.4.8	−.992498 E−1	.713458 E−3	−.114420 E−5
1.4.10	−.992498 E−1	.713458 E−3	−.114420 E−5
1.5.5	.113514 E−2	−.101196 E−5	−.316717 E−9
1.6.6	−.107132 E+0	.711300 E−3	−.107919 E−5
2.2.2	.784980 E−2	−.398950 E−4	.611870 E−7
2.2.3	.776648 E−2	−.333367 E−4	.470391 E−7
2.2.4	.473374 E−2	−.715042 E−5	.165190 E−8
2.2.5	.335086 E−2	−.147638 E−4	.220414 E−7
2.2.6	−.139981 E−1	.106230 E−3	−.162413 E−6
2.3.3	.570471 E−2	−.127157 E−4	.865358 E−8
2.3.4	−.768174 E−5	.385226 E−4	−.817506 E−7
2.3.5	.269108 E−2	−.596904 E−5	.540142 E−8
2.3.6	−.301719 E−1	.222387 E−3	−.350693 E−6
2.4.4	−.113332 E−1	.123463 E−3	−.225648 E−6
2.4.5	−.297743 E−3	.168641 E−4	−.330680 E−7

Constants for the virial coefficient $C_{ijk} = A + B \cdot T + C \cdot T^2$

i, j, k	A	B	C
2.4.6	–.506529 E – 1	.363400 E – 3	–.577241 E – 6
2.5.5	.106796 E – 2	–.252397 E – 5	.310904 E – 8
2.6.6	–.844178 E – 1	.557418 E – 3	–.835447 E – 6
3.3.3	.205130 E – 2	.348880 E – 4	–.837030 E – 7
3.3.4	–.109855 E – 1	.133800 E – 3	–.252624 E – 6
3.3.5	.430967 E – 3	.160191 E – 4	–.345955 E – 7
3.3.6	–.594074 E – 1	.430798 E – 3	–.691157 E – 6
3.4.4	–.313527 E – 1	.284509 E – 3	–.508173 E – 6
3.4.5	–.516317 E – 2	.579276 E – 4	–.105347 E – 6
3.4.6	–.944235 E – 1	.671721 E – 3	–.108080 E – 5
3.5.5	.522574 E – 4	.693387 E – 5	–.136454 E – 7
3.6.6	–.149820 E + 0	.994385 E – 3	–.152037 E – 5
4.4.4	–.621000 E – 1	.508050 E – 3	–.885260 E – 6
4.4.5	–.185994 E – 1	.163195 E – 3	–.284869 E – 6
4.4.6	–.144234 E + 0	.101275 E – 2	–.163277 E – 5
4.5.5	–.370635 E – 2	.390658 E – 4	–.684792 E – 7
4.6.6	–.216734 E + 0	.143604 E – 2	–.221182 E – 5
5.5.5	–.932310 E – 5	.283770 E – 5	–.507540 E – 8
6.6.6	–.270290 E + 0	.171040 E – 2	–.250010 E – 5
7.7.7	.190870 E – 2	.420040 E – 5	–.156800 E – 7
9.9.9	–.779620 E – 2	.491760 E – 4	–.774240 E – 7

Table 2.2.3.3 Components for which formula [2.56a] is valid

i,j,k	Component number (table 1.7)	Component	Range % (mol)
1	1	CH_4	≥ 50
2	47, 48, 42	N_2, O_2, Ar	≤ 50
3	44, 34	CO_2, C_2H_4	≤ 30
4	2	C_2H_6	≤ 20
5	46	H_2	≤ 10
6	3, 35	C_3H_8, C_3H_6	≤ 5
7	45	CO	≤ 3
8	4, 5	C_4H_{10}, C_4H_{10}	≤ 1.5
9	43	He	≤ 0.5
10	6, 7, 8, 25, –	C_5H_{12}, C_5H_{12}, C_5H_{12}, C_6H_6, C_5H_{10}*)	≤ .5
11	12, 13, 23, 27	C_6H_{14}, C_6H_{14}, C_6H_{12}**, C_8H_{10}	
12	14, 15, 26	C_7H_{16}, C_7H_{16}, C_7H_8	
13	16, 17, 18	C_8H_{18}, C_9H_{20}, $C_{10}H_{22}$	

*) C_5H_{10} (cyclopentane): Not available in this work

**) C_6H_{12} (cyclohexane)

This program is only suitable for users having access to computer facilities. To enable all users to produce the same compressibility factors, the constants used for calculation of the virial coefficients B_{ij} and C_{ijk} have been listed in tables 2.2.3.1 and 2.2.3.2. Table 2.2.3.3 gives the valid components and concentration range for formula [2.56a]

For Groningen gas (table 1.9), the program gives (table 2.2.1):

z = 0.997 7(44) (101.325 kPa; 273.15 K)

z = 0.912 2(16) (5000 kPa; 288.15 K)

2.2.1.5 Edmister

Edmister (lit. 18 b) gives a method (after Pitzer) for calculating the compressibility factor z for both gas mixtures and pure gases. Where one of the equations is implicit, the use of a computer is essential.

$$B = b_1 - b_2/T_r - b_3/T_r^2 - b_4/T_r^3 \quad [2.57]$$

$$C = c_1 - c_2/T_r + c_3/T_r^3 \quad [2.58]$$

$$D = d_1 + d_2/T_r \quad [2.59]$$

$$V_r = T_r/p_r\,(1 + B/V_r + C/V_r^2 + D/V_r^5 + + \frac{c_4}{T_r^3 \cdot V_r^2}(\beta + \gamma/V_r^2)\,e^{-\gamma/V_r^2}) \quad [2.60]$$

$$z = p_r \cdot V_r/T_r \quad [2.61]$$

where:

b, c, d, β, γ and ω are constants (table 2.2.4)

T_r	= reduced temperature (= T/T_c)	[2.66]	–
T	= temperature of the gas mixture		K
T_c	= (pseudo-) critical temperature (2.1.1)		K
p_r	= reduced pressure (= p/p_c)	[2.65]	–
p	= pressure of the gas mixture		kPa
p_c	= (pseudo-) critical pressure (2.1.1)		kPa

The above equations have to be applied twice, once using the constants for the so-called simple fluids (table 2.2.4) and once using the constants for the reference fluid (table 2.2.4). In both cases, the same values for T_r and p_r apply.

The two solutions obtained therefore yield a z^o value for simple fluids and a z^r value for the reference fluid, from which the value of z is given by:

$$z = z^o + \frac{\omega}{\omega^r}(z^r - z^o) \quad [2.62]$$

where:

z^o = compressibility factor for simple fluids –

z^r = compressibility factor for the reference fluid –

ω = acentric factor, which for mixtures is:

$$\omega = \sum_{i=1}^{n} \frac{n_i \cdot \omega_i}{100} \qquad [2.63]$$ –

ω_i = acentric factor for component i (table 2.2.5) –

n = number of components –

n_i = concentration of component i % (mol)

ω^r = 0.397 8 (table 2.2.4) –

Table 2.2.4 Constants for the Pitzer calculation model

	"Simple fluids"	"Reference fluid" (octane)
b_1	0.118 119 3	0.202 657 9
b_2	0.265 728	0.331 511
b_3	0.154 790	0.027 655
b_4	0.030 323	0.203 488
c_1	0.023 674 4	0.031 338 5
c_2	0.018 698 4	0.050 361 8
c_3	0.0	0.016 901
c_4	0.042 724	0.041 577
$d_1 \times 10^4$	0.155 488	0.487 36
$d_2 \times 10^4$	0.623 689	0.074 033 6
β	0.653 92	1.226
γ	0.060 167	0.037 54
ω^r		0.397 8*)

*) Table 2.2.5 gives ω^r = 0.4018 (octane)

2.2.2 Compressibility of pure gases

2.2.2.1 API

For hydrocarbons and non-polar gases, the compressibility factor z can be calculated using (lit. 5, 6):

$$z = 1 + p_r \cdot T_r^{-1}(0.1445 + 0.073 \cdot \omega) - (0.330 - 0.46 \cdot \omega)\, T_r^{-1} - (0.1385 + 0.50 \cdot \omega)\, T_r^{-2} - (0.0121 + 0.097 \cdot \omega)\, T_r^{-3} - 0.0073 \cdot \omega \cdot T_r^{-8}) \quad [2.64]$$

where:

p_r	= reduced pressure (= p/p_c)	[2.65]	–
p	= absolute pressure		kPa
p_c	= critical pressure (table 1.7)		kPa
T_r	= reduced temperature (= T/T_c)	[2.66]	–
T	= absolute temperature		K
T_c	= critical temperature (table 1.7)		K
ω	= acentric factor (lit. 5, 12) (table 2.2.5)		–

This formula is presented graphically in figs. 2.2.4 to 2.2.6 inclusive (see example). Table 2.2.5 gives values for z for a number of pure gases.

To a limited extent, the API formula can also be used for gas mixtures. The mixture values for the acentric factor, the pseudo-critical pressure and pseudo-critical temperature then have to be substituted. For Groningen natural gas (table 1.9) this formula yields the following values for z (compare with figures from table 2.2.1)

$z = 0.997\,7(03)$ (101.325 kPa; 273.15 K)

$z = 0.906\,5(17)$ (5000 kPa; 28815 K)

2.2.2.2 DIN

Lit. 14 describes the method according to DIN for calculating the compressibility factor z for pure gases at 273.15 K and 101.325 kPa:

$z = 1 + p \cdot B_n$ (table 2.2.5) [2.67]

where:

p = 1.013 25 bar (101.325 kPa)

B_n = virial coefficient.

The virial coefficient is known for a small number of gases only (lit 14) (table 2.2.5)

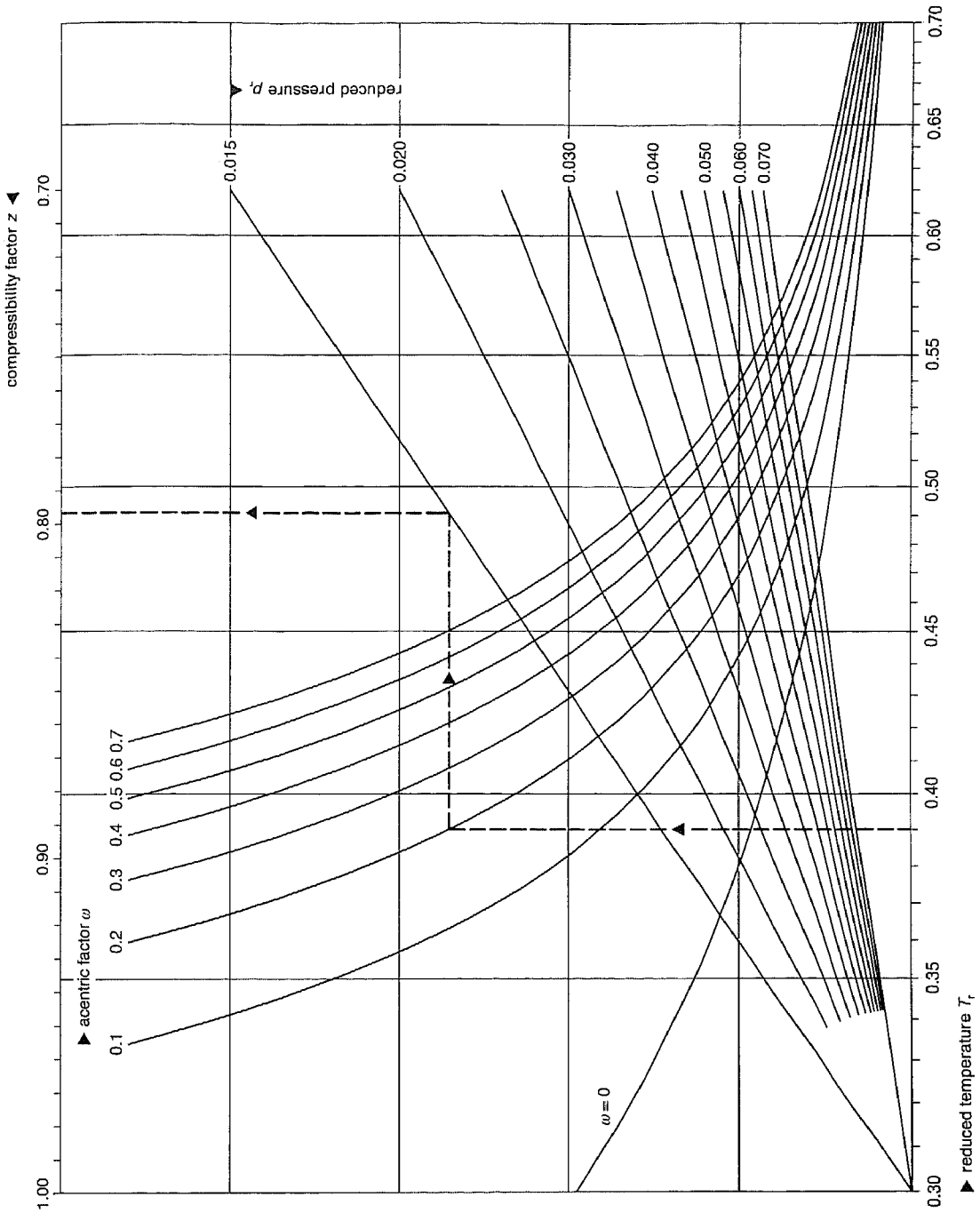


Fig. 2.2.4 Compressibility factor z for pure gases as a function of reduced pressure p_r, reduced temperature T_r and acentric factor ω ($0.30 \leq T_r \leq 0.70$)

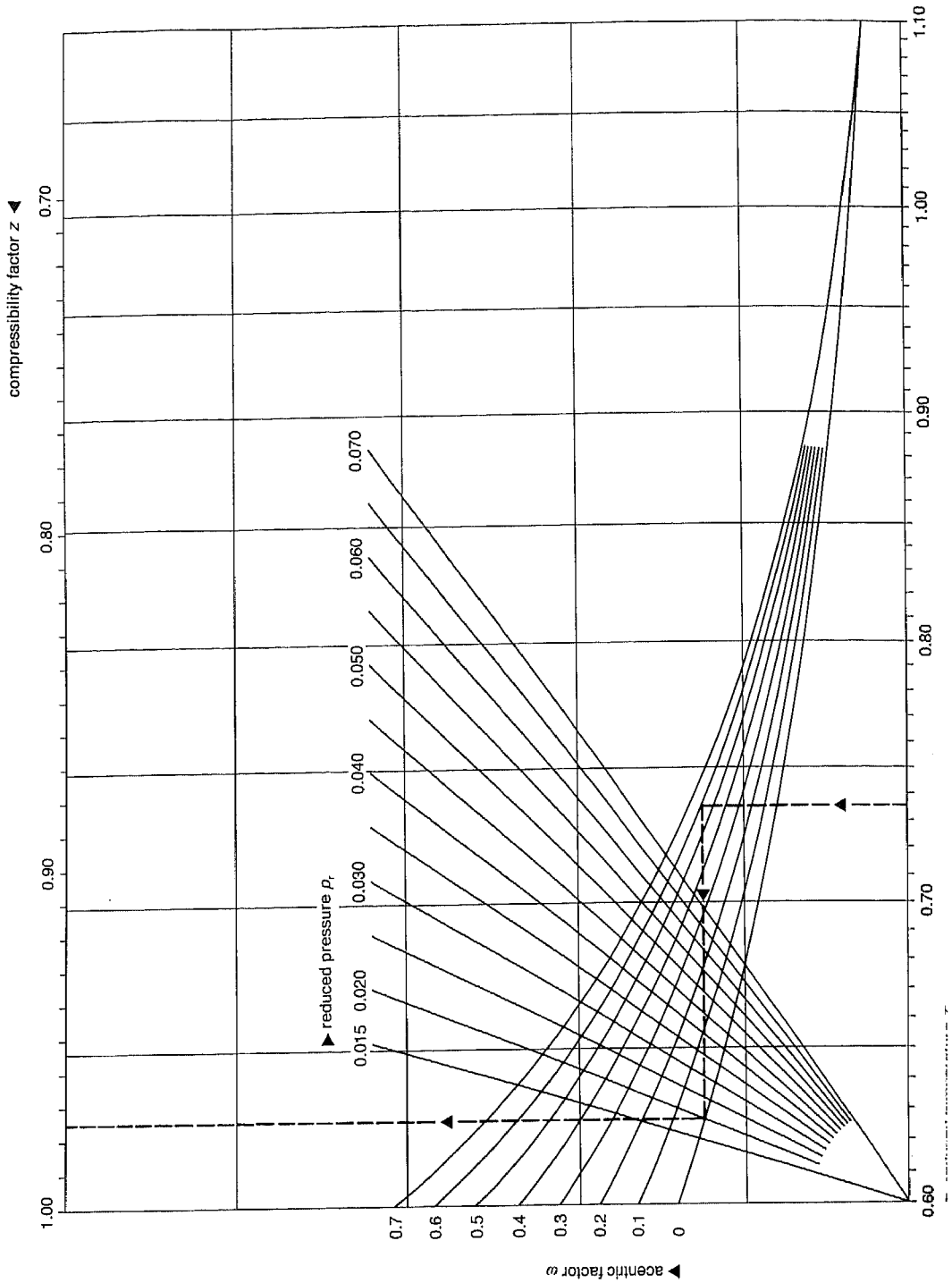


Fig. 2.2.5 Compressibility factor z for pure gases as a function of reduced pressure p_r, reduced temperature T_r and acentric factor ω ($0.60 \leq T_r \leq 1.10$)

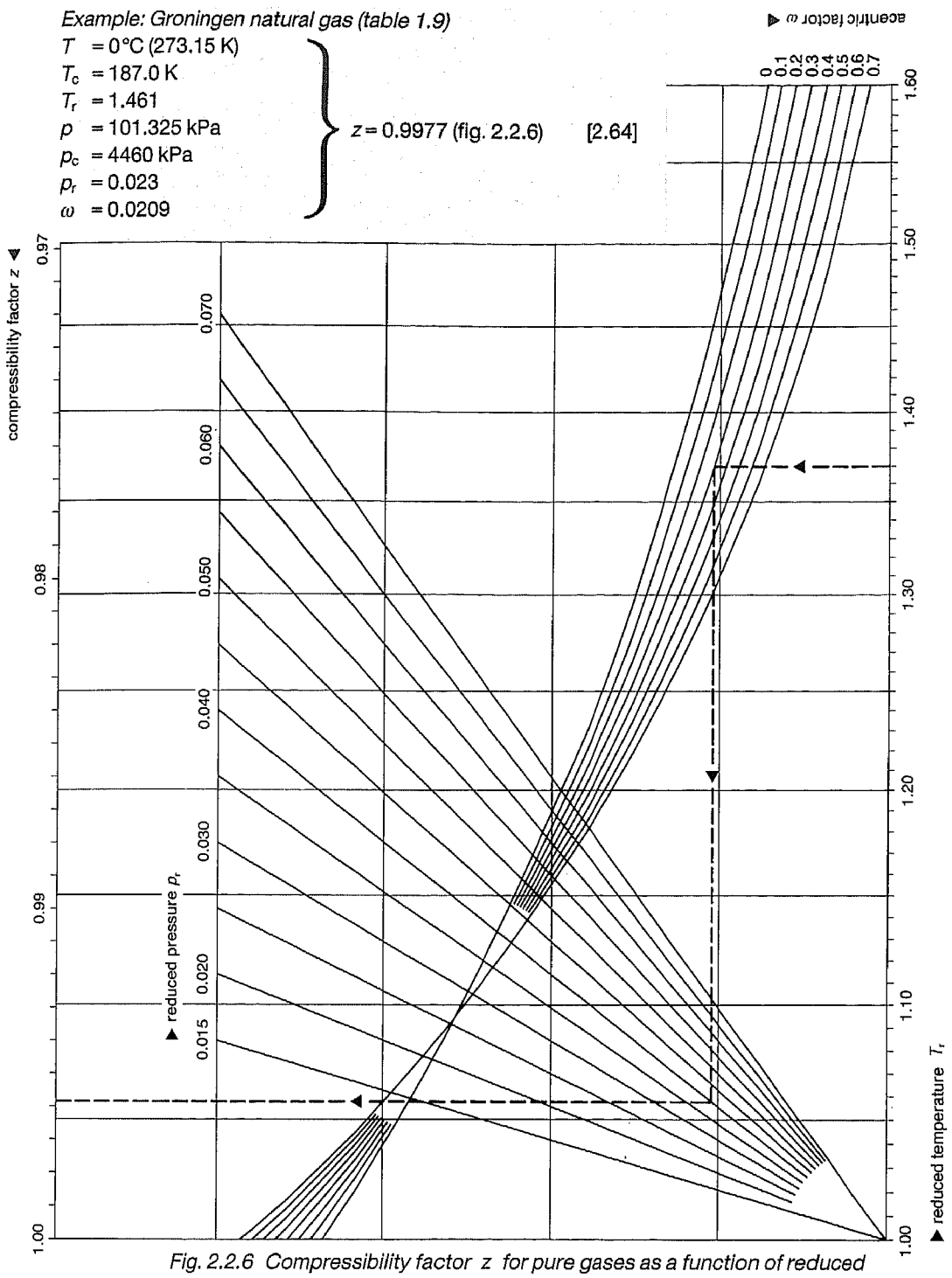


Fig. 2.2.6 Compressibility factor z for pure gases as a function of reduced pressure p_r, reduced temperature T_r and acentric factor ω ($1.00 \leq T_r \leq 1.60$)

Table 2.2.5 Compressibility factor z, summation factor $\sqrt{b}$, acentric factor ω and virial coefficient B_n of 52 pure gases at 273.15 K and 101.325 kPa

No.	Component	Formula	ISO 6976		API		DIN	
			Compressibility factor z	Summation factor $\sqrt{b}=\sqrt{(1-z)}$	Acentric factor ω	Compressibility factor z	Virial coefficient $B_n \times 10^3$	Compressibility factor z
1	methane	CH_4	0.9976	0.0490	0.0104	0.9976	− 2.4	0.9976
2	ethane	C_2H_6	0.9897	0.1015	0.0986	0.9899	− 9.5	0.9901
3	propane	C_3H_8	0.9766	0.1530	0.1524	0.9784	−21	0.9783
4	2-methylpropane (isobutane)	C_4H_{10}	0.9583	0.2042	0.1848	0.9644	−35	0.9645
5	butane	C_4H_{10}	0.9554	0.2112	0.2010	0.9601	−40	0.9595
6	2,2-dimethylpropane	C_5H_{12}	0.9496	0.2245	0.1969	0.9496		
7	2-methylbutane (isopentane)	C_5H_{12}	0.9394	0.2462	0.2223	0.9394		
8	pentane	C_5H_{12}	0.9319	0.2610	0.2539	0.9319		0.937*)
9	2,2-dimethylbutane	C_6H_{14}	0.9153	0.2910	0.2369	0.9153		
10	2,3-dimethylbutane	C_6H_{14}	0.9072	0.3046	0.2495	0.9072		
11	3-methylpentane	C_6H_{14}	0.9002	0.3159	0.2741	0.9001		
12	2-methylpentane (isohexane)	C_6H_{14}	0.9010	0.3146	0.2825	0.9009		
13	hexane	C_6H_{14}	0.8900	0.3317	0.3007	0.8898		0.915*)
14	2-methylhexane (isoheptane)	C_7H_{16}	0.8459	0.3926	0.3336	0.8458		
15	heptane	C_7H_{16}	0.8285	0.4141	0.3498	0.8282		0.870*)
16	octane	C_8H_{18}	0.7372	0.5126	0.4018	0.7371		0.848*)
17	nonane	C_9H_{20}			0.4455	0.6129		
18	decane	$C_{10}H_{22}$			0.4885	0.4389		
19	undecane	$C_{11}H_{24}$			0.5129	0.2360		
20	dodecane	$C_{12}H_{26}$			0.5573	–		
21	tridecane	$C_{13}H_{28}$			0.6026	–		
22	tetradecane	$C_{14}H_{30}$			0.6420	–		
23	cyclohexane	C_6H_{12}	0.8977	0.3198	0.2133	0.8974		

24	methylcyclohexane	C_7H_{14}	0.8481	0.3897	0.2567	0.8479		
25	benzene	C_6H_6	0.9090	0.3017	0.2125	0.9089		0.959*)
26	toluene	C_7H_8	0.8487	0.33901	0.2596	0.8477		0.937*)
27	xylene (o)	C_8H_{10}			0.3023	0.7430		0.892*)
28	methyl mercaptan	CH_3SH			0.155	0.9722		
29	ethyl mercaptan	C_2H_5SH			0.190	0.9521		
30	propyl mercaptan	C_3H_7SH			0.207	0.9175		
31	carbonyl sulphide	COS			0.099	0.9844		0.9849*)
32	hydrogen sulphide	H_2S	0.9884	0.1077	0.100	0.9899	− 9.8	0.9901
33	sulphur dioxide	SO_2			0.246	0.9790	−24	0.9757
34	ethene	C_2H_4			0.0868	0.9924	− 7.6	0.9923
35	propene	C_3H_6			0.1405	0.9811	−18	0.9818
36	1-butene	C_4H_8			0.1906	0.9644	−36	0.9635
37	1-pentene	C_5H_{10}			0.241	0.9389		
38	1,2-butadiene	C_4H_6			0.2485	0.9588		
39	1-butyne	C_4H_6			0.280	0.9521		
40	methanol	CH_3OH			0.559	0.9571		
41	ethanol	C_2H_5OH			0.635	0.9171		
42	argon	Ar	0.9990	0.0316	−0.004	0.9991	−0.95	0.9990
43	helium	He	1.0005	−0.016	−0.387	1.0009	0.52	1.0005
44	carbon dioxide	CO_2	0.9932	0.0670	0.231	0.9930	−6.6	0.9933
45	carbon monoxide	CO	0.9993	0.0265	0.093	0.9995	−0.64	0.9994
46	hydrogen	H_2	1.0006	–	0.000	1.0010	0.61	1.0006
47	nitrogen	N_2	0.9995	0.0224	0.045	0.9996	−0.45	0.9995
48	oxygen	O_2	0.9990	0.0316	0.019	0.9990	−0.97	0.9990
49	nitric oxide	NO			0.607	0.9994	−1.05	0.9989
50	nitrogen dioxide	NO_2			0.86	0.9727		
51	water vapour**)	H_2O	0.968	0.179	0.348	0.9443		0.955*)
52	air (dry)	–	0.9994	–	0.040***)	0.9994	−0.59	0.9994

*) Lit. 14
**) Polar; for H_2O: $z = 0.965\,0$ (calculated from the H_2O molar volume from table 1.7)
***) Weighted average calculated from N_2 and O_2

2.3 Thermal conductivity

The thermal conductivity of a gas mixture λ is a function of pressure and temperature (lit. 12, 15). The change with temperature is practically linear. The simplest method of determining thermal conductivity is given in lit. 15, where λ is made up of two components:

$\lambda_{t,1}$ = thermal conductivity at t °C and 101.325 kPa (fig. 2.3.1) W/(m · K)
$\lambda_{t,p}$ = thermal conductivity at t °C and p kPa (table 2.3) W/(m · K)
φ = $\lambda_{t,p}/\lambda_{t,1}$ [2.60]: ratio reflecting the gas pressure (fig. 2.3.2) –

From $\lambda_{t,1}$ (fig. 2.3.1) and φ (fig. 2.3.2) it is possible to calculate $\lambda_{t,p}$ (= $\varphi \cdot \lambda_{t,1}$). This method is valid for gas mixtures having N_2 and/or CO_2 concentrations up to 35 % (mol).

Example: Groningen natural gas (table 1.9)

t = 15 °C
M = 18.637 kg/kmol } $\lambda_{t,1}$ = 0.0299 W/(m · K) (fig. 2.3.1)
p_c = 4460 kPa
$\lambda_{t,p} = \varphi \cdot \lambda_{t,1}$ W/(m · K) (table 2.3)

Table 2.3 Thermal conductivity of Groningen natural gas

Absolute pressure p kPa	$p_r = p/p_c$	φ *)	$\lambda_{t,p}$ W/(m · K)
100	0.022	1.002	0.0300
1 000	0.224	1.027	0.0307
2 000	0.448	1.061	0.0317
3 000	0.673	1.093	0.0327
4 000	0.897	1.122	0.0335
5 000	1.121	1.14	0.0341
6 000	1.345	1.20	0.0359
7 000	1.570	1.24	0.0371
8 000	1.794	1.28	0.0383
9 000	2.018	1.37	0.0410
10 000	2.242	1.44	0.0431

*) Fig. 2.3.2

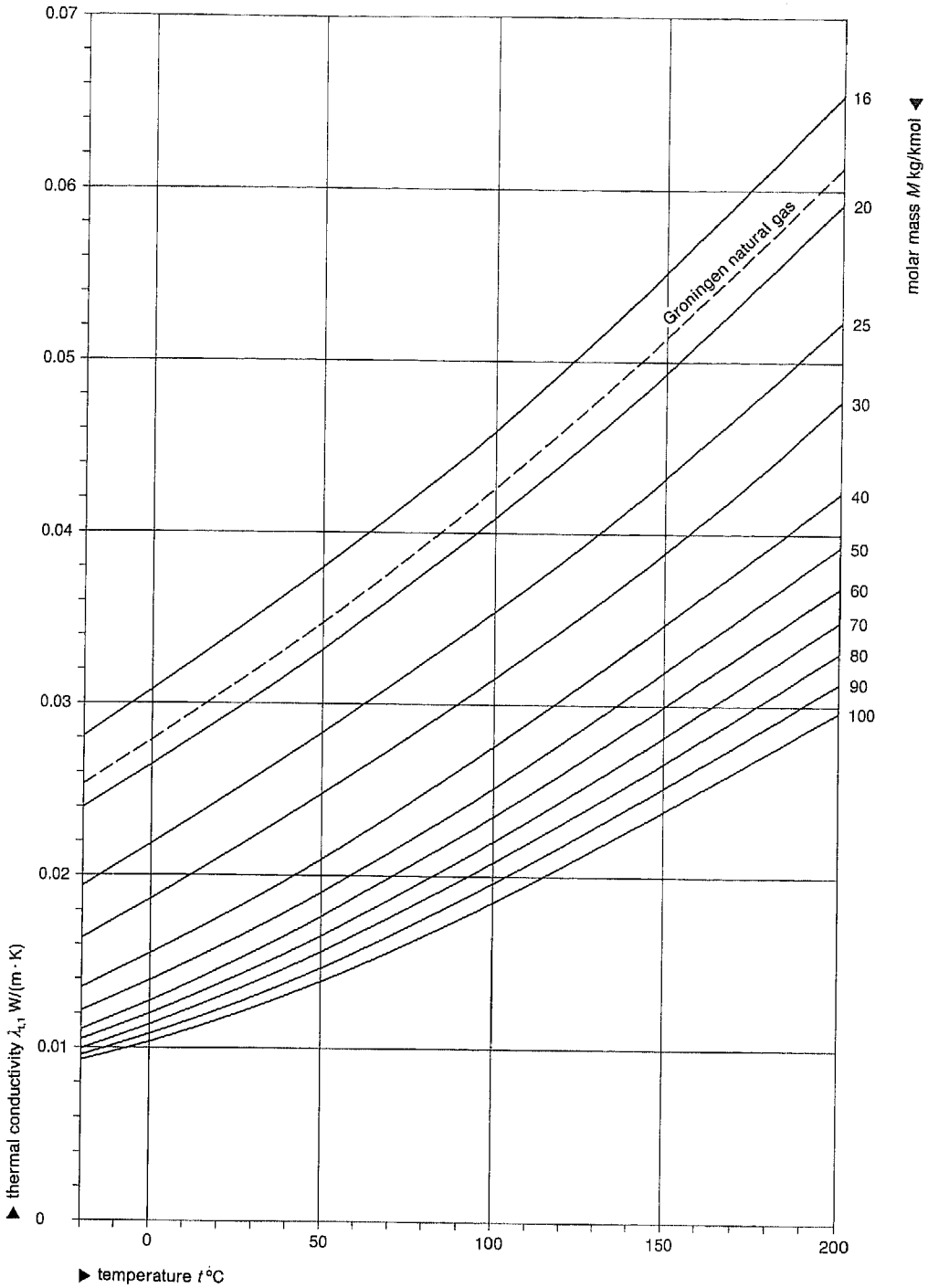


Fig. 2.3.1 Thermal conductivity $\lambda_{t,1}$ for gases as a function of gas temperature t and molar mass M

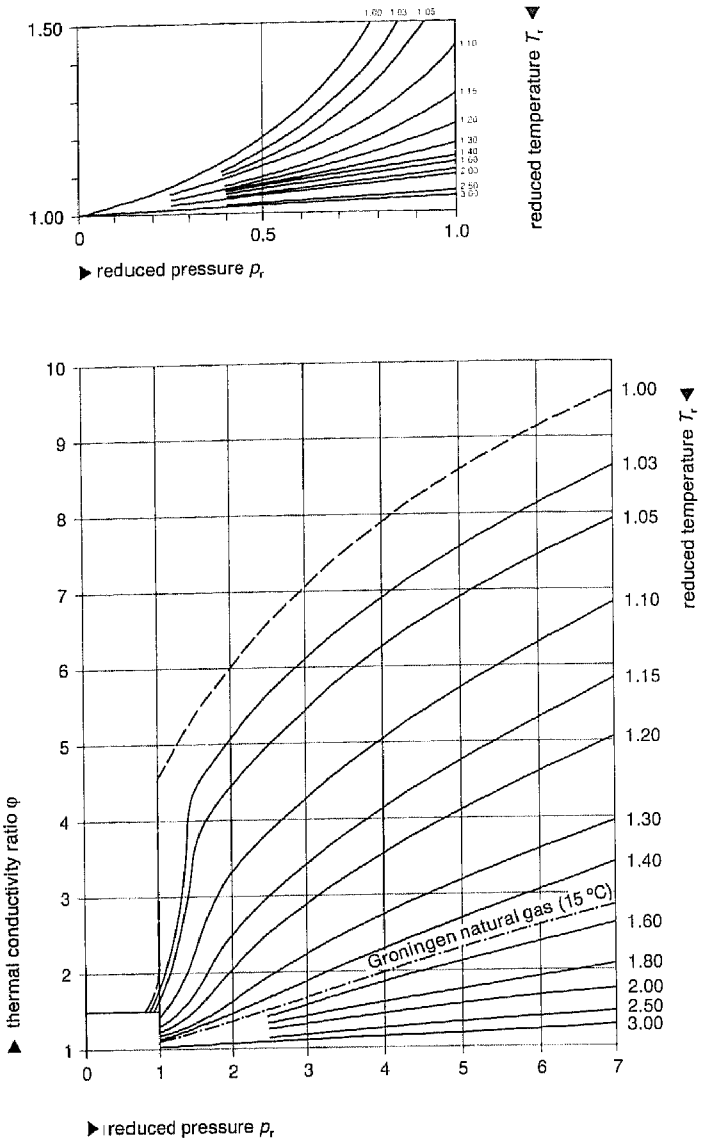


Fig. 2.3.2 Thermal conductivity ratio φ for gases as a function of the reduced pressure p_r and the reduced temperature T_r

2.4 Density

The density ϱ of a non-ideal gas or gas mixture can be determined using the formula:

$$\varrho = \frac{p \cdot M}{z \cdot R_a \cdot T} \qquad [2.69]$$

where:

ϱ	= density at p, T	kg/m³
p	= absolute pressure	kPa
z	= compressibility factor (2.2)	–
R_a	= universal gas constant (1.1.5)	kJ/(kmol · K)
T	= absolute temperature	K
M	= molar mass	kg/kmol

Fig. 2.4 provides a means of determining ϱ graphically. The accuracy is reasonably good (see example). The conversion from operating conditions (p_1, T_1) to normal conditions (101.325 kPa; 273.15 K) is performed by means of the formula:

$$\varrho_0 = \varrho_1 \frac{p_0}{p_1} \frac{T_1}{T_0} \frac{z_1}{z_0} \qquad [2.70]$$

where:
index 0 = normal conditions (101.325 kPa; 273.15 K)
index 1 = operating conditions (p_1, T_1)

ϱ	= density at p, T	kg/m³
p	= absolute pressure of the gas	kPa
T	= absolute temperature of the gas	K
z	= compressibility factor (2.2)	–

In ISO 6976 – 1983 (lit. 2), the density of a gas mixture is calculated at 101.325 kPa and T_v K from the ideal density and the compressibility factor z of the mixture (2.2.1.3) using the formula:

$$\varrho[V(T_v; 101.325)] = \frac{T_0 \sum_{i=1}^{n} n_i \cdot M_i}{100 \cdot V_m \cdot z \cdot T_v} \qquad [2.71]$$

where:

$\varrho[V(T_v; 101.325)]$	= density at 101.325 kPa and T_v K	kg/m^3
T_o	= normal temperature (1.1.4)	K
T_v	= temperature of the mixture	K
V_m	= normal molar volume (1.1.3)	m^3/kmol
z	= compressibility factor at 101.325 kPa and T_v K (2.2.1.3)	–
n	= number of components	–
n_i	= concentration of component i	% (mol)
M_i	= molar mass of component i	kg/kmol

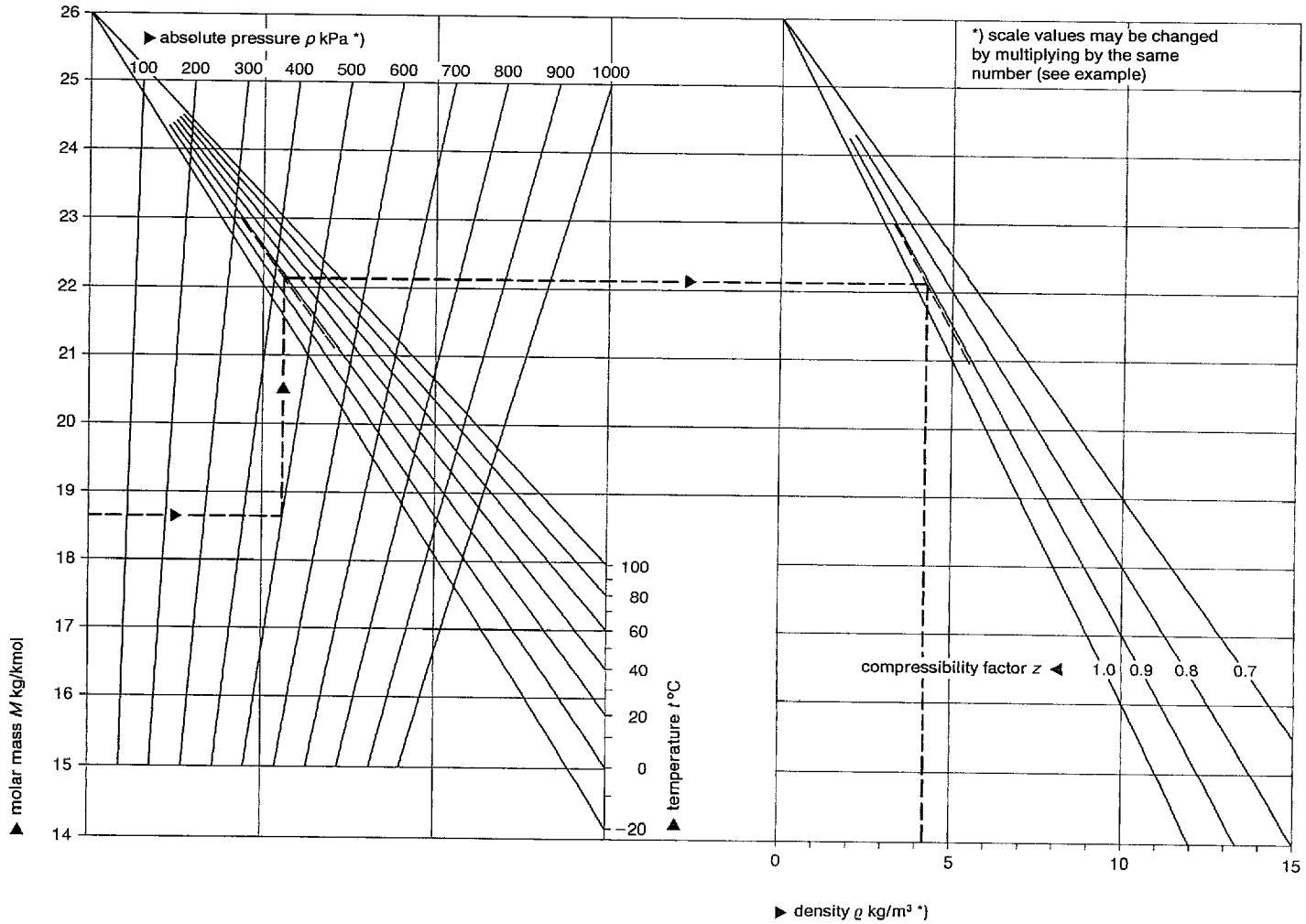
This formula is absolutely identical with the aforementioned formula [2.70] for ϱ.

Fig. 2.4 Density ϱ for gases as a function of the molar mass M, the compressibility factor z, the absolute pressure p and the temperature t

Example: Groningen natural gas (table 1.9)

p = 5000 kPa (= 10 × 500 kPa)
T = 288.15 K (15 °C)
z = 0.9117 (figs. 2.2.1 to 2.2.3)
M = 18.637 kg/kmol

$\varrho = 10 \times 4.26 = 42.6$ kg/m^3 (fig. 2.4)
$\varrho = 42.66$ kg/m^3 [2.69]


▶ absolute pressure p kPa *)
100 200 300 400 500 600 700 800 900 1000
*) scale values may be changed by multiplying by the same number (see example)
▲ molar mass M kg/kmol
26 25 24 23 22 21 20 19 18 17 16 15 14
▲ temperature t °C
100 80 60 40 20 0 −20
compressibility factor z ◀ 1.0 0.9 0.8 0.7
0 5 10 15
▶ density ϱ kg/m³ *)

2.5 Viscosity

2.5.1 Dynamic (absolute) viscosity

2.5.1.1 Herning-Zipperer method (lit. 5, 12, 15) for gas mixtures at 101.325 kPa and temperature T.

Of a number of methods for calculating the dynamic viscosity of a gas mixture, the method put forward by Herning and Zipperer appears to be most convenient. Deviations from test results are commonly less than 3 %. For gas mixtures containing a "large amount" of hydrogen, the following constraints apply:

$n_{H_2} < 10$ % (mol) – within margin of error for normal measurement

$n_{H_2} > 25$ % (mol) – not sufficiently accurate

$$\mu_{t,1} = \frac{\sum_{i=1}^{n} n_i \cdot \mu_i \sqrt{M_i}}{\sum_{i=1}^{n} n_i \sqrt{M_i}} \qquad [2.72]$$

where:

$\mu_{t,1}$ =	dynamic viscosity of the gas mixture at t °C and 101.325 kPa	Pa · s
μ_i =	dynamic viscosity of component i at t °C and 101.325 kPa (2.5.1.3)	Pa · s
n_i =	concentration of component i	% (mol)
M_i =	molar mass of component i	kg/kmol
n =	number of components	–

2.5.1.2 Method according to Carr, Kobayashi and Burrows (lit. 15) for gas mixtures at 101.325 kPa and temperature t °C.

Fig. 2.5.1 (lit. 15) gives $\mu_{t,1}$ at t °C and 101.325 kPa as a function of the molar mass M of the gas mixture. Originally, this figure was only suitable for mixtures of hydrocarbons, but by the introduction of corrections for the presence of N_2, CO_2 and H_2S – see inserted graph in fig. 2.5.1 – it becomes possible to use the graph for all natural gases.

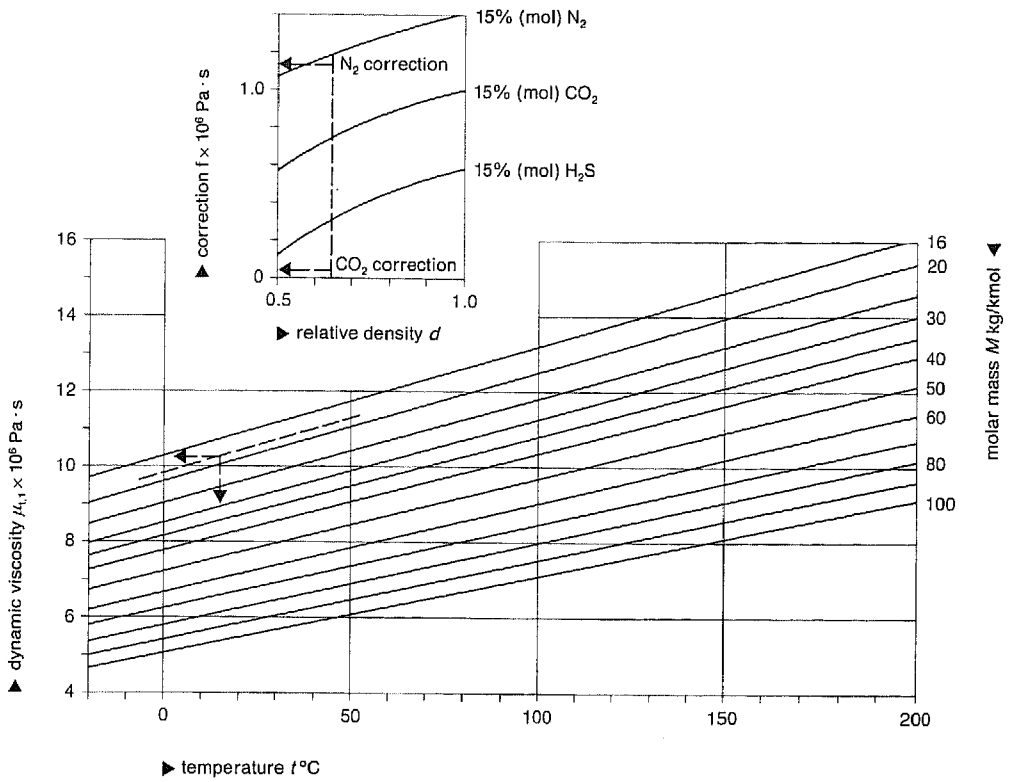


Fig. 2.5.1 Dynamic viscosity $\mu_{t,1}$ for gases as a function of the temperature t and the molar mass M. Inserted a correction factor for the presence of N_2, CO_2 and H_2S

Example: Groningen natural gas (table 1.9)	
t = 15 °C M = 18.637 kg/kmol d = 0.645 N_2 = 14.32 % (mol) CO_2 = 0.89 % (mol)	$\mu_{t,l}$ = 10.25×10^{-6} Pa · s N_2-corr = 1.13×10^{-6} Pa · s CO_2-corr = 0.04×10^{-6} Pa · s $\mu_{t,l}$ = 11.42×10^{-6} Pa · s

2.5.1.3 Method according to Chapman and Cowling (lit. 5, 12) for pure gases at 101.325 kPa and T K

Lit. 5 and 12 give a method for calculating μ for pure gases:

$$\mu = 2.669 \times 10^{-6} \frac{(M \cdot T)^{0.5}}{\sigma^2 \cdot \Omega_v} \qquad [2.73]$$

where:

μ	=	dynamic viscosity at T K and 101.325 kPa	Pa · s
M	=	molar mass (table 1.7)	kg/kmol
T	=	absolute temperature	K
σ	=	Lennard-Jones "collision diameter" (table 2.5)	Å
Ω_v	=	"collision integral" for viscosity (lit. 5) (figs. 2.5.2 to 2.5.4)	–

The value for Ω_v is obtained from figs. 2.5.2 to 2.5.4, in which Ω_v is given as a function of $k \cdot T/\varepsilon$
Table 2.5 gives values for ε/k and σ for the various components (lit. 5, 12) Although the values for these terms as calculated according to lit. 5 and lit. 12 do not always agree very well, these discrepancies are not reflected in the calculated values for the viscosity μ. It therefore makes no difference which set of formulas is used.

Lit. 5:

$$\frac{k \cdot T}{\varepsilon} = \frac{T_r}{65.3 \cdot z_c^{3.6}} \qquad [2.74]$$

$$\sigma = 1.8617 \frac{V_c^{0.333}}{z_c^{1.2}} \qquad [2.75]$$

$$\Omega_v^{-1} = \sum_{i=1}^{7} A_i \left(\ln 10 \frac{k \cdot T}{\varepsilon} \right)^i \qquad [2.76]$$

$A_1 = 9.142\,636\,2 \times 10^{-1}$
$A_2 = -1.068\,936$
$A_3 = 6.807\,779\,7 \times 10^{-1}$
$A_4 = -2.120\,867\,7 \times 10^{-1}$
$A_5 = 3.448\,718\,6 \times 10^{-2}$
$A_6 = -2.818\,822\,5 \times 10^{-3}$
$A_7 = 9.159\,034\,2 \times 10^{-5}$

Lit. 12:

$$\frac{k \cdot T}{\varepsilon} = \frac{T_r}{0.7915 + 0.1693 \cdot \omega} \qquad [2.77]$$

$$\sigma = \left(\frac{101.325 \cdot T_c}{p_c}\right)^{1/3} (2.3551 - 0.087 \cdot \omega) \qquad [2.78]$$

$$\Omega_v = \frac{1.161\,45}{\left(\frac{k \cdot T}{\varepsilon}\right)^{0.14874}} + \frac{0.524\,87}{e^{0.773\,20 \frac{k \cdot T}{\varepsilon}}} + \frac{2.161\,78}{e^{2.437\,87 \frac{k \cdot T}{\varepsilon}}} \qquad [2.79]$$

where:

T_r	=	reduced temperature (= T/T_c)	–
T	=	temperature of the gas	K
T_c	=	critical temperature (table 1.7)	K
z_c	=	critical compressibility $\left(= \frac{p_c \cdot V_c}{R_a \cdot T_c}\right)$ [2.80]	–
p_c	=	critical pressure (table 1.7)	kPa
V_c	=	critical volume (table 1.7)	m^3/kmol
R_a	=	universal gas constant (1.1.5)	kJ/(kmol · K)
ω	=	acentric factor (table 2.2.5)	–
ε/k	=	Lennard-Jones potential parameter	K

For comparison purposes, table 2.5 gives calculated values together with values from literature

2.5.1.4 Dynamic viscosity at pressure p and temperature T

Fig. 2.5.5 shows the effect of pressure on the viscosity of a gas mixture (lit. 15), according to the formula:

$$\mu_{t,p} = m \cdot \mu_{t,1} \qquad [2.81]$$

where:

$\mu_{t,p}$	=	dynamic viscosity at t °C and p kPa	Pa · s
m	=	ratio of $\mu_{t,p}$ and $\mu_{t,1}$ (pressure effect) (fig. 2.5.5)	–
$\mu_{t,1}$	=	dynamic viscosity at t °C and 101.325 kPa	Pa · s

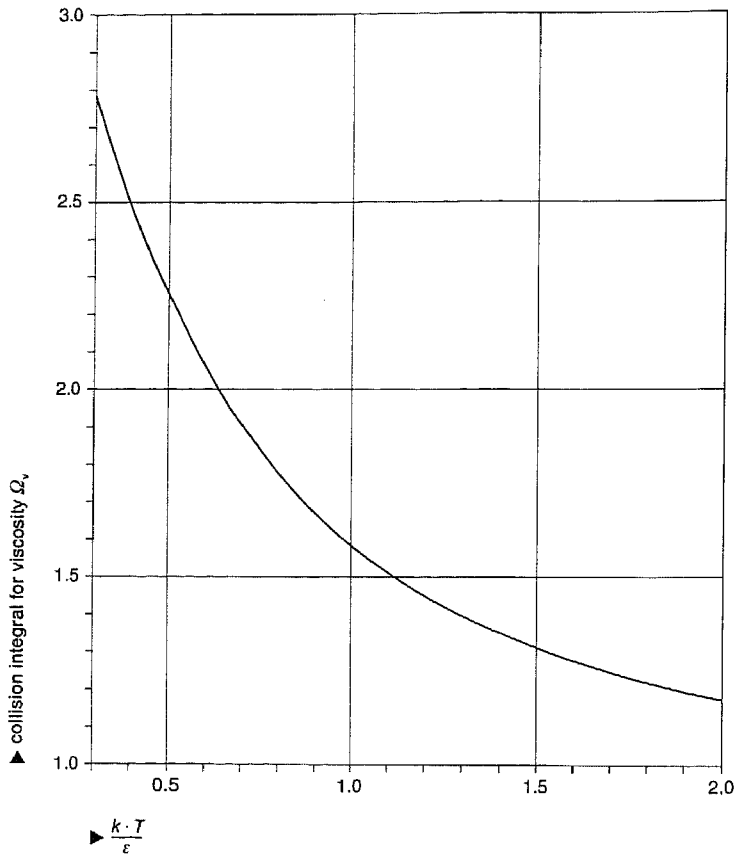


Fig. 2.5.2 The collision integral Ω_v as a function of the Lennard-Jones potential parameter ε/k and the absolute temperature T

$(0.3 \leqslant \frac{k \cdot T}{\varepsilon} \leqslant 2.0)$

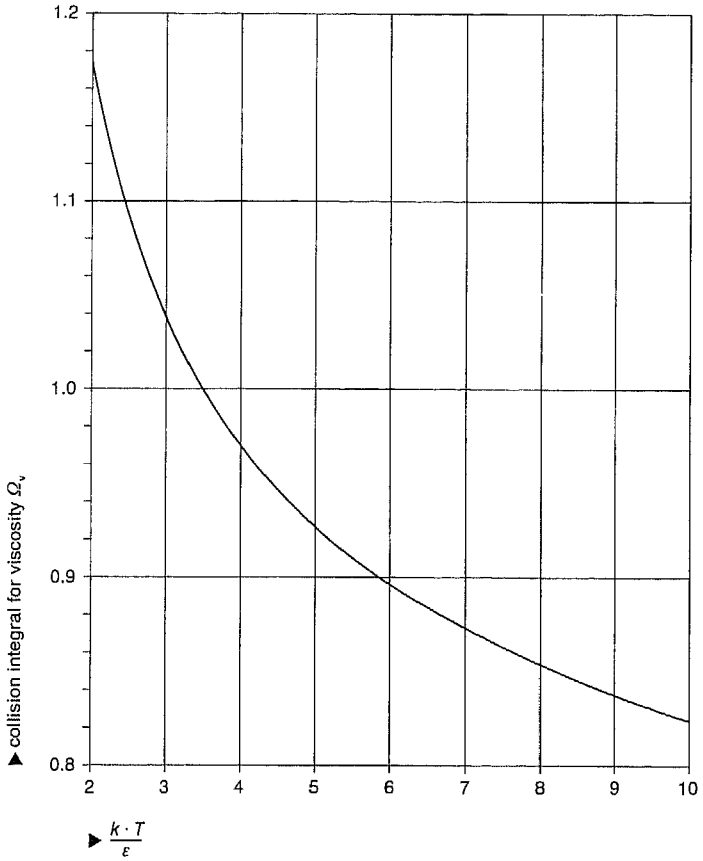


Fig. 2.5.3 The collision integral Ω_v as a function of the Lennard-Jones potential parameter ε/k and the absolute temperature T

$(2 \leq \frac{k \cdot T}{\varepsilon} \leq 10)$

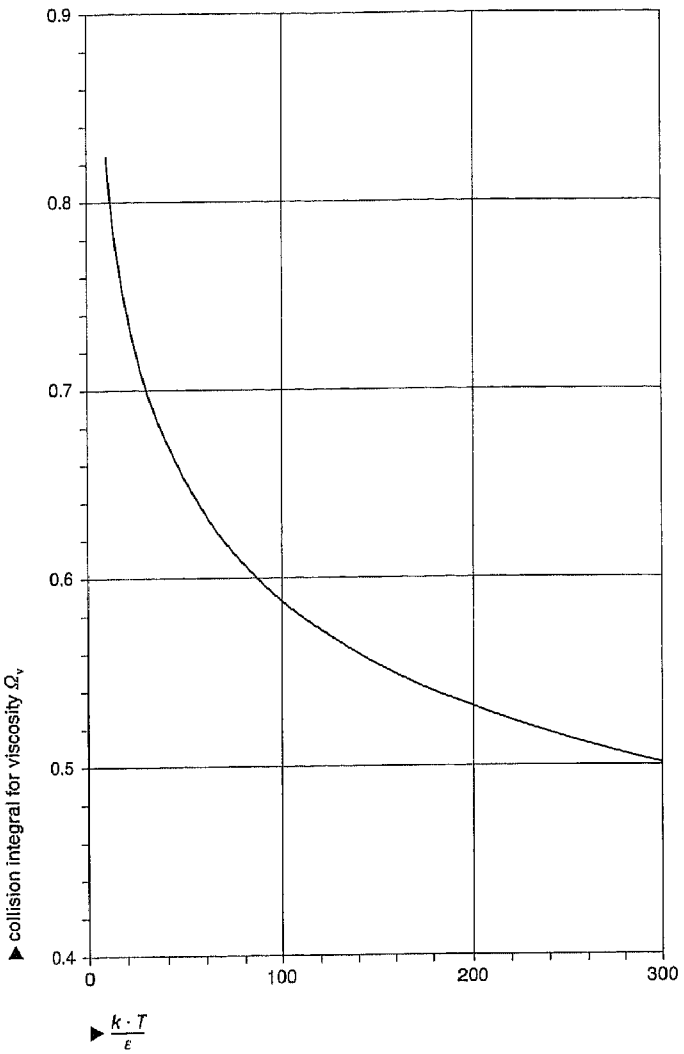


Fig. 2.5.4 The collision integral Ω_v as a function of the Lennard-Jones potential parameter ε/k and the absolute temperature T

$(10 \leqq \frac{k \cdot T}{\varepsilon} \leq 300)$

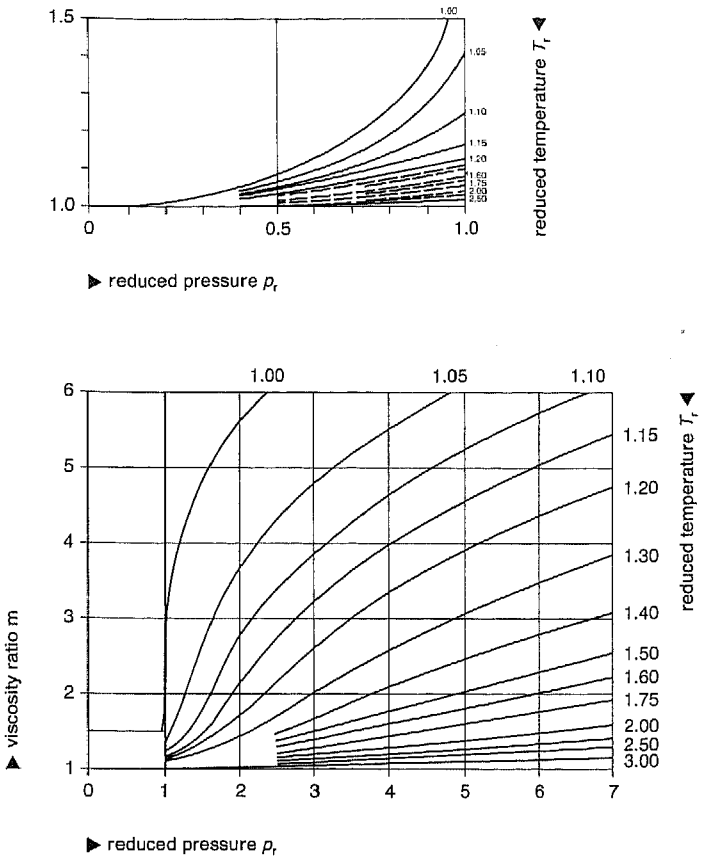


Fig. 2.5.5 The viscosity ratio m as a function of the reduced pressure p_r and the reduced temperature T_r

Example: Groningen natural gas (table 1.9)	
T = 288.15 K (15 °C) T_c = 187.0 K	$T_r = 1.54$
p = 5000 kPa p_c = 4460 kPa	$p_r = 1.12$
m = 1.10 (fig. 2.5.5) $\mu_{t,1}$ = 11.42×10^{-6} Pa·s (fig. 2.5.1) $\mu_{t,p}$ = $m \cdot \mu_{t,1} = 12.56 \times 10^{-6}$ Pa·s	

Table 2.5 Comparison between calculated values and literature values

No.	Component	Formula	ε/k				σ Å (Ångstrom)			
			API		Reid e.a.		API		Reid e.a.	
			Calculated	lit. 5	Calculated	lit. 12	Calculated	lit. 5	Calculated	lit. 12
1	methane	CH_4	140.9	140	151.2	148.6	3.839	3.808	3.797	3.758
2	ethane	C_2H_6	217.4	236	246.8	215.7	4.444	4.384	4.343	4.443
3	propane	C_3H_8	250.2	206	302.3	237.1	5.022	5.240	4.838	5.118
4	2-methylpropane (isobutane)	C_4H_{10}	283.2	217	335.8	330.1	5.428	5.819	5.254	5.278
5	butane	C_4H_{10}	262.7	208	351.0	531.4	5.585	5.869	5.253	4.687
6	2,2-dimethylpropane	C_5H_{12}	250.8	223	357.8	193.4	6.047	4.92	5.600	6.464
7	2-methylbutane (isopentane)	C_5H_{12}	273.4	–	381.8	–	6.013	–	5.602	–
8	pentane	C_5H_{12}	247.0	269	392.0	341.1	6.248	6.099	5.640	5.784
9	2,2-dimethylbutane	C_6H_{14}	294.1	266	406.5	–	6.314	7.61	5.892	–
10	2,3-dimethylbutane	C_6H_{14}	292.9	412	416.9	–	6.364	6.75	5.904	–
11	3-methylpentane	C_6H_{14}	304.8	265	422.7	–	6.332	8.59	5.919	–
12	2-methylpentane (isohexane)	C_6H_{14}	280	267	417.6	–	6.503	8.07	5.963	–
13	hexane	C_6H_{14}	259.6	423	427.5	399.3	6.732	5.916	5.997	5.949
14	2-methylhexane (isoheptane)	C_7H_{16}	275.0	–	449.7	–	6.996	–	6.278	–
15	heptane	C_7H_{16}	288.0	–	459.6	–	6.992	–	6.311	–
16	octane	C_8H_{18}	286.9	333	488.9	–	7.437	7.407	6.615	–
17	nonane	C_9H_{20}	304.1	266	515.5	–	7.673	8.302	6.889	–
18	decane	$C_{10}H_{22}$	262.7	–	540.0	–	8.424	–	7.170	–
19	undecane	$C_{11}H_{24}$	244.9	–	561.0	–	8.986	–	7.406	–
20	dodecane	$C_{12}H_{26}$	252.4	–	583.2	–	9.216	–	7.662	–
21	tridecane	$C_{13}H_{28}$	259.1	–	603.8	–	9.476	–	7.857	–
22	tetradecane	$C_{14}H_{30}$	227.6	–	622.8	–	10.219	–	8.072	–
23	cyclohexane	C_6H_{12}	337.5	313	458.2	297.1	5.973	6.143	5.602	6.182
24	methylcyclohexane	C_7H_{14}	–	–	477.8	–	–	–	5.963	–

25	benzene	C_6H_6	333.8	335	465.2	412.3	5.688	5.628	5.294	5.349
26	toluene	C_7H_8	319.8	377	494.4	–	6.271	5.932	5.700	–
27	xylene (o)	C_8H_{10}	336.0	–	531.2	–	6.634	–	6.001	–
28	methyl mercaptan	CH_3SH	268.1	–	384.3	–	4.752	–	4.389	–
29	ethyl mercaptan	C_2H_5SH	308.3	–	411.0	–	5.210	–	4.900	–
30	propyl mercaptan	C_3H_7SH	–	–	440.5	–	–	–	5.451	–
31	carbonyl sulphide	COS	191.8	–	303.1	336	4.871	–	4.371	4.130
32	hydrogen sulphide	H_2S	262.6	31.2	302.0	301.1	3.891	3.591	3.787	3.623
33	sulphur dioxide	SO_2	245.7	251.7	358.8	335.4	4.487	4.290	4.126	4.112
34	ethene	C_2H_4	179.1	230	227.6	224.7	4.412	–	4.190	4.163
35	propene	C_3H_6	228.3	303	297.4	298.9	4.960	–	4.689	4.678
36	1-butene	C_4H_8	269.6	319	345.7	–	5.402	–	5.133	–
37	1-pentene	C_5H_{10}	447.8	–	386.8	–	4.995	–	5.526	–
38	1,2-butadiene	C_4H_6	249.9	–	370.1	–	5.476	–	5.027	–
39	1-butyne	C_4H_6	271.7	–	389.0	–	5.420	–	5.017	–
40	methanol	CH_3OH	143.3	452	424.7	481.8	5.502	3.666	4.191	3.626
41	ethanol	C_2H_5OH	228.8	415	464.2	362.6	5.467	4.370	4.638	4.530
42	argon	Ar	115.7	124.9	119.3	93.3	3.472	3.423	3.450	3.542
43	helium	He	4.6	10.8	3.8	10.22	3.047	2.57	3.174	2.551
44	carbon dioxide	CO_2	188.0	190	252.8	195.2	3.578	4.00	3.760	3.941
45	carbon monoxide	CO	107.2	32.8	107.4	91.7	3.653	3.92	3.679	3.690
46	hydrogen	H_2	31.2	370.6	27.1	59.7	3.115	2.959	3.270	2.827
47	nitrogen	N_2	95.7	47.6	100.9	71.4	3.688	3.85	3.658	3.798
48	oxygen	O_2	114.4	48.9	123.0	106.7	3.515	3.541	3.427	3.467
49	nitric oxide	NO	80.1	119	161.2	116.7	3.850	3.47	3.241	3.492
50	nitrogen dioxide	NO_2	2005.6	–	404.3	–	2.490	–	3.712	–
51	water vapour	H_2O	209.6	–	550.6	809.1	4.206	–	3.340	2.641
52	air (dry)	–	–	84	105.6	78.6	–	3.689	3.591	3.711

2.5.2 Kinematic viscosity

The kinematic viscosity ν is the ratio of the dynamic viscosity μ and the density ϱ of a gas mixture:

$$\nu = \mu/\varrho \qquad [2.82]$$

where:

ν	= kinematic viscosity	m^2/s
μ	= dynamic viscosity (2.5.1)	$Pa \cdot s$
ϱ	= density (2.4)	kg/m^3

Naturally, the pressure and temperature conditions have to be the same for each of these variables

2.6 Heat capacity

2.6.1 Isobaric heat capacity

The isobaric heat capacity c_p of a gas mixture at p kPa and T K is made up of an ideal component c_p^o – which is solely a function of temperature – and a real component Δc_p – which is a function of both pressure and temperature:

$$c_p = c_p^o + \Delta c_p \qquad [2.83]$$

where:

c_p	=	isobaric heat capacity at p kPa and T K	kJ/(kmol · K)
c_p^o	=	ideal component at T K (tables 2.6.1, 2.6.2)	kJ/(kmol · K)
Δc_p	=	real component at p kPa and T K (figs. 2.6.1, 2.6.2)	kJ/(kmol · K)

The ideal component of the isobaric heat capacity is determined from the composition of the gas mixture by taking the weighted average of the heat capacity (ideal component) of the individual gases in the mixture:

$$c_p^o = \sum_{i=1}^{n} n_i \cdot c_{p,i}^o / 100 \qquad [2.84]$$

where:

c_p^o	=	isobaric heat capacity at T K	kJ/(kmol · K)
n_i	=	concentration of gas component i	% (mol)
$c_{p,i}^o$	=	isobaric heat capacity of component i at T K (tables 2.6.1, 2.6.2)	kJ/(kmol · K)
n	=	number of components in the gas mixture	–

The real component Δc_p is also made up of two components:

$$\Delta c_p = \Delta c_p^o + \omega \cdot \Delta c_p^I \qquad [2.85]$$

where:
ω = acentric factor (table 2.2.5)

Δc_p^o (fig. 2.6.1) and Δc_p^I (fig. 2.6.2) are both given as a function of the reduced pressure p_r [2.65] and the reduced temperature T_r [2.66] (lit. 18)

Table 2.6.1 Ideal isobaric heat capacity c_p^o of pure gases

No.	Component	Formula	c_p^o kJ/(kmol · K)							
			Temperature							
			253.15 K	273.15 K	288.15 K	298.15 K	373.15 K	473.15 K	573.15 K	673.15 K
1	methane	CH_4	34.490	35.080	35.581	35.942	39.212	44.674	50.725	56.792
2	ethane	C_2H_6	47.768	49.912	51.575	52.706	61.636	74.093	86.241	97.326
3	propane	C_3H_8	65.627	69.257	72.020	73.880	88.073	106.909	124.563	140.206
4	2-methylpropane (isobutane)	C_4H_{10}	85.167	90.747	94.889	97.629	117.568	142.223	164.337	183.704
5	butane	C_4H_{10}	88.014	93.151	96.986	99.533	118.282	141.940	163.547	182.724
6	2,2-dimethylpropane	C_5H_{12}	105.836	113.294	118.796	122.420	148.437	179.783	207.165	230.597
7	2-methylbutane (isopentane)	C_5H_{12}	102.505	109.982	115.468	119.068	144.657	175.106	201.718	224.868
8	pentane	C_5H_{12}	104.992	112.131	117.377	120.823	145.390	174.819	200.732	223.435
9	2,2-dimethylbutane	C_6H_{14}	118.218	128.231	135.512	140.259	173.289	210.932	242.377	268.778
10	2,3-dimethylbutane	C_6H_{14}	120.482	129.507	136.128	140.472	171.319	207.910	239.688	267.064
11	3-methylpentane	C_6H_{14}	121.488	129.770	135.987	140.126	170.653	208.415	241.198	268.627
12	2-methylpentane (isohexane)	C_6H_{14}	123.704	132.212	138.533	142.716	173.127	210.406	243.246	271.418
13	hexane	C_6H_{14}	126.843	133.923	139.368	143.049	171.321	208.133	240.749	267.716
14	2-methylhexane (isoheptane)	C_7H_{16}	143.460	152.981	160.120	164.871	199.873	243.175	280.822	312.258
15	heptane	C_7H_{16}	146.351	154.830	161.282	165.617	198.424	240.601	278.127	309.554
16	octane	C_8H_{18}	166.825	176.542	183.928	188.887	226.363	274.465	317.189	352.760
17	nonane	C_9H_{20}	186.843	197.749	206.036	211.598	253.607	307.531	355.463	395.325
18	decane	$C_{10}H_{22}$	206.755	218.706	227.848	234.008	280.909	341.208	394.017	436.973
19	undecane	$C_{11}H_{24}$	221.149	236.847	248.355	255.902	309.428	372.820	427.903	475.523
20	dodecane	$C_{12}H_{26}$	241.631	258.584	271.018	279.174	337.073	405.777	465.595	517.400
21	tridecane	$C_{13}H_{28}$	260.694	279.146	292.671	301.542	364.439	438.905	503.578	559.459
22	tetradecane	$C_{14}H_{30}$	280.445	300.255	314.778	324.302	391.847	471.834	541.317	601.365
23	cyclohexane	C_6H_{12}	83.438	93.133	100.288	105.001	138.884	179.871	215.923	247.038
24	methylcyclohexane	C_7H_{14}	107.131	118.826	127.394	133.011	172.759	219.521	259.676	293.821

25	benzene	C_6H_6	66.992	73.794	78.753	81.991	104.633	130.625	152.357	170.391
26	toluene	C_7H_8	85.949	93.983	99.848	103.684	130.611	161.809	188.199	210.380
27	xylene (o)	C_8H_{10}	114.740	123.095	129.241	133.280	162.107	196.539	226.512	252.237
28	methyl mercaptan	CH_3SH	44.972	47.070	48.608	49.617	56.762	65.210	72.539	78.873
29	ethyl mercaptan	C_2H_5SH	66.213	69.616	72.111	73.748	85.349	99.078	110.994	121.286
30	propyl mercaptan	C_3H_7SH	–	–	92.834*)	95.186**)	–	–	–	–
31	carbonyl sulphide	COS	39.654	40.614	41.307	41.757	44.835	48.202	50.864	52.965
32	hydrogen sulphide	H_2S	33.849	34.033	34.185	34.292	35.240	36.799	38.562	40.405
33	sulphur dioxide	SO_2	38.425	39.133	39.659	40.008	42.547	45.652	48.340	50.550
34	ethene	C_2H_4	39.075	40.984	42.418	43.374	50.509	59.706	68.252	75.923
35	propene	C_3H_6	56.284	59.824	62.433	64.151	76.476	91.402	104.651	116.299
36	1-butene	C_4H_8	74.095	79.283	83.086	85.579	103.254	124.172	142.345	158.074
37	1-pentene	C_5H_{10}	95.138	101.590	106.321	109.424	131.448	157.578	180.344	200.097
38	1,2-butadiene	C_4H_6	70.819	74.921	77.929	79.901	93.894	110.478	124.909	137.413
39	1-butyne	C_4H_6	73.056	77.060	79.993	81.915	95.518	111.577	125.506	137.560
40	methanol	CH_3OH	40.275	41.846	43.026	43.813	49.705	57.443	64.888	71.871
41	ethanol	C_2H_5OH	57.813	61.214	63.722	65.374	77.232	91.602	104.335	115.438
42	argon	Ar	20.704	20.704	20.704	20.704	20.704	20.706	20.708	20.711
43	helium	He	20.8	20.8	20.8	20.8	20.8	20.8	20.8	20.8
44	carbon dioxide	CO_2	35.263	36.166	36.824	37.254	40.261	43.720	46.619	49.031
45	carbon monoxide	CO	29.023	29.037	29.055	29.070	29.264	29.700	30.283	30.956
46	hydrogen	H_2	28.808	28.874	28.918	28.946	29.104	29.230	29.316	29.416
47	nitrogen	N_2	29.052	29.057	29.067	29.077	29.212	29.549	30.024	30.597
48	oxygen	O_2	29.085	29.172	29.250	29.307	29.851	30.785	31.805	32.781
49	nitric oxide	NO	29.645	29.711	29.765	29.802	30.115	30.620	31.201	31.833
50	nitrogen dioxide	NO_2	35.123	35.871	36.422	36.784	39.369	42.458	45.139	47.414
51	water vapour	H_2O	33.384	33.462	33.533	33.586	34.100	35.044	36.175	37.398
52	air (dry)	–	28.969	29.998	29.025	29.047	29.275	29.731	30.305	30.947

*) $T = 288.7$ K
**) $T = 300$ K

Table 2.6.2 Coefficients for the ideal heat capacity equation of pure gases
$c_p^o = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T^4$ *kJ/(kmol · K) (T in K)*

No.	Component	Formula	A	$B \cdot 10^3$	$C \cdot 10^6$	$D \cdot 10^9$	$E \cdot 10^{13}$	Temperature range °C	Lit.
1	methane	CH_4	38.400	− 71.167	276.271	− 239.227	685.813	−175/1200	(5)
2	ethane	C_2H_6	33.346	− 11.337	357.723	− 377.692	1203.991	−175/1200	(5)
3	propane	C_3H_8	31.866	62.503	386.796	− 461.257	1543.480	−175/1200	(5)
4	2-methylpropane (isobutane)	C_4H_{10}	11.360	293.305	34.115	− 179.627	693.433	− 75/1200	(5)
5	butane	C_4H_{10}	23.987	235.817	122.573	− 238.507	837.958	− 75/1200	(5)
6	2,2-dimethylpropane	C_5H_{12}	1.321	442.023	− 81.175	− 153.236	742.833	− 75/1200	(5)
7	2-methylbutane (isopentane)	C_5H_{12}	− 9.517	510.989	−288.577	72.572	− 46.749	− 20/1200	(5)
8	pentane	C_5H_{12}	− 0.844	478.571	−253.357	57.618	− 31.260	− 20/1200	(5)
9	2,2-dimethylbutane	C_6H_{14}	−43.116	780.037	−624.427	245.845	− 254.695	− 20/700	(5)
10	2,3-dimethylbutane	C_6H_{14}	−14.598	614.630	−337.355	68.157	0	–	(12)
11	3-methylpentane	C_6H_{14}	34.281	208.526	841.404	−1359.067	6197.914	− 75/700	(5)
12	2-methylpentane (isohexane)	C_6H_{14}	14.968	404.859	218.226	− 537.439	2384.812	− 75/700	(5)
13	hexane	C_6H_{14}	82.663	−105.950	1587.924	−2123.729	8991.790	− 75/700	(5)
14	2-methylhexane (isoheptane)	C_7H_{16}	40.567	267.472	865.062	−1407.579	6282.756	− 75/700	(5)
15	heptane	C_7H_{16}	75.603	52.452	1312.567	−1797.445	7436.114	− 75/700	(5)
16	octane	C_8H_{18}	82.779	84.038	1419.707	−1937.432	7844.206	− 75/700	(5)
17	nonane	C_9H_{20}	90.781	112.365	1527.288	−2074.253	8257.204	− 75/700	(5)
18	decane	$C_{10}H_{22}$	121.137	− 74.853	2356.998	−3205.222	13435.482	− 75/700	(5)
19	undecane	$C_{11}H_{24}$	−15.604	1085.578	−635.093	165.515	− 113.774	− 20/1200	(5)
20	dodecane	$C_{12}H_{26}$	−13.209	1165.326	−668.688	168.685	− 111.043	− 20/1200	(5)
21	tridecane	$C_{13}H_{28}$	−17.702	1276.917	−748.468	195.104	− 134.069	− 20/1200	(5)
22	tetradecane	$C_{14}H_{30}$	−18.314	1369.768	−800.615	207.576	− 141.857	− 20/1200	(5)
23	cyclohexane	C_6H_{12}	−52.801	580.060	−132.682	− 147.240	701.611	− 20/1200	(5)
24	methylcyclohexane	C_7H_{14}	−69.224	805.802	−450.284	72.033	130.764	− 20/1200	(5)

25	benzene	C_6H_6	–40.116	507.538	–361.799	114.057	– 96.947	– 20/1200	(5)
26	toluene	C_7H_8	–39.021	586.859	–398.007	120.379	– 98.017	– 20/1200	(5)
27	xylene (o)	C_8H_{10}	– 6.645	534.856	–209.150	– 47.717	397.925	– 20/1200	(5)
28	methyl mercaptan	CH_3SH	13.259	145.561	– 85.395	20.736	0	–	(12)
29	ethyl mercaptan	C_2H_5SH	14.912	234.932	–135.520	31.598	0	–	(12)
30	propyl mercaptan	C_3H_7SH	68.717	88.321	0	0	0	–	(4, 5)
31	carbonyl sulphide	COS	23.552	79.789	– 70.124	24.518	0	–	(12)
32	hydrogen sulphide	H_2S	34.037	– 12.561	56.950	– 43.308	108.471	–175/1200	(5)
33	sulphur dioxide	SO_2	29.573	31.890	23.234	– 48.372	182.002	–175/1200	(5)
34	ethene	C_2H_4	17.027	72.311	86.993	– 123.386	410.897	– 20/1200	(5)
35	propene	C_3H_6	5.428	222.764	– 84.709	– 9.295	104.083	– 20/1200	(5)
36	1-butene	C_4H_8	– 4.350	360.548	–214.764	58.758	– 43.134	– 20/1200	(5)
37	1-pentene	C_5H_{10}	– 2.019	445.092	–259.244	68.760	– 48.689	– 20/1200	(5)
38	1,2-butadiene	C_4H_6	8.959	283.704	–166.432	44.397	– 31.519	– 20/1200	(5)
39	1-butyne	C_4H_6	12.079	282.175	–176.828	55.618	– 63.475	– 20/1200	(5)
40	methanol	CH_3OH	21.138	70.877	25.853	– 28.497	0	–	(12)
41	ethanol	C_2H_5OH	9.008	213.928	– 83.847	1.372	0	–	(12)
42	argon	Ar	20.790	– 0.032	0.052	0	0	–	(12)
43	helium	He	20.8	0	0	0	0	–	(4, 16)
44	carbon dioxide	CO_2	21.085	67.085	– 47.451	14.918	– 12.708	–175/1200	(5)
45	carbon monoxide	CO	30.083	– 9.673	25.397	– 15.409	28.061	–175/1200	(5)
46	hydrogen	H_2	27.007	11.935	– 24.076	21.464	– 61.487	–175/1200	(5)
47	nitrogen	N_2	29.932	– 7.513	18.116	– 8.811	9.784	–175/1200	(5)
48	oxygen	O_2	30.477	17.992	62.899	– 57.895	174.034	–175/1200	(5)
49	nitric oxide	NO	29.326	– 0.937	9.740	– 4.184	0	–	(12)
50	nitrogen dioxide	NO_2	24.217	48.325	– 20.794	0.293	0	–	(12)
51	water vapour	H_2O	34.499	– 14.259	47.356	– 35.676	93.553	–175/1200	(5)
52	air (dry)	–	29.724	– 8.017	23.658	– 15.737	34.065	–175/1200	(17)

2.6.2 Isochoric heat capacity

Considerably less information is given in literature concerning the isochoric heat capacity c_v.

However, it is a simple matter to calculate c_v from the general formula (lit. 18, 20):

$$c_p - c_v = -T \left(\frac{\partial V}{\partial T}\right)_p^2 \Big/ \left(\frac{\partial V}{\partial p}\right)_T \qquad [2.86]$$

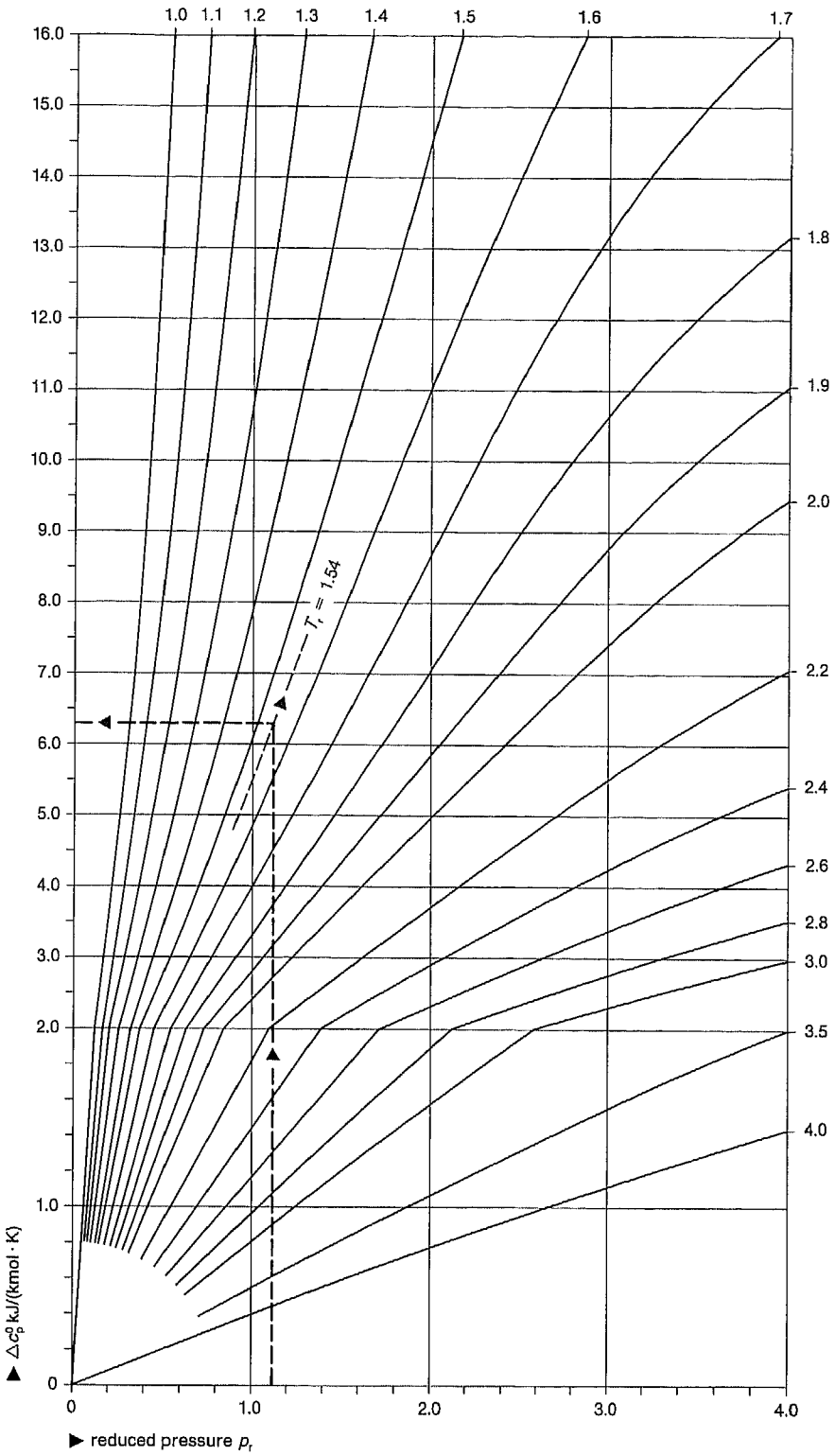
from which, for non-ideal gases, the following formula can be derived (lit. 18, 19):

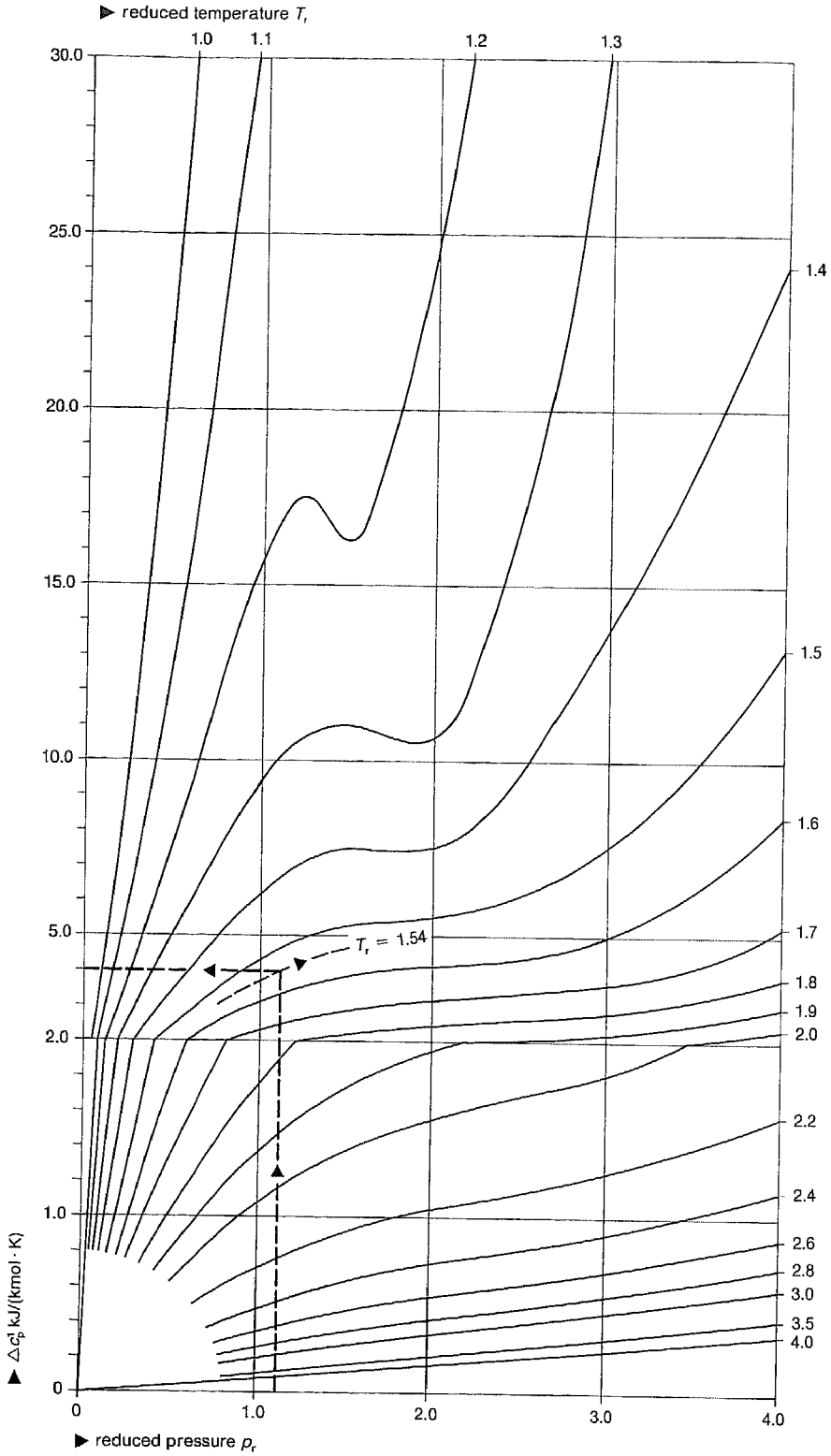
$$c_p - c_v = z \cdot R_a \frac{\left[1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right]^2}{\left[1 - \frac{p}{z}\left(\frac{\partial z}{\partial p}\right)_T\right]} \qquad [2.87]$$

where:

c_v	=	isochoric heat capacity	kJ/(kmol · K)
c_p	=	isobaric heat capacity (2.6.1)	kJ/(kmol · K)
z	=	compressibility factor at T and p (2.2)	–
R_a	=	universal gas constant (1.1.5)	kJ/(kmol · K)
p	=	absolute pressure	kPa
T	=	absolute temperature	K
$\left(\frac{\partial z}{\partial p}\right)_T$	=	partial derivative with respect to pressure at constant temperature (lit. 20) (2.2)	kPa^{-1}
$\left(\frac{\partial z}{\partial T}\right)_p$	=	partial derivative with respect to temperature at constant pressure (lit. 20) (2.2)	K^{-1}
N_1	=	$1 - \frac{p}{z}\left(\frac{\partial z}{\partial p}\right)_T$ (fig. 2.7.1)	[2.88]
N_2	=	$1 - \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p$ (fig. 2.7.2)	[2.89]

Fig. 2.6.1 Δc_p^o as a function of the reduced pressure p_r and reduced temperature T_r


1.0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
2.0
2.2
2.4
2.6
2.8
3.0
3.5
4.0
T_r = 1.54
16.0
15.0
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
▲ Δc_p^0 kJ/(kmol · K)
0
1.0
2.0
3.0
4.0
▶ reduced pressure p_r


reduced temperature T_r
1.0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
1.9
2.0
2.2
2.4
2.6
2.8
3.0
3.5
4.0
T_r = 1.54
30.0
25.0
20.0
15.0
10.0
5.0
2.0
1.0
0
Δc_p^l kJ/(kmol · K)
0
1.0
2.0
3.0
4.0
reduced pressure p_r

Substitution of N_1 and N_2 gives:

$$c_v = c_p - z \cdot R_a \frac{N_2^2}{N_1} \qquad [2.90]$$

Example: Groningen natural gas (table 1.9)	
T	= 288.15 K (15 °C)
p	= 5000 kPa (50 bar)
M	= 18.637 kg/kmol (table 1.9)
z	= 0.911 7 (2.2.1.1)

$$\left(\frac{\partial z}{\partial T}\right)_p = 1.215 \times 10^{-3}\ \mathrm{K}^{-1} \qquad (2.2.1.1, \text{lit. } 20)$$

$$\left(\frac{\partial z}{\partial p}\right)_T = -1.615 \times 10^{-5}\ \mathrm{kPa}^{-1} \qquad (2.2.1.1, \text{lit. } 20)$$

N_1 = 1.088 6 [2.88]

N_2 = 1.384 0 [2.89]

Table 2.6.3 c_p^o *of Groningen natural gas*

Component	Formula	n_i* % (mol)	$c_{p,i}^o$** kJ/(kmol · K)
methane	CH_4	81.29	35.581
ethane	C_2H_6	2.87	51.575
propane	C_3H_8	0.38	72.020
butane	C_4H_{10}	0.15	96.986
pentane	C_5H_{12}	0.04	117.377
hexane	C_6H_{14}	0.05	139.368
nitrogen	N_2	14.32	29.067
oxygen	O_2	0.01	29.250
carbon dioxide	CO_2	0.89	36.824
		100.00	35.433

* Table 1.9
** Table 2.6.1

Fig. 2.6.2 Δc_p^I *as a function of the reduced pressure* p_r *and reduced temperature* T_r

c_p^o = 35.433 kJ/(kmol · K) (table 2.6.3)
T_r = 1.54 [2.66]
p_r = 1.12 [2.65]
ω = 0.0209 (table 1.9)
Δc_p^o = 6.300 kJ/(kmol · K) (fig. 2.6.1)
Δc_p^l = 4.000 kJ/(kmol · K) (fig. 2.6.2).

This results in:
$\Delta c_p = 6.300 + 0.0209 \times 4.000 = 6.384$ kJ/(kmol · K) [2.85]

and ultimately:
$c_p = c_p^o + \Delta c_p = 41.817$ kJ/(kmol · K) = 2.244 kJ/(kg · K) [2.83]

And c_v can then be calculated from [2.90]:

$$c_v = c_p - z \cdot R_a \frac{N_2^2}{N_1} = 41.817 - 13.338 = 28.479 \text{ kJ/(kmol} \cdot \text{K)} = 1.528 \text{ kJ/(kg} \cdot \text{K)}$$

2.7 Isentropic exponents

2.7.1 Ideal gases

For ideal gases the isentropic exponent $\varkappa$ equals the heat capacity ratio c_p/c_v:

$$\varkappa = \frac{c_p}{c_v} \qquad [2.91]$$

where:
c_p = isobaric heat capacity (2.6.1) kJ/(kmol · K)
c_v = isochoric heat capacity (2.6.2) kJ/(kmol · K)

$\varkappa$ is dimensionless.

2.7.2 Non-ideal gases

In the case of non-ideal gases, it is important to bear in mind for which purpose the isentropic exponent is used.

2.7.2.1 Volume change with pressure

For an adiabatic change of state:

$$p \cdot V^k = \text{constant} \qquad [2.92]$$

From this we can derive (lit. 18, 19):

$$k = \frac{-V}{p}\left(\frac{\partial p}{\partial V}\right)_s \qquad [2.93]$$

or, according to lit. 20:

$$k = \frac{z}{[z - p\left(\frac{\partial z}{\partial p}\right)_T] - \frac{R_a}{c_p}[z + T\left(\frac{\partial z}{\partial T}\right)_p]^2} \qquad [2.94]$$

After reduction:

$$k = \frac{1}{[1 - \frac{p}{z}\left(\frac{\partial z}{\partial p}\right)_T] - \frac{R_a \cdot z}{c_p}[1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p]^2} = \frac{1}{N_1 - N_3} \qquad [2.95]$$

(figs. 2.7.1, 2.7.2, 2.7.3)

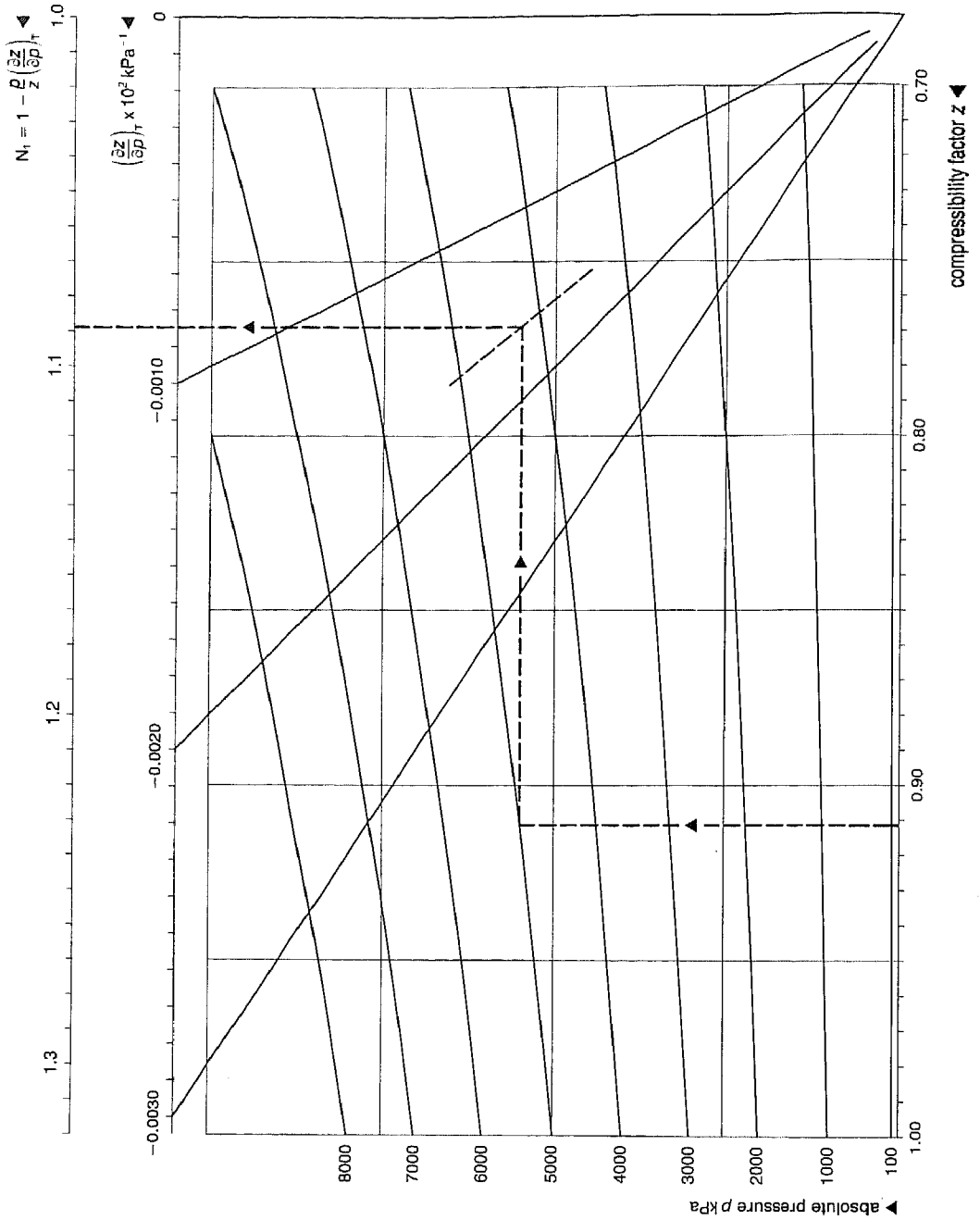


Fig. 2.7.1 N_1 *as a function of the compressibility factor z, the absolute pressure p and the derivative* $\left(\frac{\partial z}{\partial p}\right)_T$

where:

z	=	compressibility factor at p and T (2.2)	–
p	=	absolute pressure	kPa
T	=	absolute temperature	K
R_a	=	universal gas constant (1.1.5)	kJ/(kmol · K)
c_p	=	isobaric heat capacity (2.6.1)	kJ/(kmol · K)
$\left(\frac{\partial z}{\partial p}\right)_T$	=	partial derivative with respect to pressure at constant temperature (lit. 20) (2.2)	kPa^{-1}
$\left(\frac{\partial z}{\partial T}\right)_p$	=	partial derivative with respect to temperature at constant pressure (lit. 20) (2.2)	K^{-1}

$$N_3 = \frac{R_a \cdot z}{c_p} N_2^2 \qquad [2.96]$$

2.7.2.2 Temperature change with pressure

For an adiabatic change of state:

$$T \cdot p^{\frac{1-k'}{k'}} = \text{constant} \qquad [2.97]$$

From this we can derive (lit. 18, 19):

$$\frac{k'-1}{k'} = \frac{p}{T}\left(\frac{\partial T}{\partial p}\right)_s \qquad [2.98]$$

or

$$k' = \frac{1}{1-\frac{R_a}{c_p}\left[z+T\left(\frac{\partial z}{\partial T}\right)_p\right]} = \frac{1}{1-\frac{R_a \cdot z}{c_p}\left[1+\frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right]} = \frac{N_2}{N_2-N_3} \qquad [2.99]$$

(figs. 2.7.2, 2.7.3)

Example: Groningen natural gas (table 1.9)

$p = 5000$ kPa, $T = 288.15$ K (15 °C) } $z = 0.9117$ (2.2.1.1)

$\left(\frac{\partial z}{\partial p}\right)_T = -1.615 \times 10^{-5}\ kPa^{-1}$ (2.2.1.1, 2.6.2)

$N_1 = 1.089$ (fig. 2.7.1)

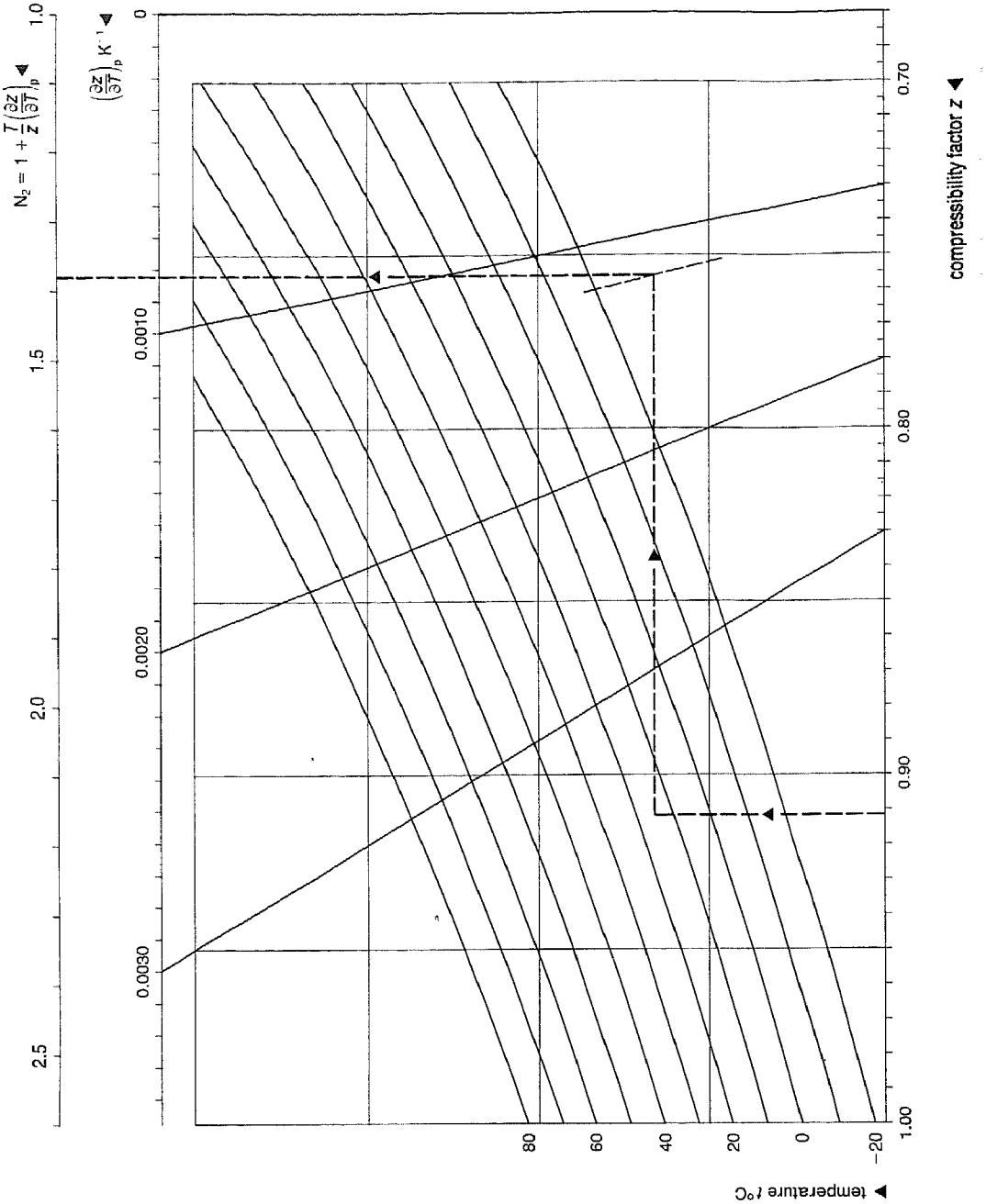


Fig. 2.7.2 N_2 *as a function of the compressibility factor z, the temperature T* and the derivative $\left(\frac{\partial z}{\partial T}\right)_p$

Example: Groningen natural gas (table 1.9)
$p = 5000$ kPa
$T = 288.15$ K (15 °C)

$z \quad = 0.9117$ (2.2.1.1)

$\left(\frac{\partial z}{\partial p}\right)_T = -1.615 \times 10^{-5}\,\text{kPa}^{-1}$ (2.2.1.1, 2.6.2)

$\left(\frac{\partial z}{\partial T}\right)_p = 1.215 \times 10^{-3}\,\text{K}^{-1}$ (2.2.1.1, 2.6.2)

$c_p \quad = 41.817$ kJ/(kmol · K) (2.6.1, 2.6.2)

Solution:

$N_1 = 1.0886$
$N_1 = 1.089$ (fig. 2.7.1) [2.88]

$N_2 = 1.3840$
$N_2 = 1.380$ (fig. 2.7.2) [2.89]

$N_3 = 0.3472$
$N_3 = 0.350$ (fig. 2.7.3) [2.96]

$$k = \frac{1}{(N_1 - N_3)} = 1.357 \qquad [2.95]$$

$k = 1.353$ (figs. 2.7.1, 2.7.2, 2.7.3)

Example: Groningen natural gas (table 1.9)	
$p = 5000$ kPa $T = 15$ °C (288.15 K)	$z = 0.9117$ (2.2.1.1)
$\left(\frac{\partial z}{\partial T}\right)_p = 1.215 \times 10^{-3}\,\text{K}^{-1}$ (2.2.1.1, 2.6.2)	
$N_2 = 1.380$ (fig. 2.7.2)	

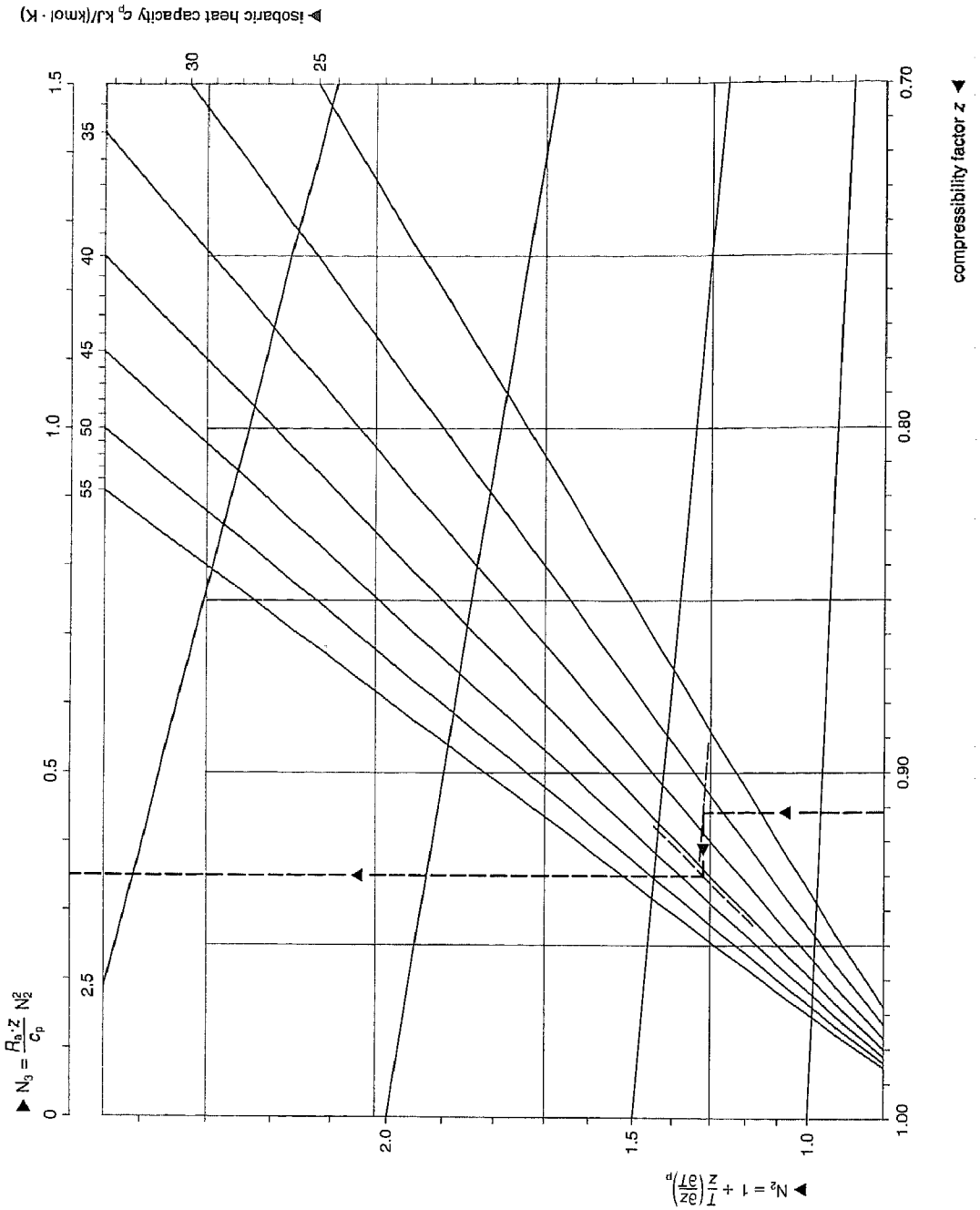


Fig. 2.7.3 N_3 *as a function of the compressibility factor z,* N_2 *(fig. 2.7.2) and the isobaric heat capacity* c_p

The difference between calculated values and graphically determined values is

$$\frac{1.357 - 1.353}{1.353} \times 100 = 0.3\,\%$$

The graphical method is thus sufficiently accurate

k' can be calculated from [2.99] or determined by using figs. 2.7.1, 2.7.2, 2.7.3:

$$k' = \frac{N_2}{N_2 - N_3} = 1.340 \qquad [2.99]$$

$\varkappa$ can be calculated from [2.91]:

$$\varkappa = \frac{41.817}{28.479} = 1.468$$

The values for c_p and c_v are calculated under 2.6.2

2.7.3 Velocity of sound

By "velocity of sound" (critical velocity) c is meant the velocity at which a pressure change is propagated in a medium (lit. 21)

In a compressible medium, the velocity of sound is represented by:

$$c = \sqrt{\left(\frac{\partial p}{\partial \varrho}\right)} \quad [2.93] \qquad [2.100]$$

For a non-ideal gas, it can be deduced that (lit. 22):

$$c = \sqrt{1000 \cdot k \cdot z \cdot R_a \cdot T/M} = \sqrt{1000 \cdot k \cdot p/\varrho} \qquad [2.101]$$

Example: Groningen natural gas (table 1.9)
$p = 5000$ kPa $T = 288.15$ K (15 °C) } $z = 0.9117$ (2.2.1.1) $N_2 = 1.380$ (fig. 2.7.2) $c_p = 41.817$ kJ/(kmol · K) (2.6.1, 2.6.2) $N_3 = 0.350$ (fig. 2.7.3)

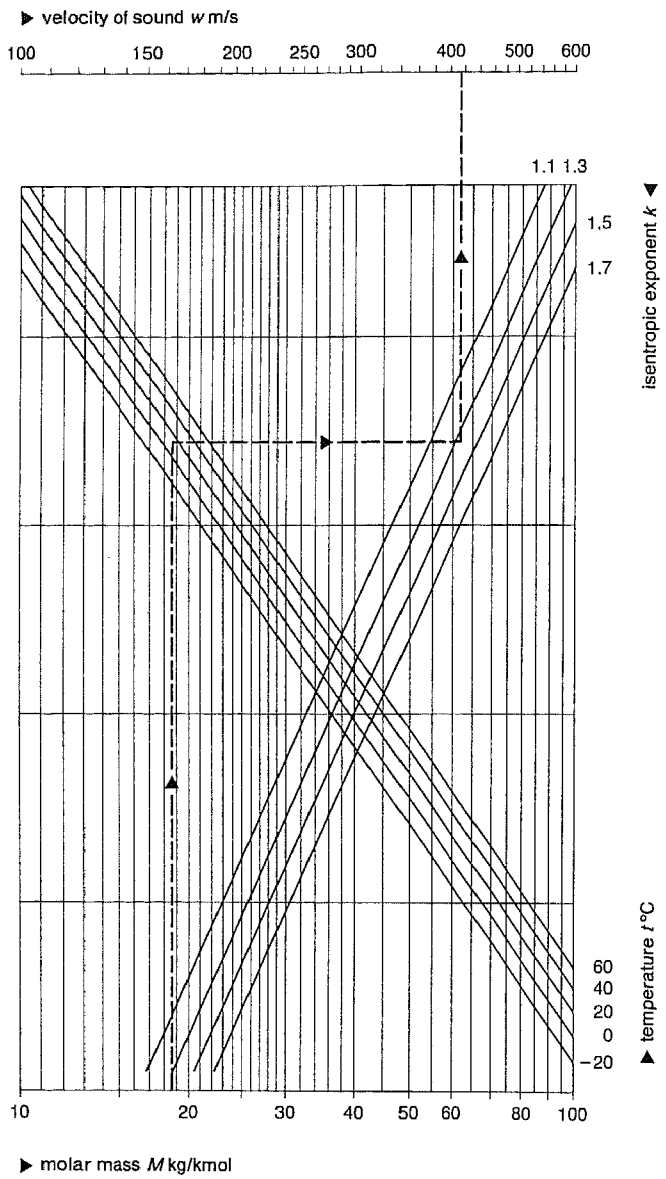


Fig. 2.7.4 Velocity of sound c for gases as a function of the molar mass M, the temperature T and the isentropic exponent k

where:

c	=	velocity of sound at p and T	m/s
k	=	isentropic exponent (2.7.2.1)	–
z	=	compressibility factor at p and T (2.2)	–
R_a	=	universal gas constant (1.1.5)	kJ/(kmol · K)
T	=	absolute temperature	K
M	=	molar mass (table 1.7)	kg/kmol
p	=	absolute pressure	kPa
ϱ	=	density at p and T (2.4)	kg/m^3

Andsager and Knapp (lit. 23) compared the results obtained using the above formula with 42 series of test data. They found that the calculated and the measured velocity of sound differed consistently by $\sqrt{z}$ (see Note).
After removing $\sqrt{z}$, the formula thus becomes (fig. 2.7.4):

$$c = \sqrt{1000 \cdot k \cdot R_a \cdot T/M} = \sqrt{\frac{1000 \cdot k \cdot p}{z \cdot \varrho}} \qquad [2.102]$$

Note: From the results of a small number of measurements of the velocity of sound of N_2, CH_4, Groningen natural gas and Ekofisk gas at Gasunie Research Laboratory we have not been able to confirm this theory. Our results agree reasonable well with those from [2.101].

Example: Groningen natural gas (table 1.9)

$p = 5000$ kPa
$T = 288.15$ K (15 °C) } $z = 0.9117$ (2.2.1.1)
$M = 18.637$ kg/kmol (table 1.9)
$k = 1.353$ (2.7.2.1, 2.7.2.2)
$c = 415$ m/s (fig. 2.7.4)
$c = 417$ m/s [2.102]
$c = 398$ m/s [2.101]

2.8 *H-S* diagram

2.8.1 Enthalpy

The enthalpy difference ($H_2 - H_1$) of a gas mixture can be calculated by the general formula (lit. 15, 18)

$$dH = c_p\,dT + [V - T\left(\frac{\partial V}{\partial T}\right)_p]\,dp \qquad [2.103]$$

Integration then gives the enthalpy difference:

$$\Delta H = H_2 - H_1 = c_p(T_2 - T_1) - R_a \cdot T^2 \left(\frac{\partial z}{\partial T}\right)_p \ln\left(\frac{p_2}{p_1}\right) \qquad [2.104]$$

where:

p_1, p_2	=	absolute pressure	kPa
T_1, T_2	=	absolute temperature	K
H_1	=	enthalpy at T_1 and p_1	kJ/kmol
H_2	=	enthalpy at T_2 and p_2	kJ/kmol
R_a	=	universal gas constant (1.1.5)	kJ/(kmol · K)
T	=	average absolute temperature $(T_1 + T_2)/2$	K
p	=	average absolute pressure $(p_2 + p_1)/2$	kPa
c_p	=	isobaric heat capacity at T and p (2.6.1)	kJ/(kmol · K)
$\left(\frac{\partial z}{\partial T}\right)_p$	=	partial derivative with respect to temperature at constant pressure (2.2)	K^{-1}

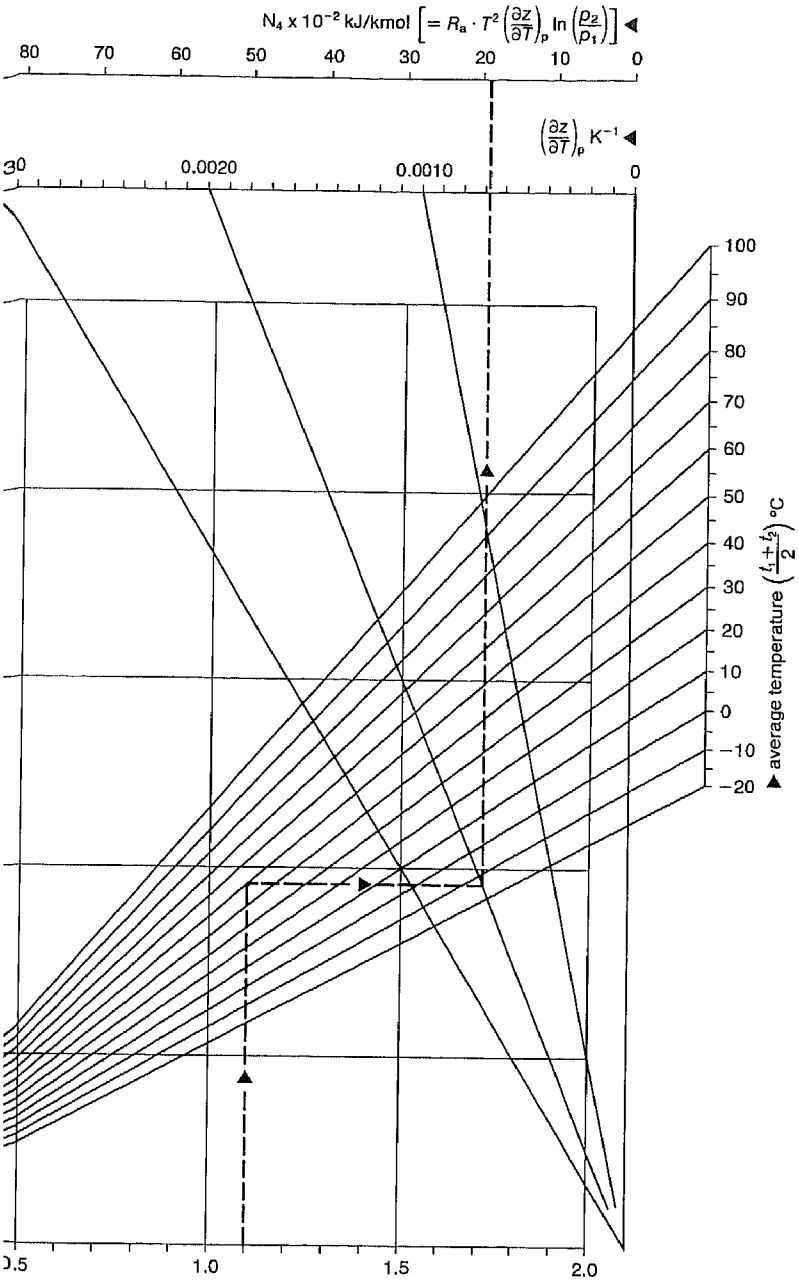
Graphic solution:

$$\Delta H = c_p(T_2 - T_1) - R_a \cdot T^2 \left(\frac{\partial z}{\partial T}\right)_p \ln\left(\frac{p_2}{p_1}\right) \qquad [2.104]$$

For $c_p\,(T_2 - T_1)$ see fig. 2.8.3

For $N_4 = R_a \cdot T^2 \left(\frac{\partial z}{\partial T}\right)_p \ln\left(\frac{p_2}{p_1}\right)$ see fig. 2.8.1 [2.105]

Fig. 2.8.1 N_4 *as a function of the average temperature T, the pressure ratio* p_2/p_1 *and the derivative* $\left(\frac{\partial z}{\partial T}\right)_p$


$N_4 \times 10^{-2}$ kJ/kmol $\left[= R_a \cdot T^2 \left(\frac{\partial z}{\partial T}\right)_p \ln\left(\frac{p_2}{p_1}\right)\right]$
80
70
60
50
40
30
20
10
0
$\left(\frac{\partial z}{\partial T}\right)_p$ K^{-1}
0.0020
0.0010
0
100
90
80
70
60
50
40
30
20
10
0
−10
−20
average temperature $\left(\frac{t_1+t_2}{2}\right)$ °C
1.0
1.5
2.0

2.8.2 Entropy

The entropy difference ($S_2 - S_1$) of a gas mixture can be calculated by means of the general formula (lit. 18, 19):

$$dS = c_p \frac{dT}{T} - \left(\frac{\partial V}{\partial T}\right)_p dp \qquad [2.106]$$

Integration gives the following formula for entropy difference:

$$\Delta S = S_2 - S_1 = c_p \ln\left(\frac{T_2}{T_1}\right) - R_a \left[z + T\left(\frac{\partial z}{\partial T}\right)_p\right] \ln\left(\frac{p_2}{p_1}\right) \qquad [2.107]$$

where:

S_1 = entropy at T_1 and p_1 kJ/(kmol · K)
S_2 = entropy at T_2 and p_2 kJ/(kmol · K)
z = compressibility at p and T
(for remaining notation see 2.8.1)

Graphic solution:

$$\Delta S = c_p \ln\left(\frac{T_2}{T_1}\right) - R_a \left[z + T\left(\frac{\partial z}{\partial T}\right)_p\right] \ln\left(\frac{p_2}{p_1}\right) \qquad [2.107]$$

For $c_p \ln\left(\frac{T_2}{T_1}\right)$ see fig. 2.8.3

For $N_5 = R_a \left[z + T\left(\frac{\partial z}{\partial T}\right)_p\right] \ln\left(\frac{p_2}{p_1}\right)$ see fig. 2.8.2 [2.108]

2.8.3 *H-S* diagram

The *H-S* diagram is constructed by plotting $\Sigma\Delta H$ against $\Sigma\Delta S$. Zero for both enthalpy and entropy is put at 0 °C and 101.325 kPa. The diagram is thus constructed step by step.

The values of ($p_2 - p_1$) and ($T_2 - T_1$) must not be too large; for c_p, z and $(\delta z/\delta T)_p$ the average of the relevant values associated with (T_1, p_1) and (T_2, p_2) should be used.

2.8.4 Isentropic expansion (S = constant)

Isentropic expansion is given by (lit. 18, 19):

$$\left(\frac{\partial T}{\partial p}\right)_s = \frac{T}{c_p}\left(\frac{\partial V}{\partial T}\right)_p \qquad [2.109]$$

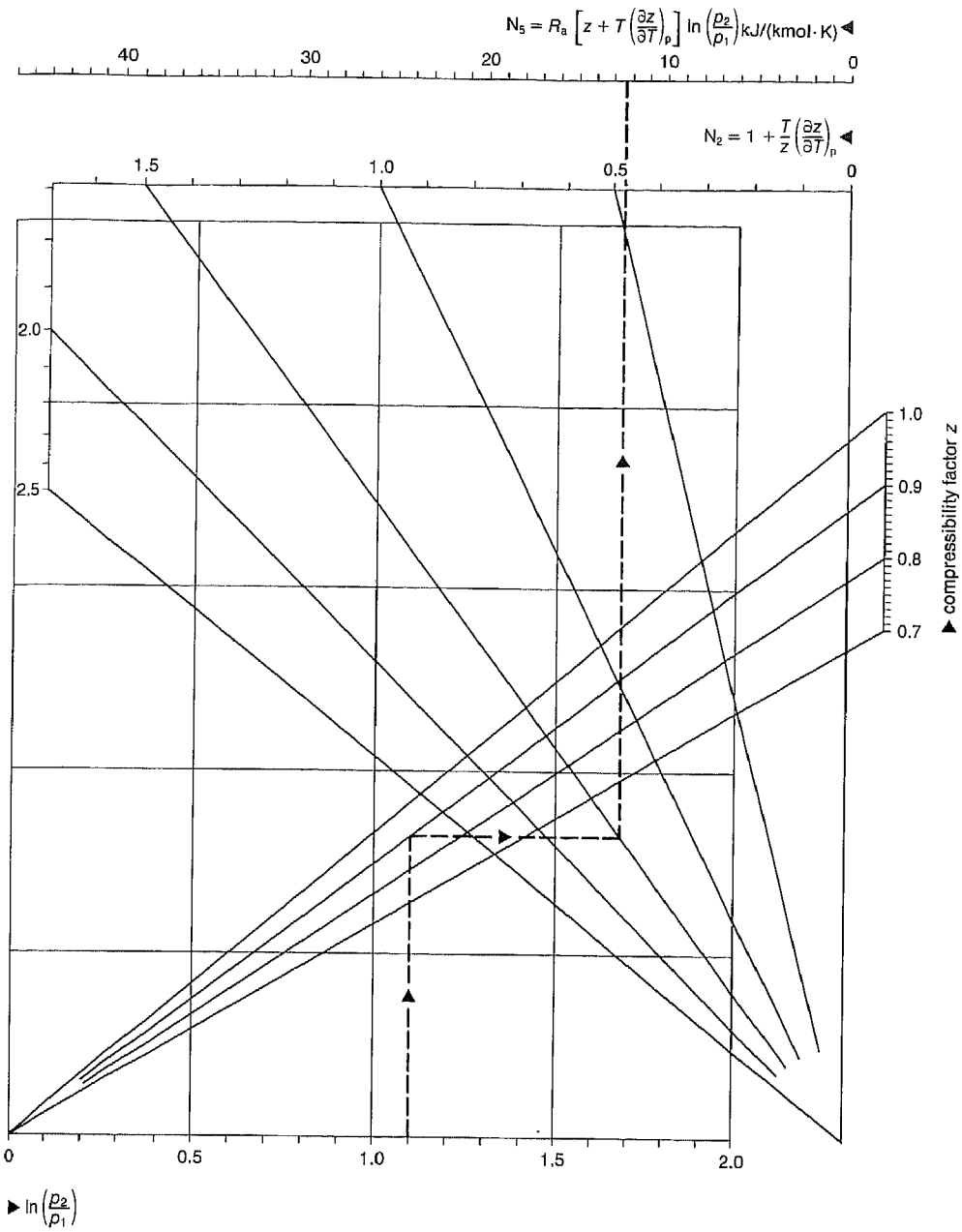


Fig. 2.8.2 N_5 *as a function of the pressure ratio* p_2/p_1, *the compressibility factor z and* N_2 *(fig. 2.7.2)*

After reduction, we have:

$$\left(\frac{\partial T}{\partial p}\right)_s = \frac{R_a \cdot T}{p \cdot c_p}\left[z + T\left(\frac{\partial z}{\partial T}\right)_p\right] \qquad [2.110]$$

or:

$$\left(\frac{\partial T}{\partial p}\right)_s = \frac{k' - 1}{k'}\frac{T}{p} \quad \text{see fig. 2.7.2.2} \qquad [2.111]$$

where:

$\left(\frac{\partial T}{\partial p}\right)_s$	= partial derivative with respect to pressure at constant entropy	[2.111]	K/kPa
k'	= isentropic exponent (2.7.2.2)		–
T	= absolute temperature		K
p	= absolute pressure		kPa

This computation can be simply performed in an *H-S* diagram

Graphic solution:

$$\left(\frac{\partial T}{\partial p}\right)_s = \frac{z \cdot R_a \cdot T}{p \cdot c_p}\left[1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p\right] \qquad [2.110]$$

or:

$$\left(\frac{\partial T}{\partial p}\right)_s = \frac{T}{p}\frac{N_3}{N_2} \qquad [2.112]$$

For $N_2 = 1 + \frac{T}{z}\left(\frac{\partial z}{\partial T}\right)_p$ see fig. 2.7.2 [2.89]

For $N_3 = \frac{R_a \cdot z \cdot N_2^2}{c_p}$ see fig. 2.7.3 [2.96]

2.8.5 Isenthalpic expansion (H = constant; choke effect)

Isenthalpic expansion – the Joule-Thomson effect – is described by (lit. 15, 18):

$$\left(\frac{\partial T}{\partial p}\right)_H = \frac{T}{c_p}\left(\frac{\partial V}{\partial T}\right)_p - \frac{V}{c_p} \quad . \qquad [2.113]$$

After reduction:

$$\left(\frac{\partial T}{\partial p}\right)_H = \frac{R_a \cdot T^2}{p \cdot c_p}\left(\frac{\partial z}{\partial T}\right)_p \qquad [2.114]$$

or

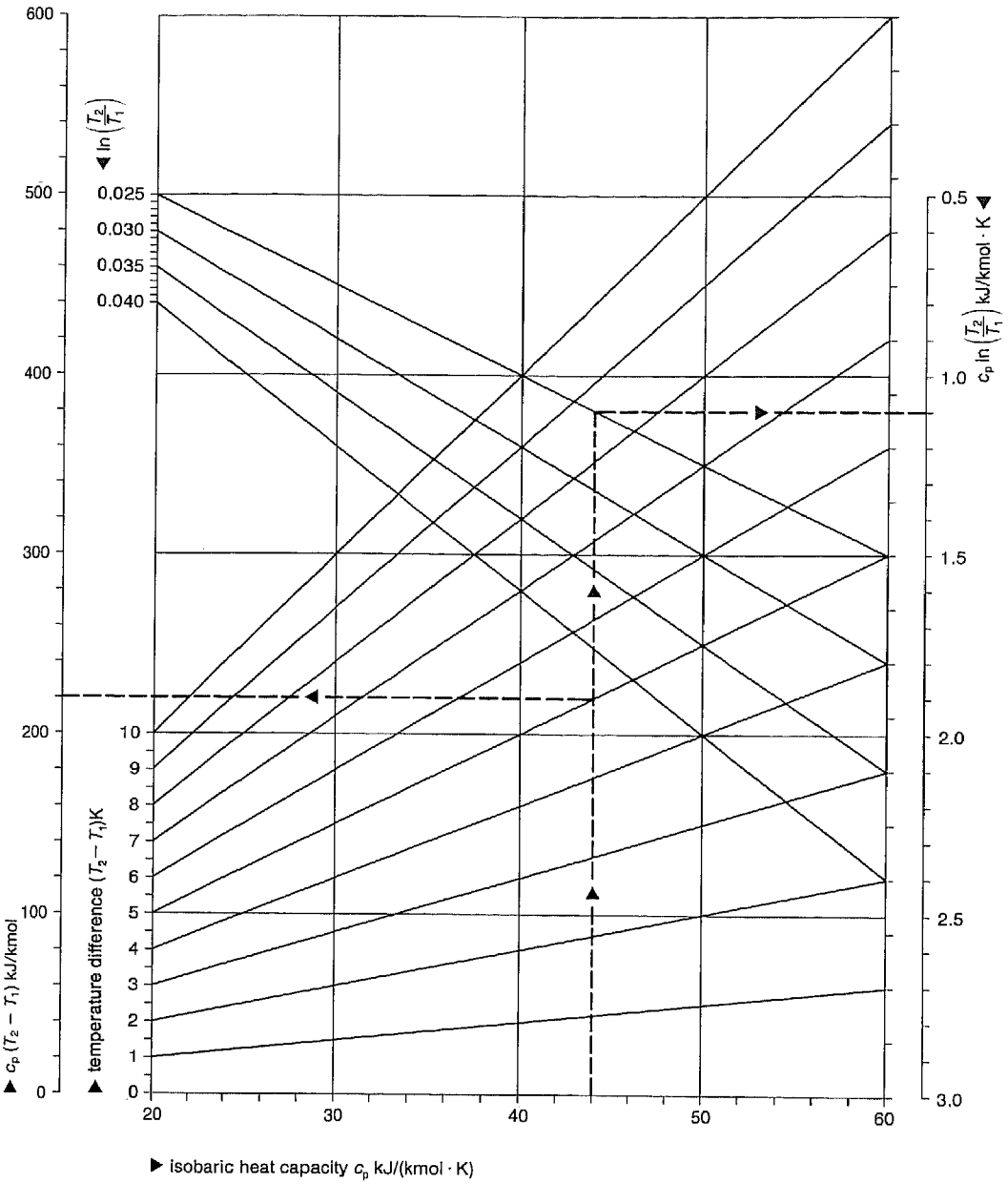


Fig. 2.8.3 Graph for quick determination of $c_p\,(T_2 - T_1)$ and $c_p \ln (T_2/T_1)$ from the heat capacity c_p and the temperature ratio T_2/T_1

$$\left(\frac{\partial T}{\partial p}\right)_H = \frac{T}{p}\frac{k'-1}{k'} - \frac{z \cdot R_a \cdot T}{p \cdot c_p} \quad (2.8.4) \qquad [2.115]$$

where:

$\left(\frac{\partial T}{\partial p}\right)_H$ = partial derivative with respect to pressure at constant enthalpy [2.115] K/kPa

$\frac{T}{p}\frac{k'-1}{k'} = \left(\frac{\partial T}{\partial p}\right)_s$ (2.8.4) [2.111]

$\frac{z \cdot R_a \cdot T}{p \cdot M} = \frac{1}{\varrho}$ (ϱ = density; fig. 2.4) [2.69]

c_p = isobaric heat capacity (2.6.1)

2.8.6 Enthalpy change with pressure and temperature (lit. 24)

The effect of pressure and temperature on enthalpy is represented by:

$$H_2 - H_1 = c_p(T_2 - T_1) - R_a \cdot T^2 \left(\frac{\partial z}{\partial T}\right)_p \ln\left(\frac{p_2}{p_1}\right) \qquad [2.104]\ (2.8.1)$$

2.8.6.1 Isothermal change (T = constant)

At constant temperature ($T_2 = T_1$) the enthalpy change with pressure is represented by:

$$H_2 - H_1 = -R_a \cdot T^2 \left(\frac{\partial z}{\partial T}\right)_p \ln\left(\frac{p_2}{p_1}\right) \qquad [2.116]$$

Graphic solution:

$H_2 - H_1 = -N_4$ kJ/kmol (fig. 2.8.1) where:

$$N_4 = R_a \cdot T^2 \left(\frac{\partial z}{\partial T}\right)_p \ln\left(\frac{p_2}{p_1}\right) \qquad [2.105]\ (2.8.1)$$

2.8.6.2 Isobaric change (p = constant)

At constant pressure ($p_2 = p_1$) the enthalpy change with temperature is represented by:

$$H_2 - H_1 = c_p(T_2 - T_1) \qquad [2.117]$$

Graphic solution:
For $H_2 - H_1 = c_p(T_2 - T_1)$ kJ/kmol (fig. 2.8.3)

2.8.7 Isentropic compression (S = constant)

The power required to compress gases is given by the formula:

$$P = \frac{\varrho_0 \cdot q_0 \cdot z_i \cdot R_a \cdot T_i \cdot k}{\eta_{ad} \cdot 3600 \cdot M(k-1)} \left[C_r^{\frac{k-1}{k}} - 1 \right] \qquad [2.118]$$

where:

P	= power supplied to compressor		kW
ϱ_0	= density (2.4) of the gas (273.15 K; 101.325 kPa)		kg/m^3
η_{ad}	= adiabatic efficiency		–
q_0	= gas flow (273.15 K; 101.325 kPa)		m^3/h
R_a	= universal gas constant (1.1.5)		kJ/(kmol · K)
M	= molar mass (table 1.7)		kg/kmol
z_i	= compressibility factor at inlet conditions p_i and T_i (2.2)		–
k	= isentropic exponent (2.7.2.1) – average value for inlet and outlet conditions		–
C_r	= compression ratio (= p_o/p_i)	[2.119]	–
o	= compressor outlet		
i	= compressor inlet		

The temperature rise due to isentropic compression is represented by:

$$\Delta T_{is} = T_i \left[C_r^{\frac{k'-1}{k'}} - 1 \right] \qquad [2.120]$$

Assuming that the "wasted" portion of the energy supplied to the compressor, i.e. $(1 - \eta_{ad})\,P$, is converted into heat and this heat is absorbed entirely by the gas, we can deduce that:

$$\Delta T_{extra} = \frac{1-\eta_{ad}}{\eta_{ad}} \frac{z_i \cdot R_a \cdot T_i}{c_p} \frac{k}{(k-1)} \left[C_r^{\frac{k-1}{k}} - 1 \right] \qquad [2.121]$$

where:

c_p = isobaric heat capacity (2.6.1) kJ/(kmol · K)

The total temperature rise is thus:

$$\Delta T_{tot} = \Delta T_{is} + \Delta T_{extra} = T_i \left[C_r^{\frac{k'-1}{k'}} - 1 \right] \left[1 + \frac{1-\eta_{ad}}{\eta_{ad}} \frac{z_i \cdot R_a \cdot k'}{c_p\,(k'-1)} \right] \qquad [2.122]$$

where:

ΔT_{tot} = total temperature rise due to compression °C

ΔT_{is} is a function of k' and ΔT_{extra} is a function of k, so that $\Delta T_{tot} = \Delta T_{is} + \Delta T_{extra}$ is not entirely correct. However, since $\Delta T_{is} \simeq 4 \cdot \Delta T_{extra}$ the error introduced is only slight.

2.9 Reynolds number

Reynolds number *Re* is a dimensionless variable which represents the nature of the flow in a pipe:

$$Re = \frac{v \cdot d}{\nu} \qquad [2.123]$$

where:

Re	=	Reynolds number (fig. 2.9)	–
v	=	flow velocity	m/s
d	=	inside diameter of pipe	m
ν	=	kinematic viscosity at p and T (2.5.2)	m^2/s

Example:

$$\left.\begin{array}{l} q_{p,t} = 4000\ m^3/h \\ d = 1\ m = 1000\ mm \end{array}\right\} v = 1.415\ m/s$$

$$\nu = 1 \times 10^{-6}\ m^2/s$$

$$Re = 1.415 \times 10^{-6} \qquad [2.123]$$

From fig. 2.9 the Reynolds number is found:

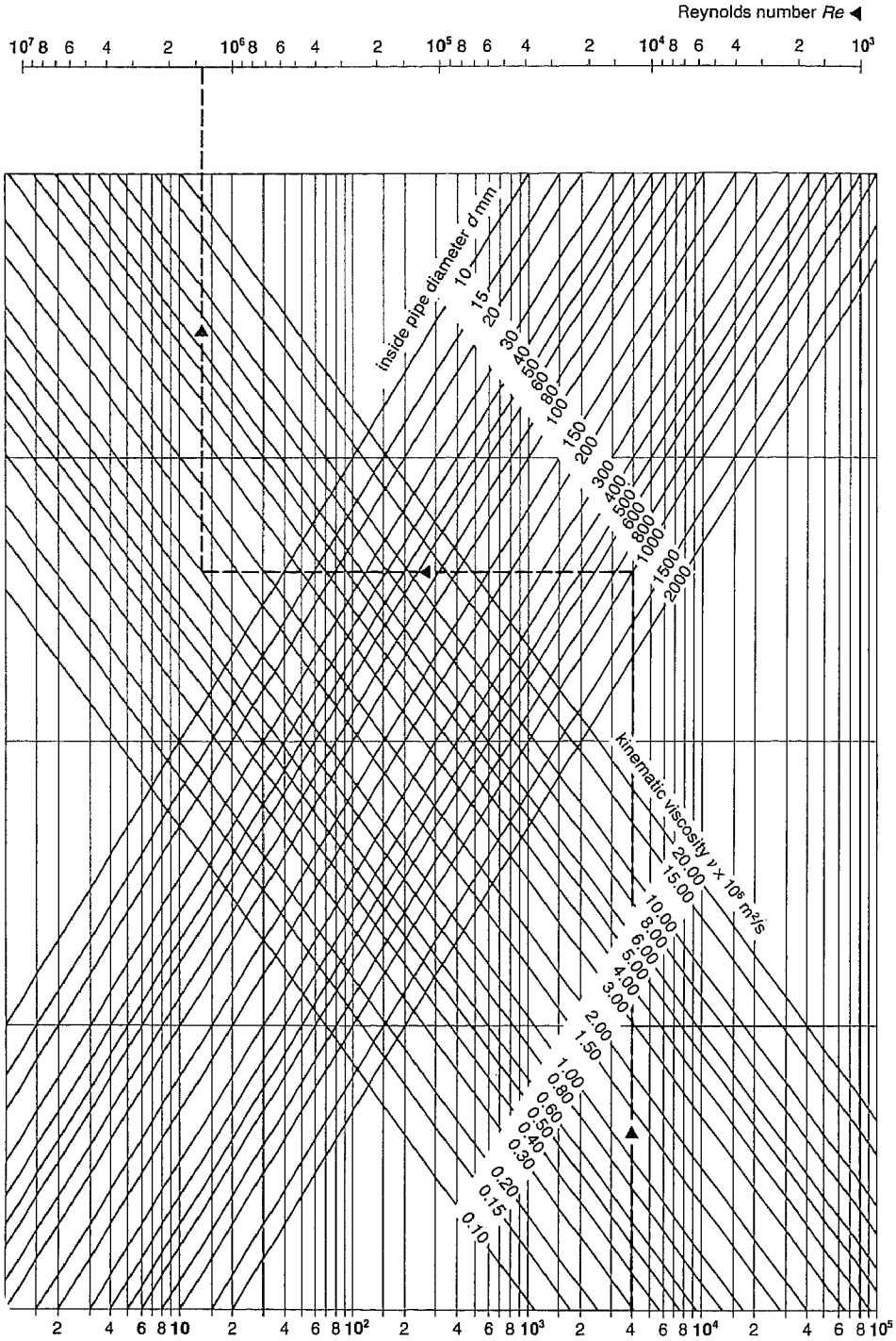
$$Re = 1.4 \times 10^6$$

This means that the flow in this pipe is turbulent

The opposite of turbulent flow is laminar flow. It is not possible to identify a clear transition from laminar to turbulent flow. The literature gives the following values:

$Re < 2000$ laminar flow
$2000 < Re < 40\,000$ transition area in which flow may be laminar or turbulent
$Re > 40\,000$ turbulent flow

Fig. 2.9 The Reynolds number as a function of flow rate $Q_{p,t}$ inside pipe diameter d and the kinematic viscosity ν ▷



flow rate $Q_{p,t}$ m³/h

2.10 Pressure loss in pipes and bends

2.10.1 Pressure loss in pipes

Pressure loss is represented by the general formula:

$$\frac{dp}{dl} = -\frac{\lambda'}{d}\ \frac{1}{2}\varrho \cdot v^2 \qquad [2.124]$$

where:

dp	=	pressure loss over length dl	Pa/m
λ'	=	friction factor (dimensionless)	–
d	=	inside diameter of pipe	m
ϱ	=	average density (2.4) over length dl	kg/m³
v	=	average flow velocity	m/s

In the American literature (such as the AGA Gas Flow Formulas) λ' is represented by f_D – the Darcy-Weisbach friction factor – which is defined as:

$$f_D = 4 \cdot f \qquad [2.125]$$

where:
f = Fanning friction factor

After reduction and integration (fig. 2.10.2):

$$\Delta p = p_1 - p_2 = \lambda' \frac{l}{d}\ \frac{1}{2}\varrho \cdot v^2 \qquad [2.126]$$

or

$$p_1^2 - p_2^2 = \frac{\lambda' \cdot l \cdot z \cdot R_a \cdot T \cdot \varrho_1^2 \cdot q_1^2 \times 10^3}{d \cdot M \cdot A^2} \qquad [2.127]$$

This formula can be rewritten as:

$$\Delta p = p_1 - \left(p_1^2 - \lambda' \frac{l}{d}\ \frac{z \cdot R_a \cdot T}{M}\ \frac{\varrho_1^2 \cdot q_1^2 \times 10^3}{A^2}\right)^{0.5} \qquad [2.128]$$

where:

p_1	=	absolute pressure at the beginning of pipe section with length l	Pa
p_2	=	absolute pressure at the end of pipe section with length l	Pa
λ'	=	friction factor (dimensionless) (fig. 2.10.1)	–
l	=	length of pipe section	m

d	=	inside diameter of pipe	m
z	=	average compressibility factor over pipe section with length l (2.2)	–
R_a	=	universal gas constant (1.1.5)	kJ/(kmol · K)
M	=	molar mass (table 1.7)	kg/kmol
T	=	average temperature over pipe section with length l	K
A	=	cross-sectional area of pipe (for cylindrical pipe $\frac{\pi \cdot d^2}{4}$) [2.129]	m^2
ϱ_1	=	density (T_1, p_1)	kg/m^3
q_1	=	flow rate through pipe (T_1, p_1)	m^3/s
T_1	=	temperature at the beginning of pipe section with length l	K
Δp	=	pressure loss over pipe section with length l	Pa

Since a number of the variables in the above formulas are a function of the magnitude of the pressure loss over pipe section with length l, it is recommended that the calculation be carried out for short pipe sections. Compressibility factor z and density ϱ can then be determined for the initial conditions p_1 and T_1.
Friction factor λ' is a function of the Reynolds number (Re) (fig. 2.10.1) and is subject to the following rules:

laminar flow

according to Hagen-Poiseuille:

$$\lambda' = 64/Re \quad (Re < 2320) \qquad [2.130]$$

turbulent flow

a) according to Blasius:

$$\lambda' = 0.3164/\sqrt[4]{Re} \quad (3000 < Re < 100000) \qquad [2.131]$$

b) according to Von Hermann:

$$\lambda' = 0.00540 + 0.3964/Re^{0.3} \quad (2 \times 10^4 < Re < 2 \times 10^6) \qquad [2.132]$$

c) according to Prandtl and Von Karmann:

$$1/\sqrt{\lambda'} = -0.8 + 2 \log (Re\sqrt{\lambda'}) \quad (Re > 10^6) \qquad [2.133]$$

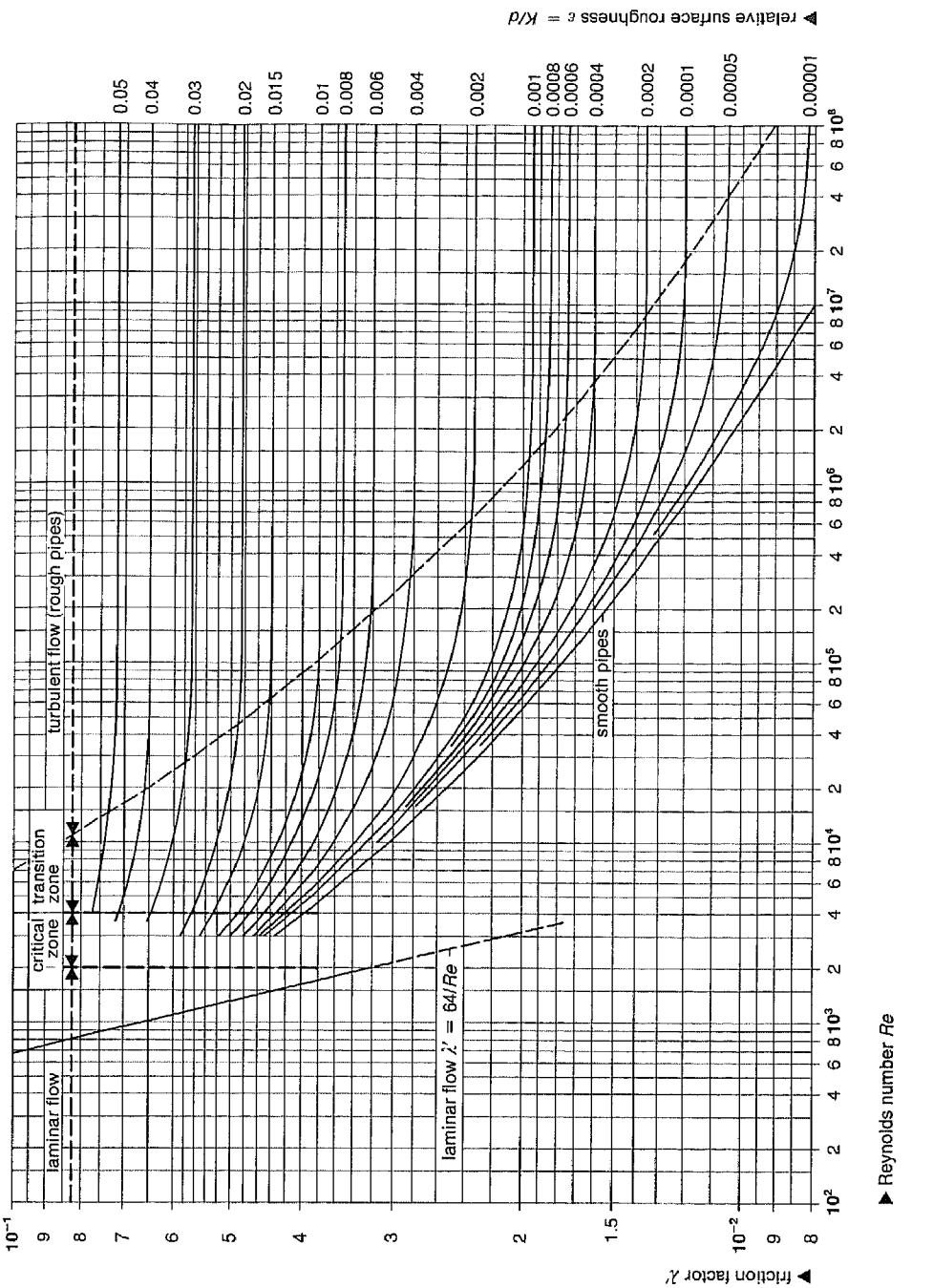
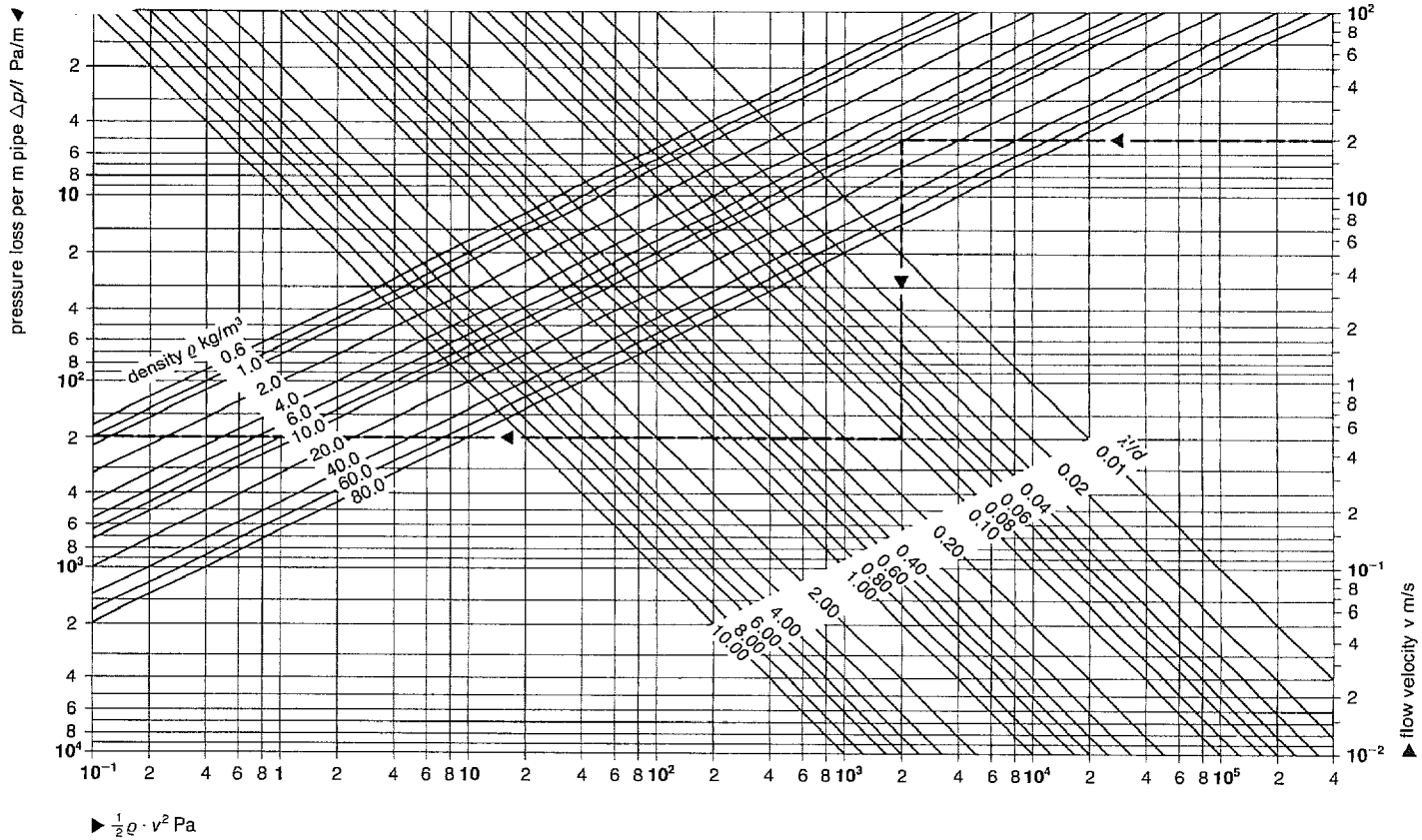


Fig. 2.10.1 The friction factor λ' as a function of the Reynolds number Re and the relative surface roughness K/d for the different flow zones


pressure loss per m pipe Δp/l Pa/m
flow velocity v m/s
▶ ½ϱ · v² Pa
density ϱ kg/m³
0.6
1.0
2.0
4.0
6.0
10.0
20.0
40.0
60.0
80.0
λ/d
0.01
0.02
0.04
0.06
0.08
0.10
0.20
0.40
0.60
0.80
1.00
2.00
4.00
6.00
8.00
10.00

Formula [2.133] gives λ' "implicitly"; a solution can only be found by trial and error. Techo (lit. 25) gives a simpler formula with similar results:

$$\lambda' = \left[0.8685 \ln\left(\frac{Re}{1.964 \ln Re - 3.8215}\right)\right]^{-2} \quad (10^4 < Re < 2.5 \times 10^8) \qquad [2.134]$$

The above rules apply only to "technically smooth" pipes.

The transition from laminar to turbulent flow ($Re \approx 2000$) is called the critical Reynolds number (Re_c). However, this value must not be applied too strictly. With technically smooth pipes, the resistance over a wide Reynolds range is a function not only of Reynolds number, but also of a given surface roughness factor; at high Reynolds numbers, resistance is only a function of surface roughness (fig. 2.10.1).

"Relative" surface roughness is defined as:

$$\varepsilon = \frac{K}{d} \qquad [2.135]$$

where:

ε	= relative surface roughness (dimensionless)	–
K	= average height of all protrusions in the pipe	mm
d	= inside diameter of pipe	mm

According to Prandtl and Von Karmann, a rough pipe is described by:

$$1/\sqrt{\lambda'} = 2 \log\left(\frac{d}{K}\right) + 1.14 = 2 \log\left(3.715 \frac{d}{K}\right) \qquad [2.136]$$

The transition from a "smooth" pipe to a "rough" pipe is given, according to Colebrook and White, by:

$$1/\sqrt{\lambda'} = -2 \log\left(\frac{2.51}{Re\sqrt{\lambda'}} + \frac{K}{3.71 \cdot d}\right) \qquad [2.137]$$

In this formula λ' is also given implicitly. The simpler Techo formula (lit. 25) reads:

$$\lambda' = \left[-0.8685 \ln\left(\frac{1.964 \ln Re - 3.8215}{Re} + \frac{K}{3.71 \cdot d}\right)\right]^{-2} \qquad [2.138]$$

Fig. 2.10.2 Pressure loss per unit length $\Delta p/l$ as a function of the flow velocity v, density ϱ and the "friction factor" λ'/d

Table 2.10 "Absolute" surface roughness factor K

Material	Nature of material	*K* mm
glass, lead, copper and brass pipe		0 – 0.0015
drawn steel pipe	new	0.04 (0.02 – 0.1)
	used (cleaned)	0.15 – 0.20
	lightly corroded	up to 0.40
	severely corroded	up to 3.0
sheet steel	smooth	0.07
galvanised steel pipe	normal galvanising	0.15
welded steel pipe	new	0.05 – 0.1
	new (bitumen coated)	0.05
	used (cleaned)	0.15 – 0.20
	uniformly corroded	up to 0.40
	light scaling	1 – 1.5
	heavy scaling	2 – 4
rivetted steel pipe		0.9 (0.5 – 10)
cast-iron pipe	new	0.26 – 1
	new (bitumen coated)	0.10 – 0.15
	corroded	1.0 – 1.5
	with scaling	1.5 – 4.0
concrete pipe	smooth finish	0.3 – 0.8
	rough	1.2 – 3
asbestos-cement pipe	eternit	0.05 – 0.1
timber	planed	0.2
	sawn	0.7
masonry (brick)	normal pointing	1.3

Table 2.10 gives a number of values for the "absolute" roughness factor K
Fig. 2.10.1 gives friction factor λ' as a function of Reynolds number Re and

"relative" roughness $\varepsilon\left(=\frac{K}{d}\right)$ [2.135] according to Colebrook and White.

Fig. 2.10.2 was constructed using equation [2.126]:

$$\Delta p = \lambda' \frac{l}{d} \frac{1}{2} \varrho \cdot v^2$$

2.10.2 Pressure loss in bends

Bends and coils in pipes have higher coefficients of friction than straight pipes due to vortices and possibly detachment of the flow from the pipe wall. If we assign λ_b' to the coefficient of friction of a coiled pipe, then according to Mishra and Gupta:

laminar flow

$$\lambda_b' = \lambda'\left(1 + 0.033\left[\log Re\sqrt{\frac{d}{D}}\right]^4\right) \qquad [2.139]$$

The formula is valid for:

$$1 < Re\sqrt{\frac{d}{D}} < Re_c\sqrt{\frac{d}{D}}$$

D = average diameter of coil m
d = inside diameter of pipe m

For straight pipes according to Hagen-Poiseuille (2.10.1):

$$\lambda' = 64/Re \quad (\mathrm{Re} < 2320) \qquad [2.130]$$

Re_c is calculated by formula:

$$Re_c = 2300\left(1 + 8.6\left[\frac{d}{D}\right]^{0.45}\right) \qquad [2.140]$$

turbulent flow

$$\lambda_b' = \lambda'\left(1 + 0.095\left[\frac{d}{D}\right]^{0.5} \cdot Re^{0.25}\right) \qquad [2.141]$$

This formula is valid for:

$$Re_c < Re < 100\,000$$

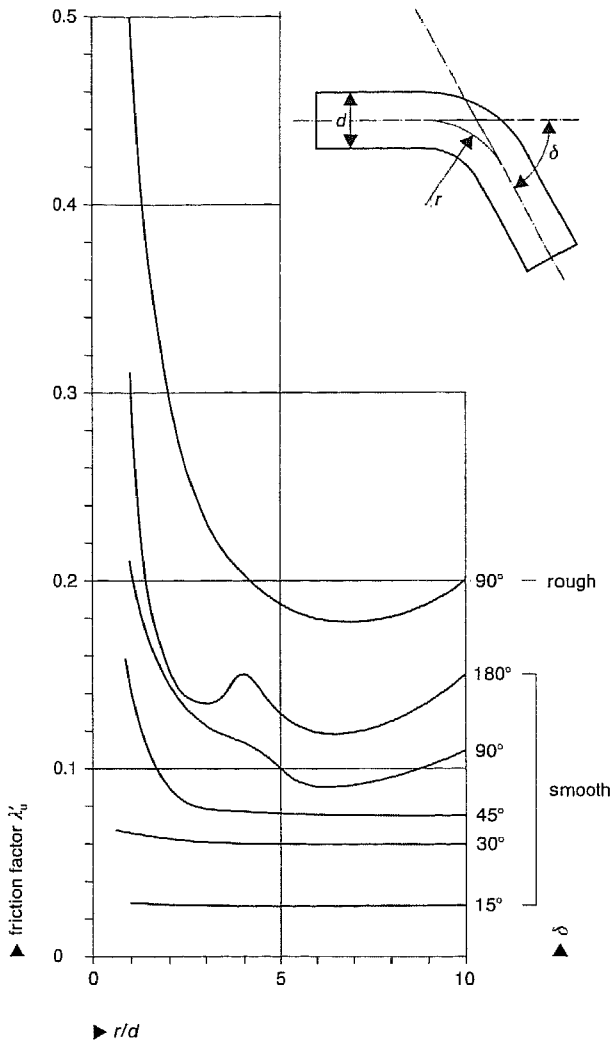


Fig. 2.10.3 The friction factor λ_u^l as a function of the ratio r/d and the angle of bending δ

For straight pipes according to Blasius (2.10.1):

$$\lambda' = \frac{0.3164}{Re^{0.25}}$$

The above formulas are valid provided $h < d$, where h is the distance (difference in height) between two coils

λ'_b is valid for the same length of pipe as λ'. If we write the formulas in the form λ'_b/λ', then the quotient of λ'_b/λ' gives the factor by which the pressure loss in a straight section of pipe of the same length has to be multiplied.

The above formulas are not valid for short bends in a pipeline system. Except the normal pressure losses (2.10.1) Hoffmann and Wasielewski (lit. 35b) account for extra pressure losses due to vortices and detachment of the flow from the pipe wall according to:

$$\Delta p = \lambda'_u \frac{1}{2} \varrho \cdot v^2 \qquad [2.142]$$

The total pressure loss in a bend is therefore:

$$\Delta p = \left(\lambda' \frac{l}{d} + \lambda'_u\right) \frac{1}{2} \varrho \cdot v^2 \qquad [2.143]$$

where:

l = length of bend (as straight pipe) m

Fig. 2.10.3 shows values for λ'_u as a function of the ratio r/d and the angle of bending δ. These values are only valid for $Re > 10^5$

Note: A substantial part of the information in subsection 2.10 was taken from lit. 35a

2.11 Water content of natural gases

The concentration of water vapour – absolute humidity – in a gas mixture is mainly a function of the vapour pressure of water, which in turn is a function of the temperature of the mixture. In addition, the water vapour concentration is further influenced to some extent by:

1. the Poynting effect: the effect of system pressure on water vapour pressure
2. the solubility effect: the effect of intermolecular energy exchange
3. composition: this has little effect in practice and is generally disregarded

The effects referred to in 1. and 2. are difficult to represent in a simple formula (lit. 26)

Fig. 2.11.1 gives the water content of saturated "sweet" natural gases (lit. 8)

The effect of H_2S and CO_2 on water content is shown by fig. 2.11.2 (lit. 27). The CO_2 content has been converted to H_2S by multiplying by a factor of 0.75

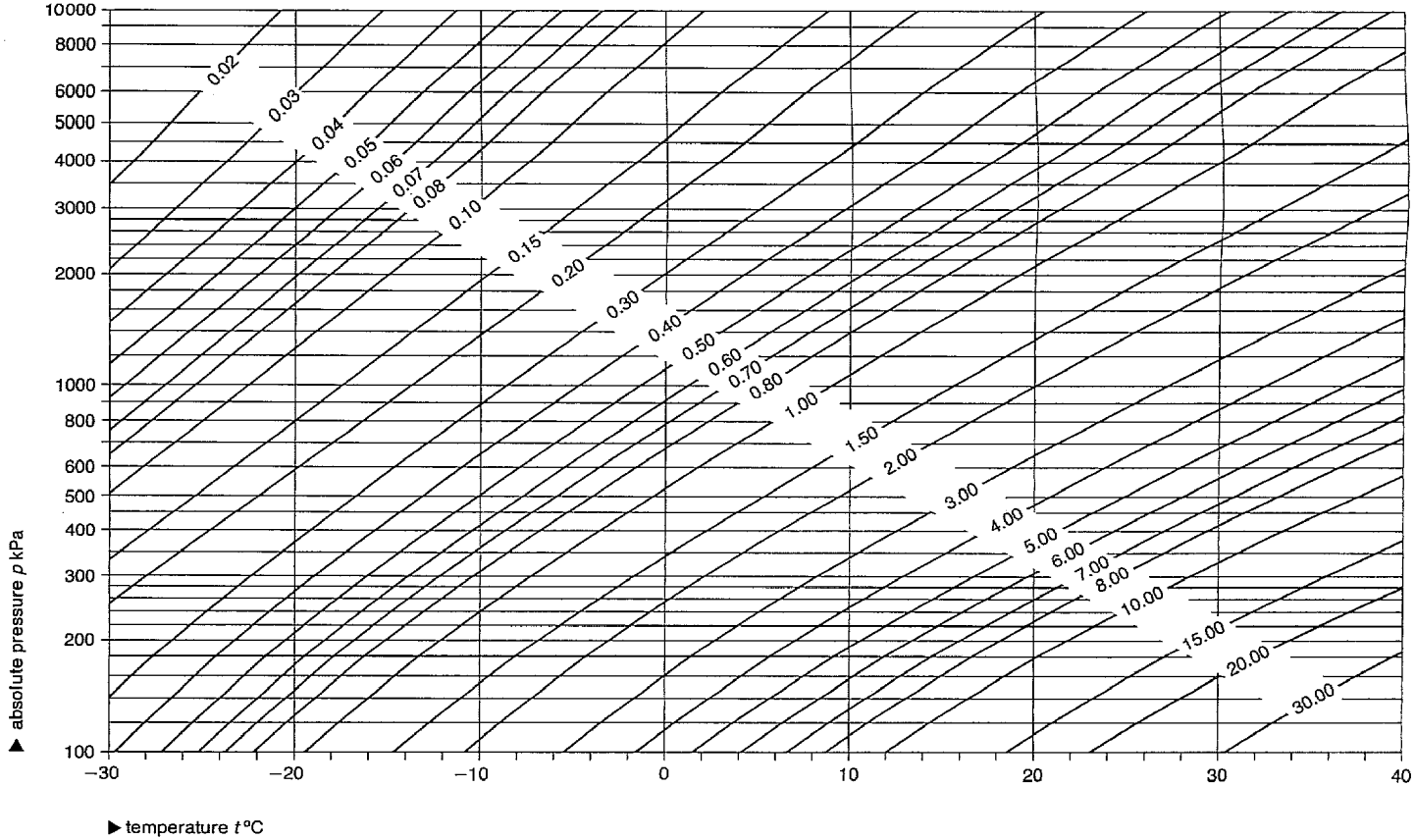
Example: A natural gas containing 10 % (mol) H_2S and 13.3 % (mol) CO_2 is represented in fig. 2.11.2 by a natural gas containing (0.75 x 13.3 + 10) = 20 % (mol) H_2S. The actual water content of a "sour" natural gas is therefore the sum of the water content given by fig. 2.11.1 and the content Δg according to fig. 2.11.2

For the aforementioned natural gas at 8000 kPa and 303.15 K (30 °C) this would amount to:

fig. 2.11.1	0.59 g H_2O/m^3 dry gas
fig. 2.11.2	0.12 g H_2O/m^3 dry gas
Total water content	0.71 g H_2O/m^3 dry gas

Fig. 2.11.1 Water content of natural gases as a function of absolute pressure p and temperature t

▶ water content of natural gases g/m³(0 °C; 101.325 kPa; dry)



▲ absolute pressure p kPa

▶ temperature t °C

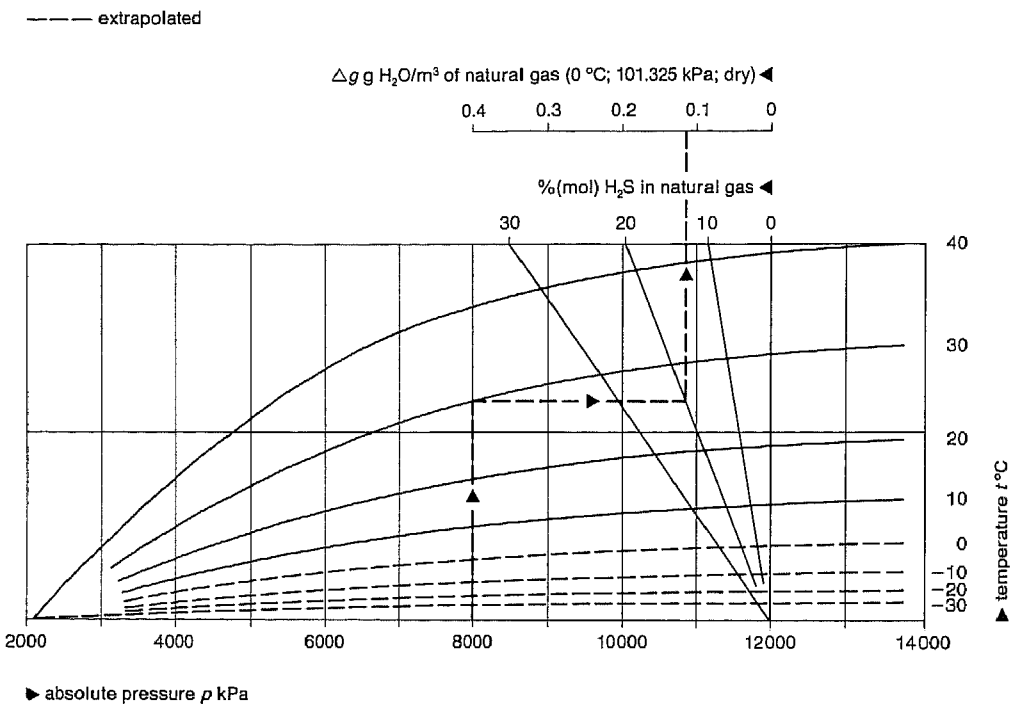


Fig. 2.11.2 Correction on water content of a natural gas Δg as a function of the absolute pressure p, temperature t and the concentration of H_2S in the natural gas. (See example 2.11).

Section 3

Combustion and flue gas properties

3.1 **Calorific values of pure gases and gas mixtures**

3.2 **Combustion of pure gases and gas mixtures**

3.3 **Air requirement**

3.4 **Flue gas composition**

3.5 **Incomplete combustion**

3.5.1 Oxygen deficiency

3.5.2 Factors associated with the combustion process

3.6 **Heat content and "average" isobaric heat capacity**

3.7 **Combustion efficiency**

3.8 **Water dew point and water content**

3.9 **Density**

3.10 **Viscosity**

3.10.1 Dynamic viscosity

3.10.1.1 Sutherland

3.10.1.2 Chapman and Cowling

3.10.1.3 Viscosity of gas mixtures (Herning and Zipperer)

3.10.2 Kinematic viscosity (Mann)

3.11 **Isobaric heat capacity**

3.12 **Thermal conductivity**

3.13 **Theoretical flame temperature**

3.14 **Heat transfer coefficient**

3.15 **Flammability limits and autoignition temperatures of gases and gas mixtures**

3.15.1 General

3.15.2 Factors affecting flammability limits

3.15.3 Calculation of flammability limits

3.15.4 Effect of pressure and temperature on flammability limits

3.1 Calorific values of pure gases and gas mixtures

The definitions of gross calorific value H_s and net calorific value H_i are given in 1.4.2

Table 3.1.1 gives the calorific values as defined in 1.4.2 for a number of hydrocarbons and other combustible gases. The calorific value is defined internationally (lit. 2) as follows:

$$H[T_H, V(T_v; p_v)] \qquad (1.4.2)$$

where:

H = calorific value (1.4.2)
T_H = temperature to which the combustion products are cooled
T_v = temperature used in definition of m^3
p_v = pressure used in definition of m^3

The molar calorific value of a gas mixture can be calculated from the composition of the mixture and the molar calorific value of its components (table 3.1.1):

$$H_s = \sum_{j=1}^{n} n_j \cdot H_{s,j}/100 \qquad [3.1]$$

$$H_i = \sum_{j=1}^{n} n_j \cdot H_{i,j}/100 \qquad [3.2]$$

where:

H_s	=	gross calorific value of gas mixture	MJ/kmol
$H_{s,j}$	=	gross calorific value of component j	MJ/kmol
H_i	=	net calorific value of gas mixture	MJ/kmol
$H_{i,j}$	=	net calorific value of component j	MJ/kmol
n_j	=	concentration of component j	% (mol)
n	=	number of components	–

Conversion from molar basis (MJ/kmol) to volume basis (MJ/m^3):

$$H_s = \left(\sum_{j=1}^{n} n_j \cdot H_{s,j}\right)/(100 \cdot z \cdot V_m) \qquad [3.3]$$

$$H_i = \left(\sum_{j=1}^{n} n_j \cdot H_{i,j}\right)/(100 \cdot z \cdot V_m) \qquad [3.4]$$

Table 3.1.1 Gross and net calorific values of a number of pure gases

No.	Component	Formula	Gross calorific value H_s [298.15, V (273.15; 101.325)]			Net calorific value H_i [298.15, V (273.15; 101.325)]		
			Lit (5)		Lit (1)*)	Lit (5)		Lit (1)*
			MJ/kmol	MJ/m³	MJ/kmol	MJ/kmol	MJ/m³	MJ/kmol
1	methane	CH_4	890.36	39.819	890.65	802.32	35.882	802.62
2	ethane	C_2H_6	1559.88	70.305	1560.69	1427.83	64.353	1428.64
3	propane	C_3H_8	2220.03	101.234	2219.27	2044.01	93.207	2043.11
4	2-methylpropane (isobutane)	C_4H_{10}	2868.72	132.747	2868.20	2648.68	122.565	
5	butane	C_4H_{10}	2877.09	133.691	2877.40	2657.05	123.466	2657.32
6	2,2-dimethylpropane	C_5H_{12}	3516.61	165.203	3514.43	3252.56	152.798	
7	2-methylbutane (isopentane)	C_5H_{12}	3528.12	167.338	3528.87	3264.06	154.814	
8	pentane	C_5H_{12}	3536.15	169.269	3535.77	3272.10	156.629	3271.67
9	2,2-dimethylbutane	C_6H_{14}	4177.89	203.800	4178.06	3869.78	188.770	
10	2,3-dimethylbutane	C_6H_{14}	4185.97	204.194	4186.12	3877.86	189.164	
11	3-methylpentane	C_6H_{14}	4189.82	204.382	4189.91	3881.71	189.352	
12	2-methylpentane (isohexane)	C_6H_{14}	4187.18	204.253	4187.32	3879.07	189.223	
13	hexane	C_6H_{14}	4194.92	204.630	4194.93	3886.81	189.601	3886.84
14	2-methylhexane (isoheptane)	C_7H_{16}	4846.49	236.414	–	4494.37	219.238	
15	heptane	C_7H_{16}	4853.57	236.760	4853.43	4501.44	219.582	4501.30
16	octane	C_8H_{18}	5511.71	268.864	5511.80	5115.57	249.540	5115.56
17	nonane	C_9H_{20}	6170.98	301.024	6171.15	5730.87	279.555	5730.99
18	decane	$C_{10}H_{22}$	6829.71	333.157	6829.77	6345.54	309.538	6345.59
19	undecane	$C_{11}H_{24}$	7488.44	365.290	7488.14	6960.25	339.525	6959.95
20	dodecane	$C_{12}H_{26}$	8147.21	397.425	8147.19	7575.01	369.513	7574.98
21	tridecane	$C_{13}H_{28}$	8805.94	429.558	8805.48	8189.72	399.499	8189.26
22	tetradecane	$C_{14}H_{30}$	9464.67	461.691	9464.15	8804.43	429.485	8803.91
23	cyclohexane	C_6H_{12}	3952.92	192.825		3688.87	179.945	
24	methylcyclohexane	C_7H_{14}	4600.64	224.422		4292.57	209.394	

25	benzene	C_6H_6	3301.51	161.049	3301.5	3169.46	154.608	
26	toluene	C_7H_8	3947.94	192.582	3948.1	3771.88	183.994	
27	xylene (o)	C_8H_{10}	4596.29	224.209	4596.3	4376.21	213.474	
28	methyl mercaptan	CH_3SH	1249.59	57.399		1161.54	53.354	
29	ethyl mercaptan	C_2H_5SH	1899.80	88.908		1767.79	82.730	
30	propyl mercaptan	C_3H_7SH	2548.31	124.156		2372.45	115.589	
31	carbonyl sulphide	COS	548.76	24.844		548.76	24.844	
32	hydrogen sulphide	H_2S	562.54	25.361		518.52	23.377	
33	sulphur dioxide	SO_2	–	–		–	–	
34	ethene	C_2H_4	1410.99	63.434	1411.2	1322.96	59.476	
35	propene	C_3H_6	2058.47	93.612	2057.7	1926.43	87.607	
36	1-butene	C_4H_8	2696.50	125.766	2716.8	2520.50	117.617	
37	1-pentene	C_5H_{10}	3350.00	159.100	3375.4	3130.00	148.730	
38	1,2-butadiene	C_4H_6	2569.50	120.299	2593.79	2437.50	114.175	
39	1-butyne	C_4H_6	2572.50	121.683		2440.50	115.496	
40	methanol	CH_3OH	764.00	36.251		675.98	32.074	
41	ethanol	C_2H_5OH	1426.02	69.374		1293.97	62.950	
42	argon	Ar	–	–		–	–	
43	helium	He	–	–		–	–	
44	carbon dioxide	CO_2	–	–		–	–	
45	carbon monoxide	CO	282.989	12.634		282.989	12.634	
46	hydrogen	H_2	285.840	12.741		241.827	10.779	
47	nitrogen	N_2	–	–		–	–	
48	oxygen	O_2	–	–		–	–	
49	nitric oxide	NO	–	–		–	–	
50	nitrogen dioxide	NO_2	–	–		–	–	
51	water vapour	H_2O	–	–		–	–	
52	air (dry)	–	–	–		–	–	

*) List not yet complete.

where:

z	=	compressibility of the gas mixture at p_v kPa and T_v K (2.2.1.3)	–
V_m	=	normal molar volume of ideal gas (1.1.3)	m^3/kmol

In cases where the consulted literature does not directly provide a figure, calorific value can be calculated on the basis of the "heat of formation".

Example: Calculation of calorific values of methanol (CH_3OH) from the heats of formation

1 mol CH_3OH + 1.5 mol O_2 → 1 mol CO_2 + 2 mol H_2O

Heat of formation:

CH_3OH	– 201.17 MJ/kmol (lit. 12)
CO_2	– 393.51 MJ/kmol (lit. 1)
H_2O (vapour)	– 241.82 MJ/kmol (lit. 1)
H_2O (liquid)	– 285.83 MJ/kmol (lit. 1)

Gross calorific value of gaseous methanol:
– 201.17 – (– 393.51) – 2 (– 285.83) = 764.00 MJ/kmol (table 3.1.1)

Net calorific value of gaseous methanol:
– 201.17 – (– 393.51) – 2 (– 241.82) = 675.98 MJ/kmol (table 3.1.1)

Table 3.1.2 Example: calculation of calorific values of Groningen natural gas (table 1.9)

Component	Formula	n_j	Calorific value MJ/kmol	
		% (mol)	$H_{s,j}$ *)	$H_{i,j}$ *)
methane	CH_4	81.29	890.36	802.32
ethane	C_2H_6	2.87	1 559.88	1 427.83
propane	C_3H_8	0.38	2 220.03	2 044.01
butane	C_4H_{10}	0.15	2 877.09	2 657.05
pentane	C_5H_{12}	0.04	3 536.15	3 272.10
hexane	C_6H_{14}	0.05	4 194.92	3 886.81
nitrogen	N_2	14.32	–	–
oxygen	O_2	0.01	–	–
carbon dioxide	CO_2	0.89	–	–
		100	784.81	708.19

H_s [298.15, V (273.15; 101.325)] = 784.81 MJ/kmol = 35.096 MJ/m^{3}**)
H_i [298.15, V (273.15; 101.325)] = 708.19 MJ/kmol = 31.669 MJ/m^{3}**)

*) Table 3.1.1
**) V = 22.363 m^3/kmol (table 1.9)

3.2 Combustion of pure gases and gas mixtures

The complete combustion of methane with oxygen is described by:

$$1 \text{ mol } CH_4 + 2 \text{ mol } O_2 \rightarrow 1 \text{ mol } CO_2 + 2 \text{ mol } H_2O$$

A reaction equation of this kind can be drawn up for each combustible component in a gas mixture (table 3.2.1). The aggregate of all the quantities of oxygen given by the reaction equations for each of the combustible components present in the mixture gives the total quantity of oxygen required for complete – stoichiometric (1.4.7) – combustion of a gas mixture. Allowance has to be made, however, for any oxygen which may already be present in the mixture.

Similarly, the total quantity of CO_2 and H_2O – and SO_2 where sulphur compounds are present – can be determined by adding the quantities indicated by each of the reaction equations. It is assumed that no nitrogen oxides are formed by the combustion.

Table 3.2.2 gives the theoretical oxygen (O_2) requirement – from which one can determine the "dry" and "wet" air requirement – and the theoretical quantities of carbon dioxide (CO_2), water (H_2O) and sulphur dioxide (SO_2) formed by the stoichiometric combustion with oxygen (O_2) of a number of combustible gases. Table 3.2.3 gives an example of the combustion of 1 m^3 of Groningen natural gas (table 1.9). The necessary data have been derived from table 2.2.5 and 3.2.1

Combustion of Groningen natural gas with oxygen thus requires:

– 1.763 0 mol O_2/mol gas or $\frac{1.763\,0 \times 0.999\,0}{0.997\,7} = 1.765\,3 \text{ m}^3 \text{ O}_2/\text{m}^3 \text{ gas}$

and yields:

– 0.901 6 mol CO_2/mol gas or $\frac{0.901\,6 \times 0.993\,0}{0.997\,7} = 0.897\,4 \text{ m}^3 \text{ CO}_2/\text{m}^3 \text{ gas}$

– 1.740 5 mol H_2O/mol gas or $\frac{1.740\,5 \times 0.965\,0}{0.997\,7} = 1.683\,5 \text{ m}^3 \text{ H}_2\text{O}/\text{m}^3 \text{ gas}$

– 0.143 2 mol N_2/mol gas or $\frac{0.143\,2 \times 0.999\,6}{0.997\,7} = 0.143\,5 \text{ m}^3 \text{ N}_2/\text{m}^3 \text{ gas}$

Table 3.2.3 Stoichiometric combustion of Groningen natural gas

Component	Formula	n_i *) % (mol)	Quantity O_2 required mol/mol	Quantity formed CO_2 mol/mol	Quantity formed H_2O mol/mol
methane	CH_4	81.29	1.625 8	0.812 9	1.625 8
ethane	C_2H_6	2.87	0.100 5	0.057 4	0.086 1
propane	C_3H_8	0.38	0.019 0	0.011 4	0.015 2
butane	C_4H_{10}	0.15	0.009 8	0.006 0	0.007 5
pentane	C_5H_{12}	0.04	0.003 2	0.002 0	0.002 4
hexane	C_6H_{14}	0.05	0.004 8	0.003 0	0.003 5
nitrogen	N_2	14.32			
oxygen	O_2	0.01	−0.000 1		
carbon dioxide	CO_2	0.89		+0.008 9	
		100.00	1.763 0	0.901 6	1.740 5

*) Table 1.9

3.2.1 Stoichiometric combustion of gases

No.	Component	Formula	Stoichiometric combustion of 1 mol of gas with oxygen					
			Needed:			Formed:		
			O_2 mol/mol	Dry air*) mol/mol	Wet air*) mol/mol	CO_2 mol/mol	H_2O mol/mol	SO_2/NO_2 mol/mol
1	methane	CH_4	2	9.5465	9.6618	1	2	–
2	ethane	C_2H_6	3.5	16.7064	16.9082	2	3	–
3	propane	C_3H_8	5	23.8663	24.1546	3	4	–
4	2-methylpropane (isobutane)	C_4H_{10}	6.5	31.0263	31.4010	4	5	–
5	butane	C_4H_{10}	6.5	31.0263	31.4010	4	5	–
6	2,2-dimethylpropane	C_5H_{12}	8	38.1862	38.6473	5	6	–
7	2-methylbutane (isopentane)	C_5H_{12}	8	38.1862	38.6473	5	6	–
8	pentane	C_5H_{12}	8	38.1862	38.6473	5	6	–
9	2,2-dimethylbutane	C_6H_{14}	9.5	45.3461	45.8937	6	7	–
10	2,3-dimethylbutane	C_6H_{14}	9.5	45.3461	45.8937	6	7	–
11	3-methylpentane	C_6H_{14}	9.5	45.3461	45.8937	6	7	–
12	2-methylpentane (isohexane)	C_6H_{14}	9.5	45.3461	45.8937	6	7	–
13	hexane	C_6H_{14}	9.5	45.3461	45.8937	6	7	–
14	2-methylhexane (isoheptane)	C_7H_{16}	11	52.5060	53.1401	7	8	–
15	heptane	C_7H_{16}	11	52.5060	53.1401	7	8	–
16	octane	C_8H_{18}	12.5	59.6659	60.3865	8	9	–
17	nonane	C_9H_{20}	14	66.8258	67.6329	9	10	–
18	decane	$C_{10}H_{22}$	15.5	73.9857	74.8792	10	11	–
19	undecane	$C_{11}H_{24}$	17	81.1456	82.1256	11	12	–
20	dodecane	$C_{12}H_{26}$	18.5	88.3055	89.3720	12	13	–
21	tridecane	$C_{13}H_{28}$	20	95.4654	96.6184	13	14	–
22	tetradecane	$C_{14}H_{30}$	21.5	102.6253	103.8647	14	15	–
23	cyclohexane	C_6H_{12}	9	42.9594	43.4783	6	6	–
24	methylcyclohexane	C_7H_{14}	10.5	50.1193	50.7246	7	7	–

25	benzene	C_6H_6	7.5	35.7995	36.2319	6	3	–
26	toluene	C_7H_8	9	42.9594	43.4783	7	4	–
27	xylene (o)	C_8H_{10}	10.5	50.1193	50.7246	8	5	–
28	methyl mercaptan	CH_3SH	3	14.3198	14.4928	1	2	SO_2 : 1
29	ethyl mercaptan	C_2H_5SH	4.5	21.4797	21.7391	2	3	SO_2 : 1
30	propyl mercaptan	C_3H_7SH	6	28.6396	28.9855	3	4	SO_2 : 1
31	carbonyl sulphide	COS	1.5	7.1599	7.2464	1	–	SO_2 : 1
32	hydrogen sulphide	H_2S	1.5	7.1599	7.2464	–	1	SO_2 : 1
33	sulphur dioxide	SO_2	–	–		–	–	–
34	ethene	C_2H_4	3	14.3198	14.4928	2	2	–
35	propene	C_3H_6	4.5	21.4797	21.7391	3	3	–
36	1-butene	C_4H_8	6	28.6396	28.9835	4	4	–
37	1-pentene	C_5H_{10}	7.5	35.7995	36.2319	5	5	–
38	1,2-butadiene	C_4H_6	5.5	26.2530	26.5700	4	3	–
39	1-butyne	C_4H_6	5.5	26.2530	26.5700	4	3	–
40	methanol	CH_3OH	1.5	7.1599	7.2464	1	2	–
41	ethanol	C_2H_5OH	3	14.3198	14.4928	2	3	–
42	argon	Ar	–	–		–	–	–
43	helium	He	–	–		–	–	–
44	carbon dioxide	CO_2	–	–		–	–	–
45	carbon monoxide	CO	0.5	2.3866	2.4155	1	–	–
46	hydrogen	H_2	0.5	2.3866	2.4155	–	1	–
47	nitrogen	N_2	–	–		–	–	–
48	oxygen	O_2	–	–		–	–	–
49	nitric oxide	NO**)	0.5	2.3866	2.4155	–	–	NO_2 : 1
50	nitrogen dioxide	NO_2	–	–		–	–	–
51	water vapour	H_2O	–	–		–	–	–
52	air (dry)	–	–	–		–	–	–

*) 3.3.
**) Non combustible: O_2 or air needed to form NO_2

Table 3.2.2 Stoichiometric combustion of gases

No.	Component	Formula	Stoichiometric combustion of 1 m^3 of gas with oxygen					
			Needed:			Formed:		
			O_2 m^3/m^3	Dry air* m^3/m^3	Wet air* m^3/m^3	CO_2 m^3/m^3	H_2O m^3/m^3	Remarks
1	methane	CH_4	2.0028	9.5645	9.6754	0.9954	1.9346	
2	ethane	C_2H_6	3.5322	16.8682	17.0638	2.0063	2.9245	
3	propane	C_3H_8	5.1053	24.3806	24.6633	3.0448	3.9452	
4	2-methylpropane (isobutane)	C_4H_{10}	6.7332	32.1547	32.5275	4.1186	5.0031	
5	butane	C_4H_{10}	6.7634	32.2989	32.6734	4.1371	5.0255	
6	2,2-dimethylpropane	C_5H_{12}	8.4162	40.1920	40.6580	5.2285	6.0973	
7	2-methylbutane (isopentane)	C_5H_{12}	8.5076	40.6285	41.0995	5.2853	6.1635	
8	pentane	C_5H_{12}	8.5760	40.9551	41.4300	5.3278	6.2131	
9	2,2-dimethylbutane	C_6H_{14}	10.3687	49.5162	50.0903	6.5093	7.3801	
10	2,3-dimethylbutane	C_6H_{14}	10.3765	49.5535	50.1280	6.5142	7.3856	
11	3-methylpentane	C_6H_{14}	10.3765	49.5535	50.1280	6.5142	7.3856	
12	2-methylpentane (isohexane)	C_6H_{14}	10.3765	49.5535	50.1280	6.5142	7.3856	
13	hexane	C_6H_{14}	10.3765	49.5535	50.1280	6.5142	7.3856	
14	2-methylhexane (isoheptane)	C_7H_{16}	12.0149	57.3777	58.0430	7.5999	8.4407	
15	heptane	C_7H_{16}	12.0149	57.3777	58.0430	7.5999	8.4407	
16	octane	C_8H_{18}	13.6533	65.2020	65.9580	8.6856	9.4958	
17	nonane	C_9H_{20}	15.2917	73.0263	73.8729	9.7713	10.5509	
18	decane	$C_{10}H_{22}$	16.9301	80.8505	81.7879	10.8570	11.6060	
19	undecane	$C_{11}H_{24}$	18.5685	88.6748	89.7029	11.9427	12.6611	
20	dodecane	$C_{12}H_{26}$	20.2069	96.4990	97.6179	13.0284	13.7162	
21	tridecane	$C_{13}H_{28}$	21.8453	104.3233	105.5329	14.1142	14.7712	
22	tetradecane	$C_{14}H_{30}$	23.4837	112.1476	113.4478	15.1999	15.8263	
23	cyclohexane	C_6H_{12}	9.8304	46.9456	47.4899	6.5142	6.3305	
24	methylcyclohexane	C_7H_{14}	11.4688	54.7698	55.4048	7.5999	7.3856	

25	benzene	C_6H_6	8.192 0	39.121 3	39.5749	6.514 2	3.165 3	
26	toluene	C_7H_8	9.830 4	46.945 6	47.489 9	7.599 9	4.220 4	
27	xylene (o)	C_8H_{10}	11.468 8	54.769 8	55.404 8	8.685 6	5.275 4	
28	methyl mercaptan	CH_3SH	3.082 7	14.721 6	14.892 3	1.021 4	1.9852	SO_2: 1.007 0 m^3/m^3
29	ethyl mercaptan	C_2H_5SH	4.721 7	22.548 7	22.810 1	2.085 9	3.040 6	SO_2: 1.028 3 m^3/m^3
30	propyl mercaptan	C_3H_7SH	6.533 0	31.198 7	31.560 4	3.246 9	4.207 1	SO_2: 1.067 0 m^3/m^3
31	carbonyl sulphide	COS	1.522 3	7.269 8	7.354 1	1.007 7	–	SO_2: 0.994 5 m^3/m^3
32	hydrogen sulphide	H_2S	1.513 8	7.229 2	7.313 0	–	0.974 8	SO_2: 0.989 0 m^3/m^3
33	sulphur dioxide	SO_2	–	–	–	–	–	
34	ethene	C_2H_4	3.019 9	14.421 7	14.588 9	2.001 2	1.944 8	
35	propene	C_3H_6	4.582 1	21.882 0	22.135 7	3.036 4	2.950 8	
36	1-butane	C_4H_8	6.215 3	29.681 5	30.025 6	4.118 6	4.002 5	
37	1-pentene	C_5H_{10}	7.980 1	38.109 4	38.551 2	5.288 1	5.139 0	
38	1,2-butadiene	C_4H_6	5.730 6	27.3668	27.684 1	4.142 7	3.019 4	
39	1-butyne	C_4H_6	5.770 9	27.559 2	27.878 7	4.171 8	3.040 6	
40	methanol	CH_3OH	1.565 7	7.477 1	7.563 8	1.037 5	2.016 5	
41	ethanol	C_2H_5OH	3.267 9	15.606 0	15.787 0	2.165 5	3.156 7	
42	argon	Ar	–	–	–	–	–	
43	helium	He	–	–	–	–	–	
44	carbon dioxide	CO_2	–	–	–	–	–	
45	carbon monoxide	CO	0.499 7	2.386 3	2.414 0	0.993 5	–	
46	hydrogen	H_2	0.499 0	2.383 0	2.410 6	–	0.964 0	
47	nitrogen	N_2	–	–	–	–	–	
48	oxygen	O_2	–	–	–	–	–	
49	nitric oxide	NO**)	0.499 8	2.386 8	2.414 5	–	–	NO_2: 0,973 3 m^3/m^3
50	nitrogen dioxide	NO_2	–	–	–	–	–	
51	water vapour	H_2O	–	–	–	–	–	
52	air (dry)	–	–	–	–	–	–	

*) 3.3
**) Noncombustible: O_2 or air needed to form NO_2

3.3 Air requirement

The air required for the combustion of a gas is calculated from the quantity of oxygen required (table 3.2.2) and the oxygen content of the "combustion air" (table 3.3.1 and 3.3.2). The average composition of "dry" air is taken as that given in lit. 17 (table 3.3.1)

Since dry air never occurs in practice, the calculation is generally based on "wet" combustion air. The absolute water vapour content of this "wet" air can be calculated using a simply derived formula:

$$x = 1000 \frac{R_{da}}{R_{wv}} \frac{\Phi \cdot p}{p_o - \Phi \cdot p} \qquad [3.5]$$

where:

x	=	water vapour content of "wet" air	g H_2O/kg dry air
R_{da}	=	gas constant for dry air (= 8 314.41/28.964)	J/(kg · K)
R_{wv}	=	gas constant for water vapour (= 8 314.41/18.015)	J/(kg · K)
Φ	=	relative humidity ($0 \leq \Phi \leq 1$)	–
p	=	saturation pressure of water vapour [3.36]; (fig. 3.8.2)	kPa
p_o	=	total system pressure (in this case 101.325)	kPa

The water vapour concentration in % (vol.) can be calculated from:

$$x' = \left(\frac{\Phi \cdot p}{p_o}\right) \times 100\ \%\ \text{(vol.)} \qquad [3.6]$$

The average relative humidity of air at 20 °C is 50 %. The water vapour content can be determined from the above formulas:

$$x = 1000 \frac{18.015}{28.964} \frac{0.5 \times 2.337}{101.325 - 0.5 \times 2.337} = 7.256\ \text{g}H_2O\text{/kg dry air}$$

$$x' = (0.5 \times 2.337/101.325) \times 100\ \% = 1.15\ \%\ \text{(vol.)}$$

It is thus possible to calculate the composition of "wet" air (table 3.3.2)

Table 3.2.2 gives the theoretical "dry" and "wet" air requirement for a number of combustible gases – components of natural gases or other gas mixtures – based on the oxygen content of "dry" air given in table 3.3.1 and that of "wet" air given in table 3.3.2.

Table 3.3.1 Composition of "dry" air

Component	Formula	n_i *) % (mol)	Real molar volume**) V m^3/kmol	x_i % (vol.)
nitrogen	N_2	78.09	22.404 8	78.10
oxygen	O_2	20.95	22.391 4	20.94
argon	Ar	0.93	22.393 6	0.93
carbon dioxide	CO_2	0.03	22.256 9	0.03
		100.00		100.00

*) Lit. 17
**) Table 1.7

Table 3.3.2 Composition of "wet" air

Component	Formula	x*) % (vol.)	Real molar volume**) V m^3/kmol	n_i % (mol)
nitrogen	N_2	77.20	22.404 8	77.16
oxygen	O_2	20.70	22.391 4	20.70
argon	Ar	0.92	22.393 6	0.92
carbon dioxide	CO_2	0.03	22.256 9	0.03
water vapour	H_2O	1.15	21.629	1.19
		100.00		100.00

*) Table 3.3.1
**) Table 1.7

The theoretical air requirement for gas mixtures is calculated from:

$$a = \frac{z_{O_2}\left[\left(\sum_{i=1}^{n} n_i \cdot O_{2,i}\right) - n_{O_2,g}\right]}{z_g \cdot x_{O_2,a}} \qquad [3.7]$$

where:

a	=	theoretical air requirement	m^3/m^3 gas
n_i	=	concentration of component i	% (mol)
$O_{2,i}$	=	oxygen requirement for complete combustion of component i (table 3.2.1)	mol/mol gas
$n_{O_2,g}$	=	concentraton of O_2 in gas (see example table 3.2.3)	% (mol)
$x_{O_2,a}$	=	concentration of O_2 in "dry" or "wet" air (table 3.3.1 or 3.3.2)	% (vol.)
z_{O_2}	=	compressibility of oxygen at 0 °C and 101.325 kPa (table 2.2.5 – API)	–
z_g	=	compressibility of gas mixture at 0 °C and 101.325 kPa (2.2)	–
n	=	number of components	–

The theoretical air requirement a for the combustion of 1 m^3 of Groningen natural gas is:

"dry" air (table 3.2.3 and 3.3.1) = 8.430 3 m^3
"wet" air (table 3.2.3 and 3.3.2) = 8.528 0 m^3

The definition of air factor a_f is given in 1.4.8

Note: In this reference manual, "wet" air is understood in all cases to mean air with a water vapour content corresponding to a relative humidity of 50 % at 20°C and 101.325 kPa

3.4 Flue gas composition

The flue gas composition is a function of the composition of the combustible gas and may consists of:

nitrogen	N_2
argon	Ar
carbon dioxide	CO_2
carbon monoxide	CO
water vapour	H_2O
hydrogen	H_2
oxygen	O_2
sulphur dioxide	SO_2

Any NO_x which may be formed is disregarded

The total quantity of combustion products q_{tot} per m^3 of combustible gas consists of the sum of the products formed by stoichiometric combustion q_{st} (table 3.4.1 and 3.4.2) and the excess ($a_f - 1$) of combustion air which does not take part in the combustion reaction:

$$q_{tot} = q_{st} + (a_f - 1)\, a \qquad [3.8]$$

where:

q_{tot}	=	total quantity of combustion products	m^3/m^3 gas
q_{st}	=	quantity of combustion products formed by stoichiometric combustion ($a_f = 1$) (table 3.4.1 and 3.4.2)	m^3/m^3 gas
a_f	=	air factor	–
$a_f - 1$	=	excess air	–
a	=	theoretical air requirement (table 3.2.2)	m^3/m^3 gas

The composition of the combustion products for $a_f = 1$ is given by table 3.4.1 and 3.4.2:

$$q_{CO_2} = \left(\sum_{i=1}^{n} n_i \cdot CO_{2,i} + n_{CO_2,g} + a_f \cdot n_{CO_2,a} \cdot a\right) \frac{z_{CO_2}}{z_g \cdot 100} \qquad m^3\ CO_2/m^3\ \text{gas}\ [3.9]$$

$$q_{H_2O} = \left(\sum_{i=1}^{n} n_i \cdot H_2O_i + a_f \cdot n_{H_2O,a} \cdot a\right) \frac{z_{H_2O}}{z_g \cdot 100} \qquad m^3 H_2O/m^3\ \text{gas}\ [3.10]$$

$$q_{N_2} = (n_{N_2,g} + a_f \cdot n_{N_2,a} \cdot a) \frac{z_{N_2}}{z_g \cdot 100} \qquad m^3 N_2/m^3\ \text{gas}\ [3.11]$$

$$q_{Ar} = a_f \cdot n_{Ar,a} \cdot a \frac{z_{Ar}}{z_g \cdot 100} \qquad m^3\ Ar/m^3\ \text{gas}\ [3.12]$$

Table 3.4.1 Flue gas products formed by stoichiometric combustion of 1 m³ of gas with "dry" air

No.	Component	Formula	Flue gas products formed by stoichiometric combustion of 1 m³ of gas with "dry" air					
			CO_2 m³	N_2 m³	Ar m³	H_2O m³	SO_2 or NO_2 m³	Total m³
1	methane	CH_4	0.998 2	7.469 8	0.088 9	1.934 6		10.491 5
2	ethane	C_2H_6	2.011 3	13.173 9	0.156 8	2.924 5		18.266 5
3	propane	C_3H_8	3.052 1	19.041 1	0.226 7	3.945 2		26.265 1
4	2-methylpropane (isobutane)	C_4H_{10}	4.128 2	25.112 7	0.298 9	5.003 1		34.542 9
5	butane	C_4H_{10}	4.146 8	25.225 2	0.300 3	5.025 5		34.697 8
6	2,2-dimethylpropane	C_5H_{12}	5.240 5	31.389 7	0.373 6	6.097 3		43.101 1
7	2-methylbutane (isopentane)	C_5H_{12}	5.297 4	31.730 5	0.377 7	6.163 5		43.569 1
8	pentane	C_5H_{12}	5.340 0	31.985 9	0.380 7	6.213 1		43.919 7
9	2,2-dimethylbutane	C_6H_{14}	6.524 0	38.672 1	0.460 3	7.380 1		53.036 5
10	2,3-dimethylbutane	C_6H_{14}	6.529 0	38.701 7	0.460 7	7.385 7		53.077 1
11	3-methylpentane	C_6H_{14}	6.529 0	38.701 7	0.460 7	7.385 7		53.077 1
12	2-methylpentane (isohexane)	C_6H_{14}	6.529 0	38.701 7	0.460 7	7.385 7		53.077 1
13	hexane	C_6H_{14}	6.529 0	38.701 7	0.460 7	7.385 7		53.077 1
14	2-methylhexane (isoheptane)	C_7H_{16}	7.617 0	44.812 5	0.533 4	8.440 8		61.403 7
15	heptane	C_7H_{16}	7.617 0	44.812 5	0.533 4	8.440 8		61.403 7
16	octane	C_8H_{18}	8.705 1	50.923 3	0.606 2	9.496 0		69.730 6
17	nonane	C_9H_{20}	9.793 0	57.034 1	0.678 9	10.551 1		78.057 1
18	decane	$C_{10}H_{22}$	10.881 3	63.144 9	0.751 6	11.606 2		86.384 0
19	undecane	$C_{11}H_{24}$	11.969 4	69.255 7	0.824 4	12.661 3		94.710 8
20	dodecane	$C_{12}H_{26}$	13.057 4	75.366 5	0.897 1	13.716 4		103.037 4
21	tridecane	$C_{13}H_{28}$	14.145 6	81.477 3	0.969 9	14.771 5		111.364 3
22	tetradecane	$C_{14}H_{30}$	15.233 6	87.588 1	1.042 6	15.826 6		119.690 9
23	cyclohexane	C_6H_{12}	6.528 3	36.664 8	0.436 4	6.330 6		49.960 1
24	methylcyclohexane	C_7H_{14}	7.616 3	42.775 6	0.509 2	7.385 7		58.286 8

25	benzene	C_6H_6	6.5260	30.5540	0.3637	3.1653		40.6090
26	toluene	C_7H_8	7.6140	36.6648	0.4364	4.2204		48.9356
27	xylene (o)	C_8H_{10}	8.7021	42.7756	0.5092	5.2755		57.2624
28	methyl mercaptan	CH_3SH	1.0258	11.4975	0.1369	1.9852	SO_2: 1.0070	15.6524
29	ethyl mercaptan	C_2H_5SH	2.0926	17.6103	0.2096	3.0405	SO_2: 1.0283	23.9813
30	propyl mercaptan	C_3H_7SH	3.2562	24.3659	0.2900	4.2071	SO_2: 1.0670	33.1862
31	carbonyl sulphide	COS	1.0109	5.6775	0.0676	–	SO_2: 0.9945	7.7505
32	hydrogen sulphide	H_2S	0.0022	5.6460	0.0672	0.9748	SO_2: 0.9890	7.6792
33	sulphur dioxide	SO_2	–	–	–	–		–
34	ethene	C_2H_4	2.0055	11.2635	0.1341	1.9448		15.3479
35	propene	C_3H_6	3.0429	17.0898	0.2034	2.9508		23.2869
36	1-butene	C_4H_8	4.1274	23.1810	0.2759	4.0025		31.5868
37	1-pentene	C_5H_{10}	5.2995	29.7632	0.3543	5.1390		40.5560
38	1,2-butadiene	C_4H_6	4.1509	21.3733	0.2544	3.0194		28.7980
39	1-butyne	C_4H_6	4.1800	21.5237	0.2562	3.0406		29.0005
40	methanol	CH_3OH	1.0398	5.8394	0.0695	2.0165		8.9652
41	ethanol	C_2H_5OH	2.1701	12.1883	0.1451	3.1567		17.6602
42	argon	Ar	–	–	–	–		–
43	helium	He	–	–	–	–		–
44	carbon dioxide	CO_2	–	–	–	–		–
45	carbon monoxide	CO	0.9942	1.8639	0.0222	–		2.8803
46	hydrogen	H_2	0.0007	1.8611	0.0222	0.9640		2.8480
47	nitrogen	N_2	–	–	–	–		–
48	oxygen	O_2	–	–	–	–		–
49	nitric oxide	NO	0.0007	1.8641	0.0222	–	NO_2: 0.9733	2.8603
50	nitrogen dioxide	NO_2	–	–	–	–		–
51	water vapour	H_2O	–	–	–	–		–
52	air (dry)	–	–	–	–	–		–

Table 3.4.2 Flue gas products formed by stoichiometric combustion of 1 m³ of gas with "wet" air

No.	Component	Formula	Flue gas products formed by stoichiometric combustion of 1 m³ of gas with "wet" air					
			CO_2 m³	N_2 m³	Ar m³	H_2O m³	SO_2 or NO_2 m³	Total m³
1	methane	CH_4	0.998 3	7.470 0	0.089 0	2.045 9		10.603 2
2	ethane	C_2H_6	2.011 4	13.174 2	0.157 0	3.120 7		18.463 3
3	propane	C_3H_8	3.052 2	19.041 5	0.226 9	4.228 7		26.549 3
4	2-methylpropane (isobutane)	C_4H_{10}	4.128 3	25.113 3	0.299 3	5.377 0		34.917 9
5	butane	C_4H_{10}	4.146 9	25.225 8	0.300 6	5.401 1		35.074 4
6	2,2-dimethylpropane	C_5H_{12}	5.240 7	31.390 4	0.374 1	6.564 7		43.569 9
7	2-methylbutane (isopentane)	C_5H_{12}	5.297 6	31.731 3	0.378 2	6.635 9		44.043 0
8	pentane	C_5H_{12}	5.340 1	31.986 7	0.381 2	6.689 4		44.397 4
9	2,2-dimethylbutane	C_6H_{14}	6.524 2	38.673 0	0.460 9	7.955 9		53.614 0
10	2,3-dimethylbutane	C_6H_{14}	6.529 2	38.702 6	0.461 2	7.962 0		53.655 0
11	3-methylpentane	C_6H_{14}	6.529 2	38.702 6	0.461 2	7.962 0		53.655 0
12	2-methylpentane (isohexane)	C_6H_{14}	6.529 2	38.702 6	0.461 2	7.962 0		53.655 0
13	hexane	C_6H_{14}	6.529 2	38.702 6	0.461 2	7.962 0		53.655 0
14	2-methylhexane (isoheptane)	C_7H_{16}	7.617 2	44.813 6	0.534 1	9.108 1		62.073 0
15	heptane	C_7H_{16}	7.617 2	44.813 6	0.534 1	9.108 1		62.073 0
16	octane	C_8H_{18}	8.705 3	50.924 5	0.606 9	10.254 2		70.490 9
17	nonane	C_9H_{20}	9.793 3	57.035 5	0.679 7	11.400 2		78.908 7
18	decane	$C_{10}H_{22}$	10.881 6	63.146 4	0.752 5	12.546 3		87.326 8
19	undecane	$C_{11}H_{24}$	11.969 7	69.257 3	0.825 4	13.692 4		95.744 8
20	dodecane	$C_{12}H_{26}$	13.057 7	75.368 3	0.898 2	14.838 5		104.162 7
21	tridecane	$C_{13}H_{28}$	14.145 9	81.479 2	0.971 0	15.984 6		112.580 7
22	tetradecane	$C_{14}H_{30}$	15.234 0	87.590 2	1.043 8	17.130 7		120.998 7
23	cyclohexane	C_6H_{12}	6.528 5	36.665 7	0.437 0	6.876 5		50.507 7
24	methylcyclohexane	C_7H_{14}	7.616 5	42.776 6	0.509 8	8.022 6		58.925 5

25	benzene	C_6H_6	6.5262	30.5547	0.3641	3.6202		41.0652
26	toluene	C_7H_8	7.6142	36.6657	0.4370	4.7663		49.4832
27	xylene (o)	C_8H_{10}	8.7023	42.7766	0.5098	5.9124		57.9011
28	methyl mercaptan	CH_3SH	1.0258	11.4978	0.1370	2.1564	SO_2: 1.0070	15.8240
29	ethyl mercaptan	C_2H_5SH	2.0927	17.6108	0.2099	3.3028	SO_2: 1.0283	24.2445
30	propyl mercaptan	C_3H_7SH	3.2563	24.3665	0.2904	4.5699	SO_2: 1.0670	33.5501
31	carbonyl sulphide	COS	1.0109	5.6776	0.0677	0.0845	SO_2: 0.9945	7.8352
32	hydrogen sulphide	H_2S	0.0022	5.6461	0.0673	1.0589	SO_2: 0.9890	7.7635
33	sulphur dioxide	SO_2	–	–	–	–		–
34	ethene	C_2H_4	2.0056	11.2637	0.1342	2.1125		15.5160
35	propene	C_3H_6	3.0430	17.0902	0.2037	3.2052		23.5421
36	1-butene	C_4H_8	4.1275	23.1815	0.2763	4.3476		31.9329
37	1-pentene	C_5H_{10}	5.2996	29.7639	0.3547	5.5821		41.0003
38	1,2-butadiene	C_4H_6	4.1510	21.3739	0.2547	3.3376		29.1172
39	1-butyne	C_4H_6	4.1801	21.5243	0.2565	3.3611		29.3220
40	methanol	CH_3OH	1.0398	5.8396	0.0696	2.1035		9.0525
41	ethanol	C_2H_5OH	2.1702	12.1886	0.1453	3.3382		17.8423
42	argon	Ar	–	–	–	–		–
43	helium	He	–	–	–	–		–
44	carbon dioxide	CO_2	–	–	–	–		–
45	carbon monoxide	CO	0.9942	1.8640	0.0222	0.0278		2.9082
46	hydrogen	H_2	0.0007	1.8612	0.0222	0.9917		2.8758
47	nitrogen	N_2	–	–	–	–		–
48	oxygen	O_2	–	–	–	–		–
49	nitric oxide	NO	0.0007	1.8641	0.0222	0.0278	NO_2: 0.9733	2.8881
50	nitrogen dioxide	NO_2	–	–	–	–		–
51	water vapour	H_2O	–	–	–	–		–
52	air (dry)	–	–	–	–	–		–

$$q_{SO_2} = \left(\sum_{i=1}^{n} n_i \cdot SO_{2,i}\right) \frac{z_{SO_2}}{z_g \cdot 100} \qquad m^3SO_2/m^3\,gas\ [3.13]$$

$$q_{O_2} = (a_f - 1)\, n_{O_2,a} \cdot a \frac{z_{O_2}}{z_g \cdot 100} \qquad m^3O_2/m^3\,gas\ [3.14]$$

$$q_{st} = \sum_{i=1}^{n} q_i \quad (a_f = 1) \qquad m^3/m^3\,gas\ [3.15]$$

$$q_{tot} = \sum_{i=1}^{n} q_i \quad (a_f \neq 1) \qquad m^3/m^3\,gas\ [3.16]$$

where:

q_i	=	quantity of product i (table 3.4.1 and 3.4.2)	m^3/m^3 gas
n	=	number of components	
n_i	=	concentration of component i	% (mol)
$CO_{2,i}$	=	quantity of CO_2 formed by complete combustion of component i with oxygen (table 3.2.1)	mol/mol
H_2O_i	=	quantity of H_2O formed by complete combustion of component i with oxygen (table 3.2.1)	mol/mol
$SO_{2,i}$	=	quantity of SO_2 formed by complete combustion of component i with oxygen (table 3.2.1)	mol/mol
$n_{CO_2,g}$	=	concentration of CO_2 in gas	% (mol)
$n_{CO_2,a}$	=	concentration of CO_2 in air (table 3.3.1 and 3.3.2)	% (mol)
$n_{H_2O,a}$	=	concentration of H_2O in air (table 3.3.2)	% (mol)
$n_{N_2,g}$	=	concentration of N_2 in gas	% (mol)
$n_{N_2,a}$	=	concentration of N_2 in air (table 3.3.1 and 3.3.2)	% (mol)
$n_{Ar,a}$	=	concentration of Ar in air (table 3.3.1 and 3.3.2)	% (mol)
$n_{O_2,a}$	=	concentration of O_2 in air (table 3.3.1 and 3.3.2)	% (mol)
z_g	=	compressibility factor of gas (0 °C; 101.325 kPa) (2.2)	–
z_{CO_2}	=	compressibility factor of CO_2 (table 2.2.5, API)	–
z_{H_2O}	=	compressibility factor of H_2O (table 2.2.5; see**)	–
z_{N_2}	=	compressibility factor of N_2 (table 2.2.5, API)	–
z_{Ar}	=	compressibility factor of Ar (table 2.2.5, API)	–
z_{SO_2}	=	compressibility factor of SO_2 (table 2.2.5, API)	–
z_{O_2}	=	compressibility factor of O_2 (table 2.2.5, API)	–

Example: Groningen natural gas (table 1.9)

For the requisite data, refer to tables 3.2.1, 3.2.2, 3.2.3, 3.3.1, 3.3.2

Table 3.4.3 Stoichiometric combustion of Groningen natural gas with "wet" air

Component	Formula	"Wet" air		Combustion products		
	(vol.)	% (vol.)	m^3	see 3.2	Total	% (vol.)
nitrogen	N_2	77.20	6.583 6	0.143 5	6.727 1	70.91
oxygen	O_2	20.70	1.765 3	–	–	–
argon	Ar	0.92	0.078 4	–	0.078 4	0.82
carbon dioxide	CO_2	0.03	0.002 6	0.897 4	0.900 0	9.49
water vapour	H_2O	1.15	0.098 1	1.683 5	1.781 6	18.78
		100.00	8.528 0		9.487 1	100.00

Table 3.4.4 Stoichiometric combustion of Groningen natural gas with "dry" air

Component	Formula	"Dry" air		Combustion products		
	(vol.)	% (vol.)	m^3	see 3.2	Total	% (vol.)
nitrogen	N_2	78.10	6.584 1	0.143 5	6.727 6	71.65
oxygen	O_2	20.94	1.765 3	–	–	–
argon	Ar	0.93	0.078 4	–	0.078 4	0.84
carbon dioxide	CO_2	0.03	0.002 5	0.897 4	0.899 9	9.58
water vapour	H_2O	–	–	1.683 5	1.683 5	17.93
		100.00	8.430 3		9.389 4	100.00

3.5 Incomplete combustion

Incomplete combustion may occur as a result of:

- oxygen deficiency (inert gas production)
- factors connected with the combustion process, although sufficient oxygen is available for complete combustion

3.5.1 Oxygen deficiency

In the manufacture of shield gases, the oxygen admitted to the combustion process is intentionally kept below the level required for complete combustion. In this process, the composition of the combustion products is a function of the composition of the combustible gas mixture and the temperature of the reaction. The product composition can be calculated from the following equations:

1. $V_{CO_2} + V_{CO} + V_{CH_4} = \sum_{i=1}^{n} C_i$ [3.17]

2. $V_{H_2O} + V_{H_2} + 2\,V_{CH_4} = \sum_{i=1}^{n} H_{2,i}$ [3.18]

3. $V_{CO_2} + 0.5\,V_{CO} + 0.5\,V_{H_2O} = \sum_{i=1}^{n} O_{2,i}$ [3.19]

4. $\frac{V_{H_2O} \cdot V_{CO_2}}{V_{CO} \cdot V_{H_2O}} = k$ "homogeneous water gas reaction" [3.20]

5. $\frac{V_{CH_4} \cdot V_{CO_2}}{V_{H_2}^2 \cdot V_{CO}^2} = l$ "homogeneous methane formation reaction" [3.21]

6. $V_{CO_2} + V_{CO} + V_{H_2O} + V_{H_2} + V_{N_2} + V_{CH_4} = 1$ [3.22]

where:

V_{CO_2} etc. = volume fraction of CO_2 etc.
C_i = carbon (C) content of all carbon-containing components
$H_{2,i}$ = hydrogen (H_2) content of all hydrogen-containing components
$O_{2,i}$ = oxygen (O_2) content of all oxygen-containing components
k = equilibrium constant for the "homogeneous water-gas reaction" (function of reaction temperature)
l = equilibrium constant for the "homogeneous methane formation reaction" (function of reaction temperature)
n = number of components

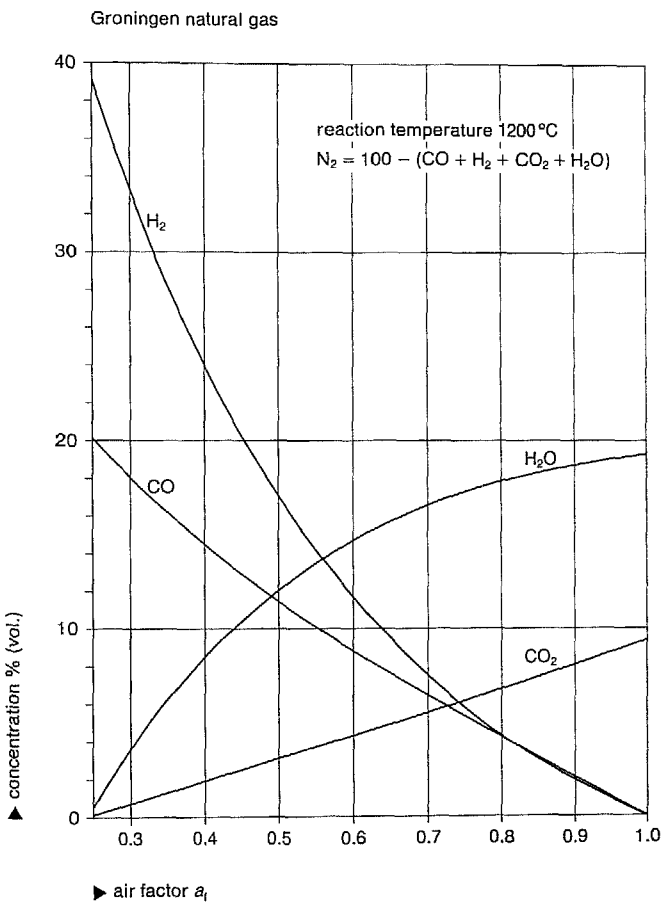


Fig. 3.5.1 The "wet" combustion products for Groningen natural gas at a reaction temperature of 1200 °C and air factors of $0.25 < a_l < 1$

Resolving the six equations above gives the flue gas composition (= shield gases). Constants k and l are both functions of the reaction temperature.

$\sum_{i=1}^{n} C_i$, $\sum_{i=1}^{n} H_{2,i}$ en $\sum_{i=1}^{n} O_{2,i}$ are derived from the gas composition and the various combustion reaction equations. The above system of equations is applicable to air factors of $0.25 < a_f < 1$

N.V. Nederlandse Gasunie has at its disposal a computer program (set up by Ruhrgas AG, FRG) for calculating the composition of the combustion products and the dew point from the composition of the gas mixture and the reaction temperature.

Fig. 3.5.1 gives the composition of the "wet" combustion products for Groningen natural gas at a temperature of 1200°C and air factors of $0.25 < a_f < 1$

3.5.2 Incomplete combustion due to factors associated with the combustion process

These factors include, for example, insufficient burn-out length.

The reaction equation then becomes:

$$CH_4 + 2O_2 \rightarrow x\,CO_2 + (1 - x)\,CO + 2H_2O + 0.5\,(1\text{-}x)\,O_2$$

The portion of the methane (CH_4) which is not "completely" converted into carbon dioxide (CO_2) is converted instead into carbon monoxide (CO), with a small amount of oxygen (O_2) being left over. The equation has been used to construct fig. 3.5.2 (Ostwald triangel) (lit. 33) for Groningen natural gas.

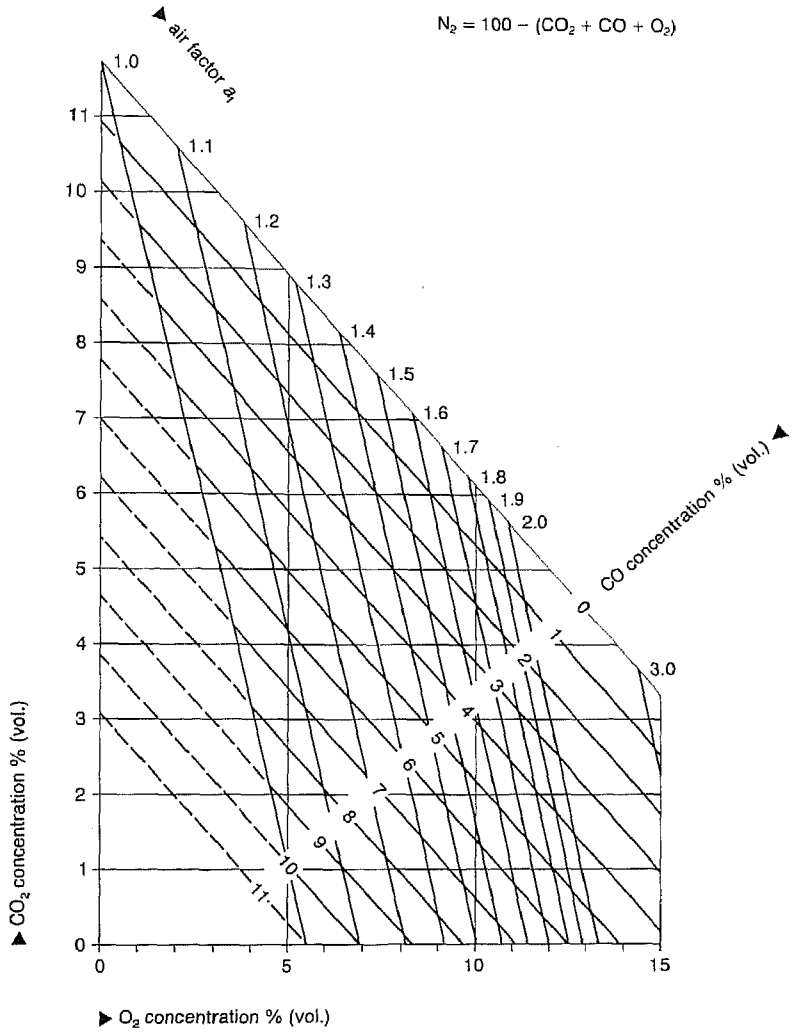


Fig. 3.5.2 Flue gas composition due to incomplete combustion of Groningen natural gas as a function of the air factor a_f ($1.0 \leq a_f \leq 3.0$)

3.6 Heat content and "average" isobaric heat capacity

The heat content of flue gases is given by:

$$I = q_{tot} \cdot c_{pm} \times 10^{-3} \cdot \Delta t \qquad [3.23]$$

where:

I	= heat content of flue gases (fig. 3.6.2)	MJ/m³ gas
q_{tot}	= total quantity of flue gases (3.4)	m³/m³ gas
c_{pm}	= average isobaric heat capacity of gas mixture over the temperature range (0 – t) °C (table 3.6)	kJ/m³ · K
Δt	= temperature range (0 – t)	°C

able 3.6 and fig. 3.6.1 give the average isobaric heat capacity c_{pm} of a number of pure gases over the temperature range (0 – t)°C. By definition c_{pm} represents the average quantity of heat needed to raise 1 m³ of gas through 1 °C in the range between 0 and t°C · c_{pm} can be derived from c_p – the "true" isobaric heat capacity – by the integral:

$$c_{pm} = \frac{1}{t} \int_0^t c_p \cdot dt \qquad [3.24]$$

For gas mixtures, c_{pm} is calculated from:

$$c_{pm} = \sum_{i=1}^{n} x_i \cdot c_{pm,i}/100 \qquad [3.25]$$

where:

c_{pm}	= average isobaric heat capacity of gas mixture	kJ/(m³ · K)
x_i	= concentration of component i	% (vol.)
$c_{pm,i}$	= average isobaric heat capacity of component i (table 3.6)	kJ/(m³ · K)
n	= number of components	

Table 3.6 The average isobaric heat capacity of pure gases c_{pm} at 101.325 kPa over the temperature range (0 – t) °C

temperature range (0 – t) °C	c_{pm} kJ/(m³ · K)							
	CO_2	O_2	N_2	H_2O	SO_2*)	CO	H_2	Air**)
0	1.620	1.310	1.302	1.491	1.712	1.302	1.281	1.302
0– 100	1.721	1.319	1.302	1.503	1.822	1.306	1.290	1.306
0– 200	1.809	1.336	1.306	1.520	1.908	1.310	1.298	1.310
0– 300	1.884	1.357	1.310	1.541	1.981	1.319	1.298	1.319
0– 400	1.955	1.377	1.319	1.562	2.043	1.331	1.302	1.331
0– 500	2.018	1.398	1.331	1.587	2.104	1.344	1.306	1.344
0– 600	2.068	1.419	1.344	1.612	2.153	1.361	1.310	1.357
0– 700	2.119	1.436	1.361	1.637	2.202	1.373	1.315	1.373
0– 800	2.160	1.453	1.373	1.662	2.238	1.390	1.319	1.386
0– 900	2.198	1.470	1.386	1.687	2.275	1.403	1.327	1.398
0–1000	2.232	1.482	1.398	1.717	2.312	1.415	1.331	1.411
0–1200	2.290	1.503	1.424	1.767	2.361	1.440	1.344	1.436
0–1400	2.336	1.524	1.440	1.817	2.397	1.461	1.361	1.457
0–1600	2.378	1.541	1.461	1.863	2.434	1.478	1.377	1.474
0–1800	2.412	1.557	1.478	1.905	2.471	1.495	1.394	1.491
0–2000	2.441	1.574	1.491	1.947	2.495	1.507	1.407	1.503
0–2200	2.466	1.587	1.503	1.985	2.520	1.520	1.424	1.516
0–2400	2.491	1.599	1.516	2.018	2.532	1.532	1.440	1.528

*) calculated from c_p (lit. 35)
**) compare CO

Note: c_{pm} for argon (Ar) is constant over the entire temperature range and is 0.926 kJ/(m³ · K)

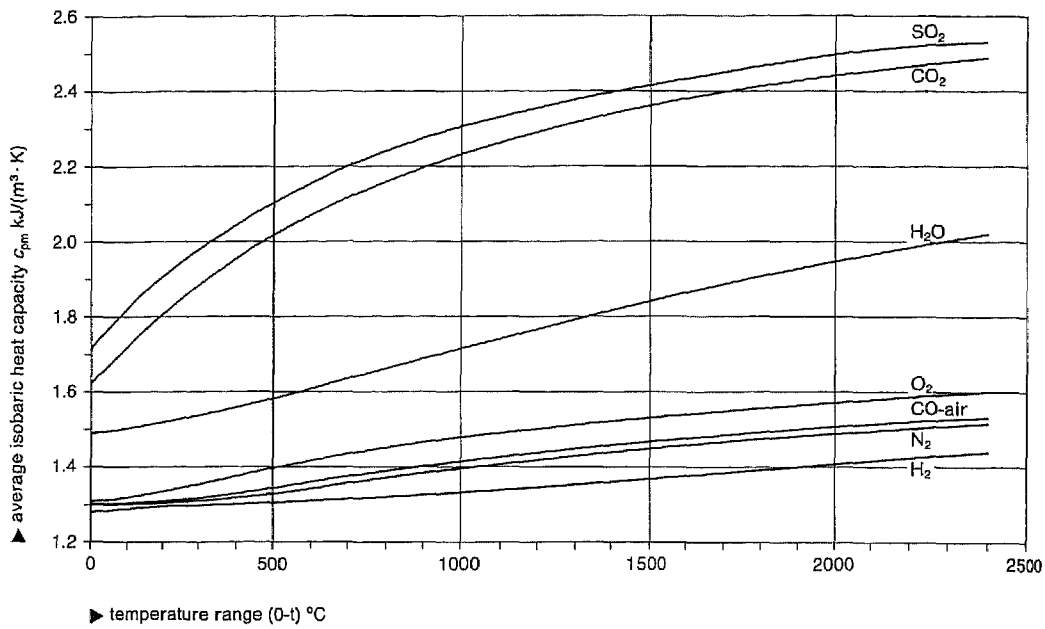


Fig. 3.6.1 The average isobaric heat capacity of pure gases c_{pm} (table 3.6) as a function of the temperature range (0 – t) °C

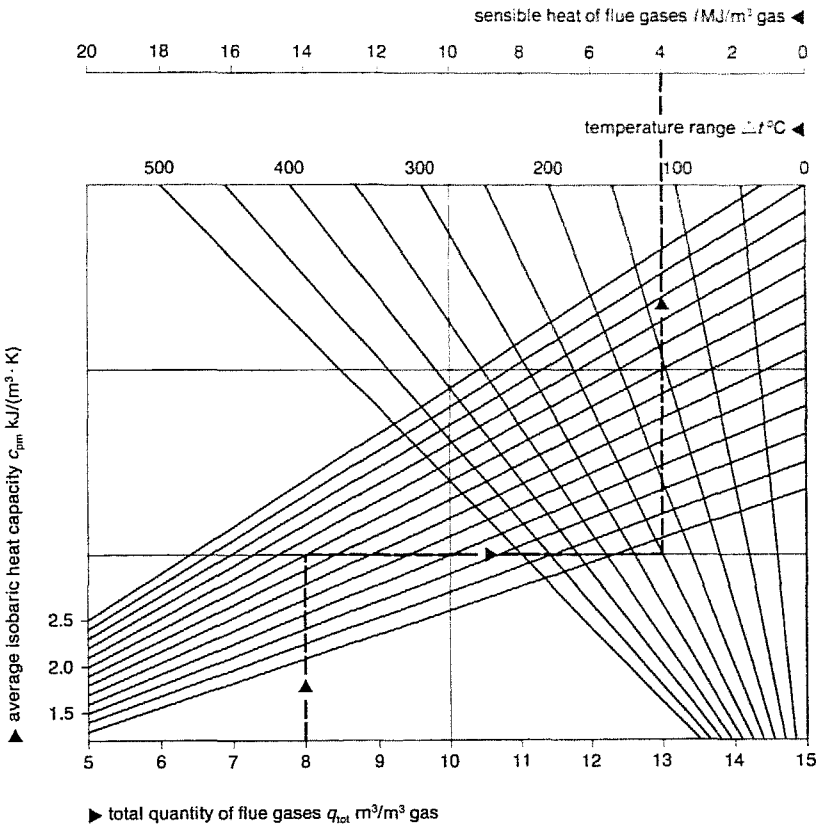


Fig. 3.6.2 Heat content of flue gases I as a function of the total quantity q_{tot}, the average isobaric heat capacity c_{pm} and the temperature range (0 – t) °C

3.7 Combustion efficiency

Efficiency can be defined in simple terms as the ratio of useful energy produced to the total quantity of energy supplied. A number of different measures of efficiency in use in the gas industry are defined in 1.4.18
Efficiency can be referred either to the gross calorific value H_s or to the net calorific value H_i of a gas.
Indirect efficiency η_{ind} is the measure of efficiency in most widespread use and it is the easiest to determine.
The flue losses – the heat or energy content of the flue gases leaving the installation via the flue – can be found from:

$$l = q_{tot} \cdot c_{pm} \times 10^{-3} \cdot \Delta t \quad \text{(3.6 and fig. 3.6.2)} \qquad [3.23]$$

where:

l	= the heat or energy content of the flue gases in the flue (fig. 3.6.2)	MJ/m³ gas
q_{tot}	= total quantity of flue gases (3.4)	m³/m³ gas
c_{pm}	= average isobaric heat capacity of the flue gases	kJ/(m³ · K)
Δt	= difference in temperature between flue gases and ambient air	°C

Indirect efficiency referred to net and gross calorific value, respectively, is given by:

$$\eta_{ind,i} = \frac{H_i - l}{H_i} \times 100\,\% \qquad [3.26]$$

$$\eta_{ind,s} = \frac{H_s - l - (H_s - H_i)}{H_s} \times 100\,\% = \frac{H_i - l}{H_s} \qquad [3.27]$$

The term $(H_s - H_i)$ represents the latent heat of vaporisation of the chemically formed water vapour

The ratio between these indirect efficiencies is therefore:

$$\frac{\eta_{ind,s}}{\eta_{ind,i}} = \frac{H_i - l}{H_s} \frac{H_i}{H_i - l} = \frac{H_i}{H_s} \qquad [3.28]$$

For most natural gases and their components (table 3.1.1) a reasonable approximation is:

$$\frac{\eta_{ind,s}}{\eta_{ind,i}} = \frac{H_i}{H_s} = 0.9$$

Fig. 3.7.1 gives $\eta_{ind,i}$ for cases where the flue losses l are known

Example: Groningen natural gas (table 1.9)
Stoichiometric combustion with "wet" air: $a_f = 1$
Flue gas temperature: $T = 423.15\,K\,(150\,°C)$
Ambient temperature: $T_{amb} = 298.15\,K\,(25\,°C)$
Gas temperature: $T_g = 298.15\,K\,(25\,°C)$

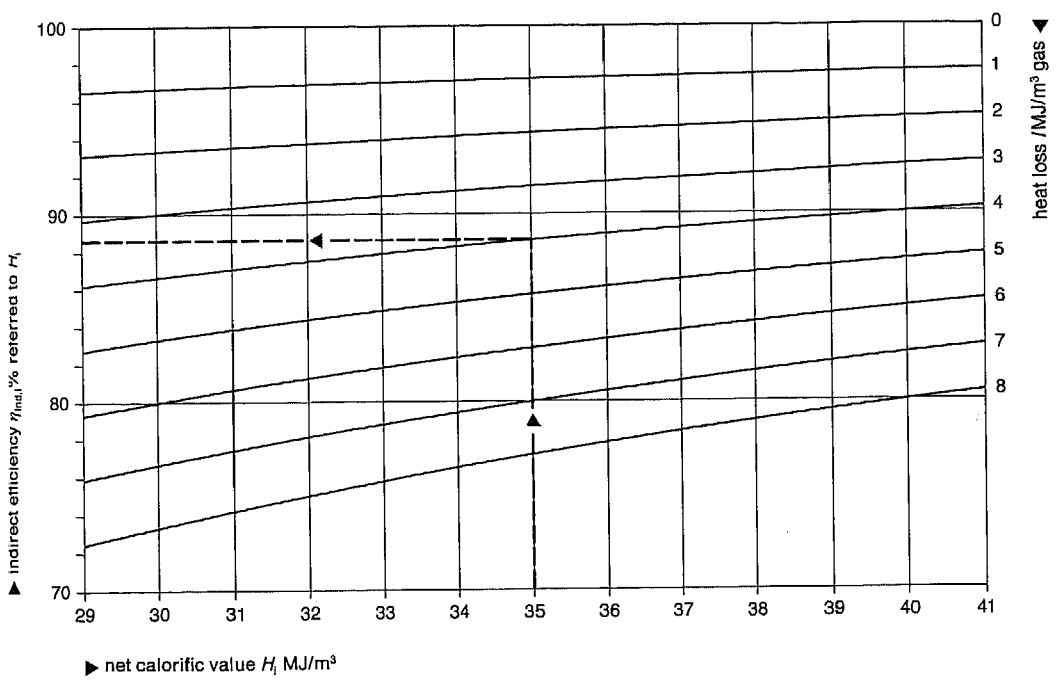


Fig. 3.7.1 Indirect efficiency referred to net calorific value $\eta_{ind,l}$ as a function of net calorific value H_i and heat loss l from flue gases

Example: $H_i = 35\,MJ/m^3$
$l = 4\,MJ/m^3$ } $\eta_{ind,l} = 88.6\,\%$
$\eta_{ind,s} = 0.9 \cdot \eta_{ind,l} = 79.7\,\%$

For combustion data see (3.4)
$I = 1.650\ MJ/m^3$ gas (for c_{pm} over temperature range (0 – 150) °C)
$I = 1.640\ MJ/m^3$ gas (for c_{pm} over temperature range (25 – 150) °C)

Difference: $\frac{1650-1640}{1650} 100\,\% = 0.6\,\%$

The influence of c_{pm} on the efficiency ([3.26] and [3.27]):

$$\Delta\eta = \frac{0.01}{35.096} 100 = 0.03\,\%$$

For a fast and easy calculation of the indirect combustion efficiency of Groningen natural gas (lit. 36) a Siegert type formula (lit. 33) is used:

$$\eta_{ind,s} = 90.2 - (0.303/x_{CO_2} + 0.01371)\,\Delta t \qquad [3.29]$$

or, according to VEG-Gasinstituut (4.2):

$$\eta_{ind,s} = 90 - (0.34/x_{CO_2} + 0.0077)\,\Delta t \qquad [3.30]$$

where:

x_{CO_2} =	CO_2 concentration in dry flue gases	% (vol.)
Δt =	temperature difference between ambient air and flue gases	°C

Against the background of declining energy resources, increasing attention is being devoted to better energy utilisation. It is clear from the efficiency formulas presented above that any improvements in efficiency will have to be sought through reduction in heat loss l ($= q_{tot} \cdot c_{pm} \cdot \Delta t$), in other words through reduction in Δt. However, the minimum limit to Δt is set by the water dew point of the combustion products. If the flue gas temperature passes below this limit, the water vapour in the combustion products will condense, and these formulas are no longer valid.

New developments in this area make deliberate use of this condensation, recovering the considerable latent heat of vaporisation of water to achieve a significant gain in efficiency.

Where this latent heat of vaporisation is recovered, the above formulas become:

$$\eta_{ind,i} = \frac{H_i - I + Q_{cond}}{H_i} \times 100\,\% \qquad [3.31]$$

$$\eta_{ind,s} = \frac{H_i - I + Q_{cond}}{H_s} \times 100\,\% \qquad [3.32]$$

where:

Q_{cond} = total quantity of heat liberated by condensation of water vapour from the combustion products and cooling of the water thus formed — kJ/m³ gas

For Q_{cond} it can be deduced (lit. 37) that:

$$Q_{cond} = \varrho_w \cdot q_{tot} \left[\int_t^{t_d} r(\tau) \frac{d(\Delta p(\tau))}{d\tau} d\tau + c_{p,w}(t_d - t) \int_t^{t_d} \frac{d(\Delta p(\tau))}{d\tau} d\tau \right] +$$
$$+ q_{tot} \left\{ c_{pm,t_d} \cdot t_d - c_{pm,t} \cdot t \left[1 - \int_t^{t_d} \frac{d(\Delta p(\tau))}{d\tau} d\tau \right] \right\} \qquad [3.33]$$

where:

t	=	temperature of the flue gases	°C
t_d	=	dew-point temperature flue gases	°C
q_{tot}	=	total quantity of flue gases (3.4)	m³/m³ gas
ϱ_w	=	density of water vapour (table 1.7)	kg/m³
r_t	=	latent heat of vaporisation released on condensation of water vapour at t °C and 101.325 kPa (fig. 3.7.2)	kJ/kg
Δp	=	$\frac{p_d - p_t}{p_{tot} - p_t} = (\Delta p(\tau))$ (fig. 3.7.3)	[3.34]
		τ = "running" temperature of flue gases where: $t \leq \tau \leq t_d$ °C	
p_{tot}	=	total absolute system pressure (= 101.325)	kPa
p_t	=	absolute saturation pressure of water vapour at t °C (fig. 3.8.2)	kPa
p_d	=	absolute saturation pressure of water vapour at t_d °C (fig. 3.8.2)	kPa
$c_{p,w}$	=	isobaric heat capacity of water (= 4.19)	kJ/(kg · K)
$c_{pm,t}$	=	average isobaric heat capacity of flue gases over temperature range (0 – t) °C	kJ/(m³ · K)
c_{pm,t_d}	=	average isobaric heat capacity of flue gases over temperature range (0 – t_d) °C	kJ/(m³ · K)

The formula for Q_{cond} can also be given simply as:

$$Q_{cond} = \varrho_w \cdot \Delta p \cdot q_{tot} [r_{av} + c_{p,w} (t_d - t)] + c_{pm,t_d} \cdot q_{tot} (t_d - t + t \cdot \Delta p) \qquad [3.35]$$

where the average latent heat r_{av} is found from fig. 3.7.2 for an average flue gas temperature $t_{av} = (t_d + t)/2$ °C

Δp is given by fig. 3.7.3

A worked example (lit. 37) shows that there is only a slight difference between the results obtained by the "integration method" (Q_{cond} = 144.06 kW) and the "simple method" (Q_{cond} = 144.11 kW)

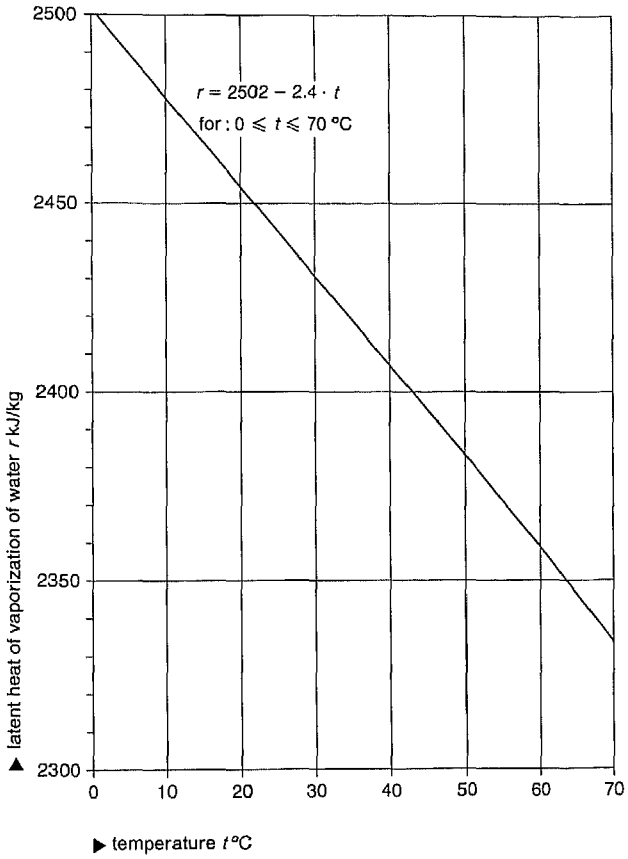


Fig. 3.7.2 Latent heat of vaporization r of water as a function of the flue gas temperature t at 101.325 kPa

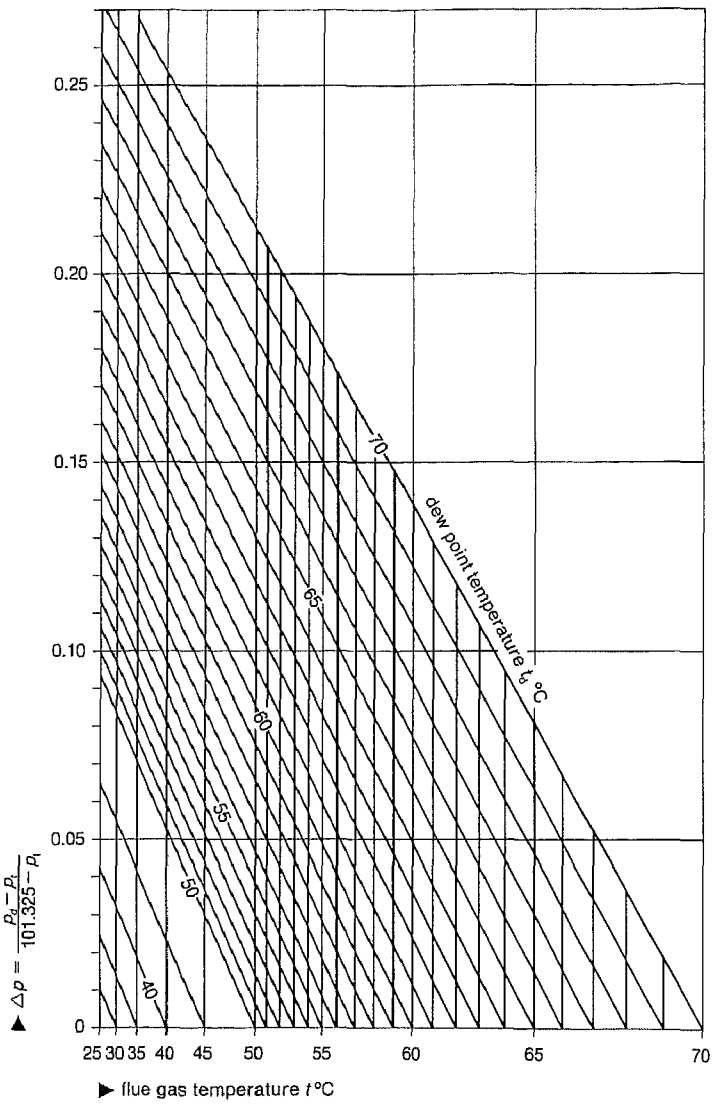


Fig. 3.7.3 Δp as a function of t_d and t where p_{tot} = 101.325 kPa [3.34]

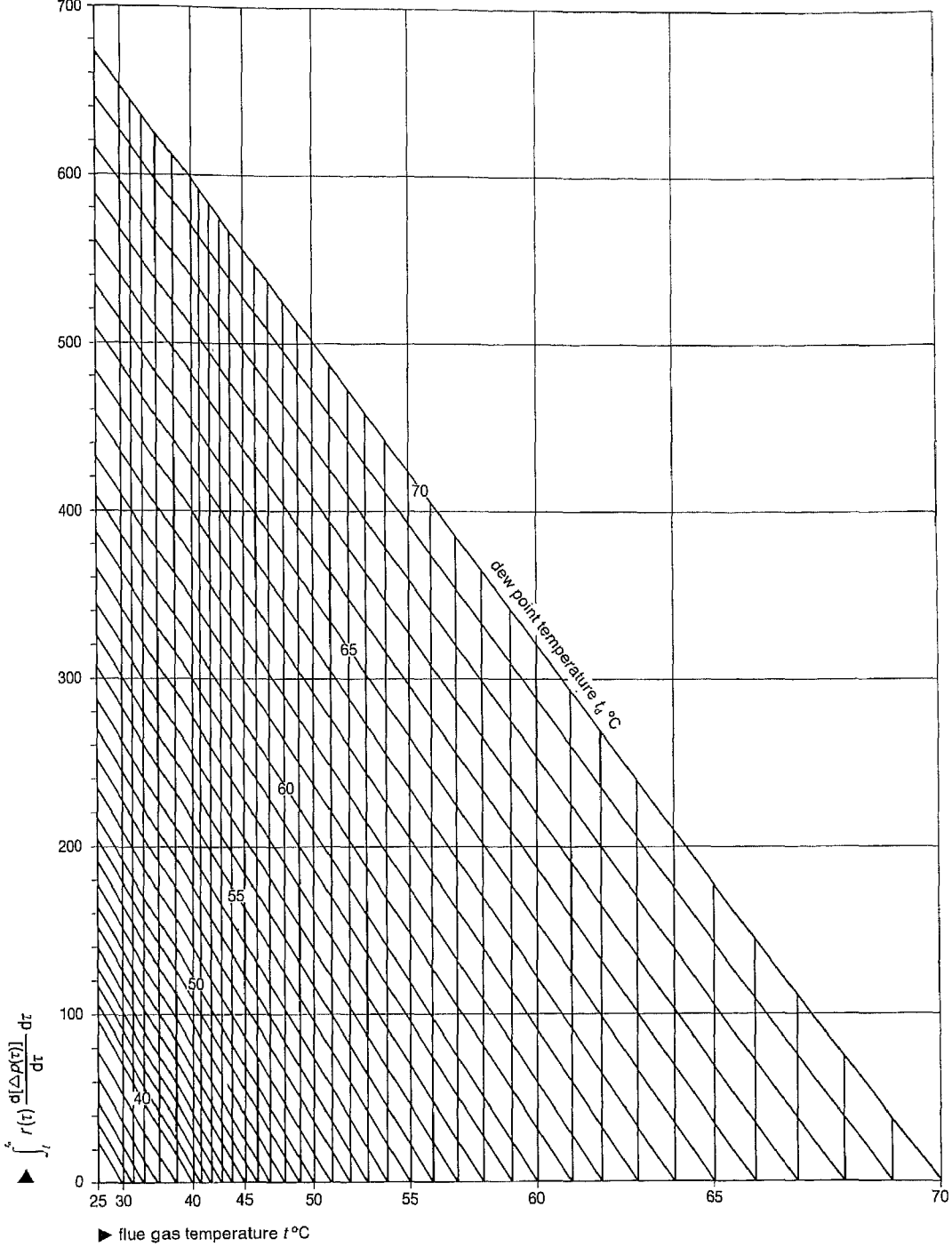


Fig. 3.7.4 Solution of integral $\int_t^{t_d} r(\tau)\,\frac{d(\Delta p(\tau))}{d\tau}\,d\tau$ [3.33]

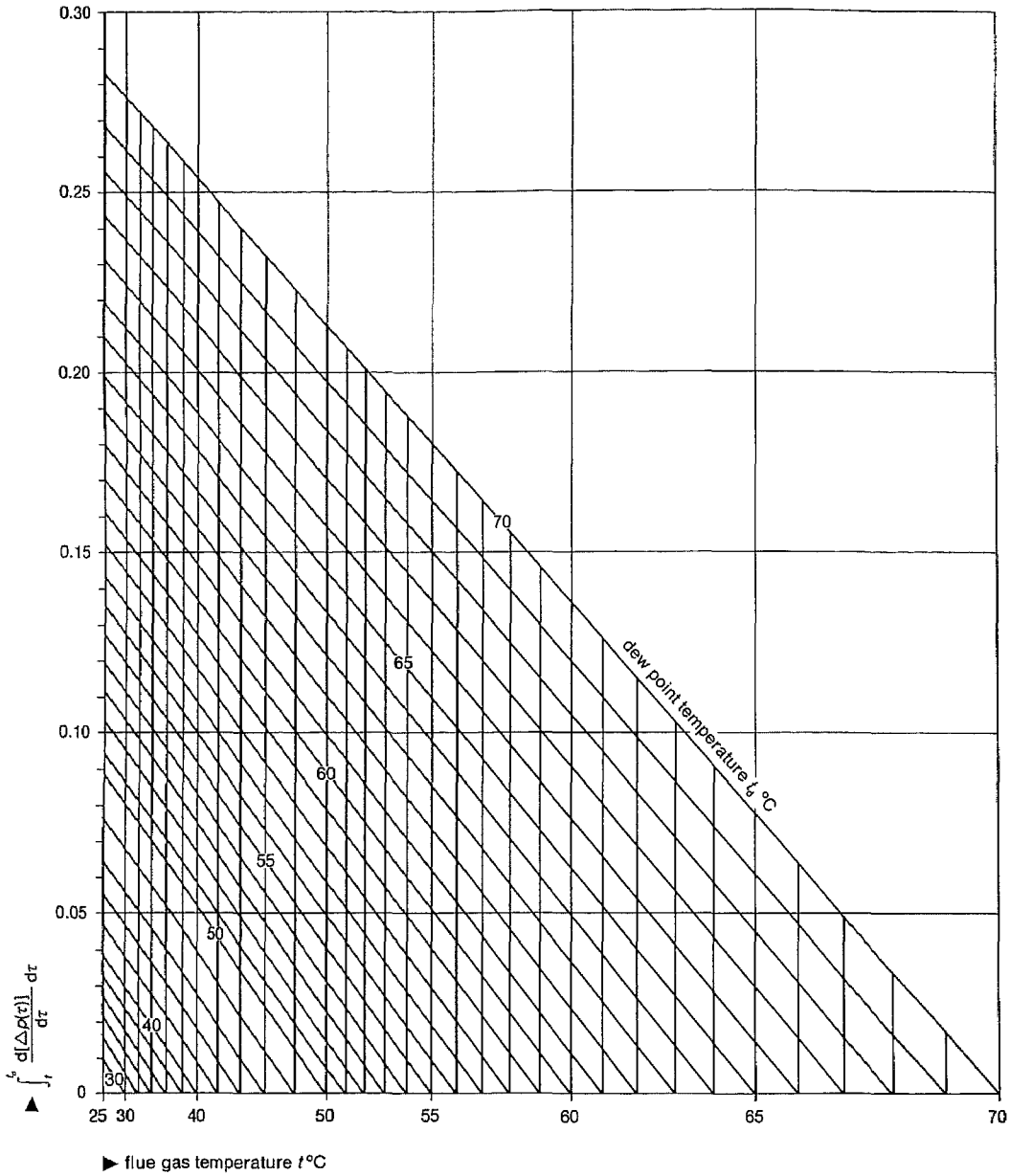


Fig. 3.7.5 Solution of integral $\int_t^{t_d} \frac{d(\Delta p(\tau))}{d\tau} d\tau$ [3.33]

3.8 Water dew point and water content

The dew point is dependent on the relationship between the quantity of water vapour actually present and the maximum quantity potentially present at the prevailing pressure and temperature of a gas mixture.

As shown in 3.3, the water vapour content of air can be determined by means of the formula:

$$x = 1000 \frac{R_{da}}{R_{wv}} \frac{\Phi \cdot p}{p_o - \Phi \cdot p} \quad \text{g } H_2O/\text{kg dry air} \qquad [3.5]$$

or

$$x' = \left(\frac{\Phi \cdot p}{p_o}\right) \times 100\ \%\ (\text{vol.}) \quad (\text{fig. } 3.8.1) \qquad [3.6]$$

Refer to 3.3 for notation

p is the saturated water vapour pressure, which is a function only of temperature (fig. 3.8.2, lit. 47)

For $0 \leq t \leq 70\ °C$, p can be represented with sufficient accuracy by:

$$p = 0.1 \cdot e^{\left(17.433 - \frac{19513.7}{T^{1.270\,95}}\right)} \quad \text{kPa} \qquad [3.36]$$

in which $T (= t + 273.15)$ must be expressed in K

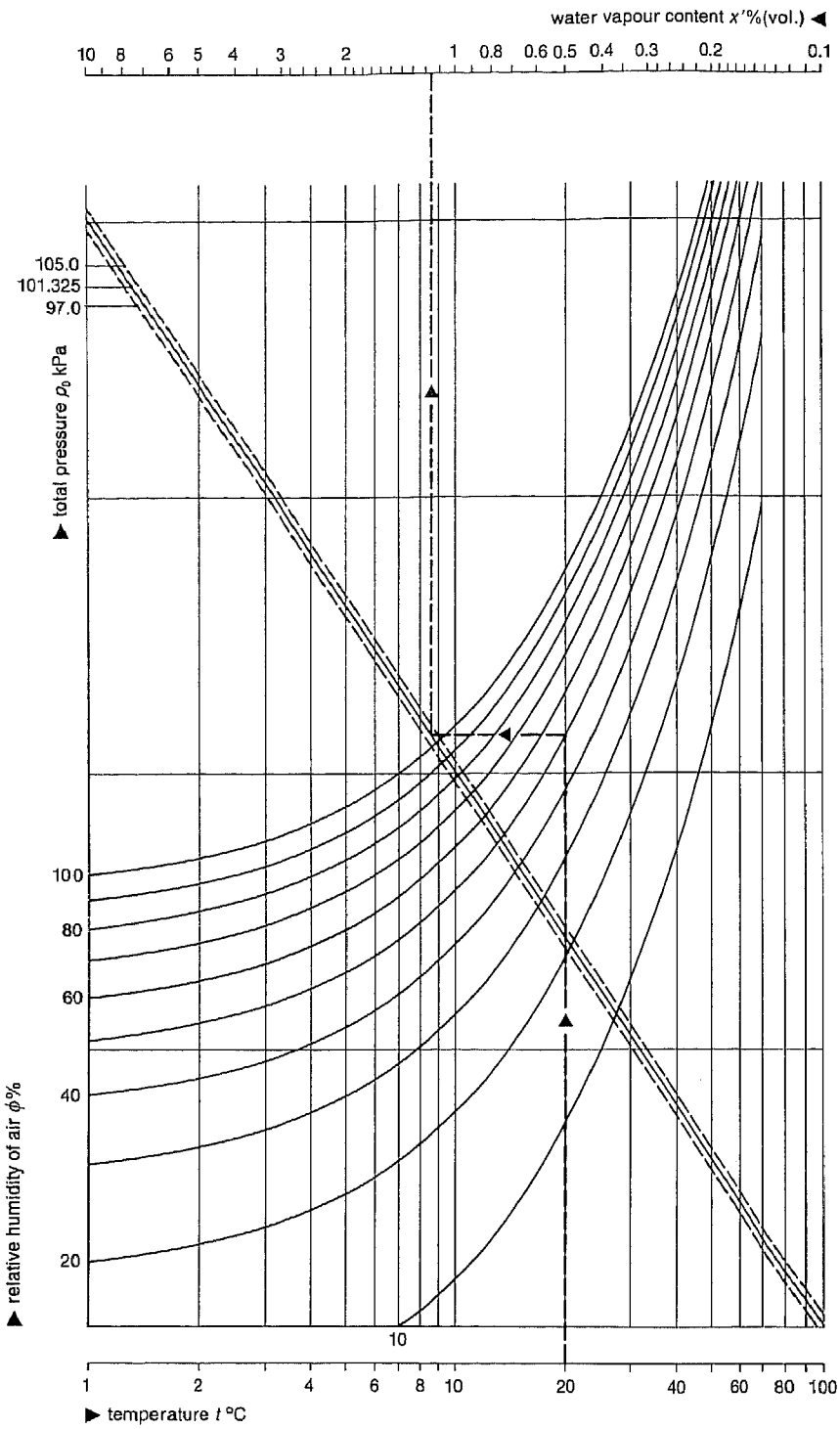
The total quantity of water vapour present in the flue gases can be subdivided into:

a. the chemically formed water vapour ($= q_{chem}$)
b. the water vapour introduced with the combustion air

$$\left(= \frac{x'}{100} a_f \cdot a\right) \qquad [3.37]$$

so that

$$q_{H_2O} = q_{chem} + \frac{x'}{100} a_f \cdot a \qquad [3.38]$$


water vapour content x'%(vol.)
10 8 6 5 4 3 2 1 0.8 0.6 0.5 0.4 0.3 0.2 0.1
105.0
101.325
97.0
total pressure p_0 kPa
100
80
60
40
20
10
relative humidity of air ϕ%
1 2 4 6 8 10 20 40 60 80 100
temperature t °C

where:

q_{H_2O}	=	total quantity of water vapour present in the flue gases (3.4)	m^3/m^3 gas
q_{chem}	=	chemically formed water (3.2)	m^3/m^3 gas
x^l	=	concentration of water vapour in combustion air [3.6]	% (vol.)
a_f	=	air factor (1.4.8)	–
a	=	"wet" air requirement (3.3)	m^3/m^3 gas

The partial water vapour pressure in the combustion products is given by:

$$p_{part} = \frac{q_{H_2O}}{q_{tot}} p_o \qquad [3.39]$$

where:

p_{part}	=	partial water vapour pressure	kPa
q_{tot}	=	total quantity of flue gases (3.4)	m^3/m^3 gas
p_o	=	total system pressure (generally 101.325)	kPa

The dew point is a function of p (= p_{part}) and is given in fig. 3.8.2

Example: Combustion of Groningen natural gas with "wet" air (R_v = 50 % at 20 °C and 101.325 kPa). Air factor a_f = 1

Solution:

$$q_{H_2O} = q_{chem} + \frac{x^l}{100} a_f \cdot a \qquad [3.38] \qquad m^3\ H_2O/m^3\ gas$$

q_{chem}	=	1.6835 (table 3.2.2)		$m^3\ H_2O/m^3$ gas
x^l	=	1.15 (H_2O in "wet" air)	[3.6]	% (vol.)
a	=	8.5280 (3.3)		m^3 air/m^3 gas

$$q_{H_2O} = 1.6835 + \frac{1.15}{100} 8.5280 = 1.7816 \qquad m^3\ H_2O/m^3\ gas$$

$$p_{part} = \frac{q_{H_2O}}{q_{tot}} p_o \qquad [3.39] \qquad kPa$$

$$q_{tot} = 9.4874 \text{ (table 3.4.3)} \qquad m^3/m^3\ gas$$

Fig. 3.8.1 The water vapour content of air x^l as a function of the temperature t and the relative humidity Φ

p_o = 101.325 kPa

$p_{part} = \frac{1.7816}{9.4874} \times 101.325 = 19.0$ kPa

Fig. 3.8.2 shows that for p_{part} = 19.0 kPa the dew point t_d = 59.1 °C

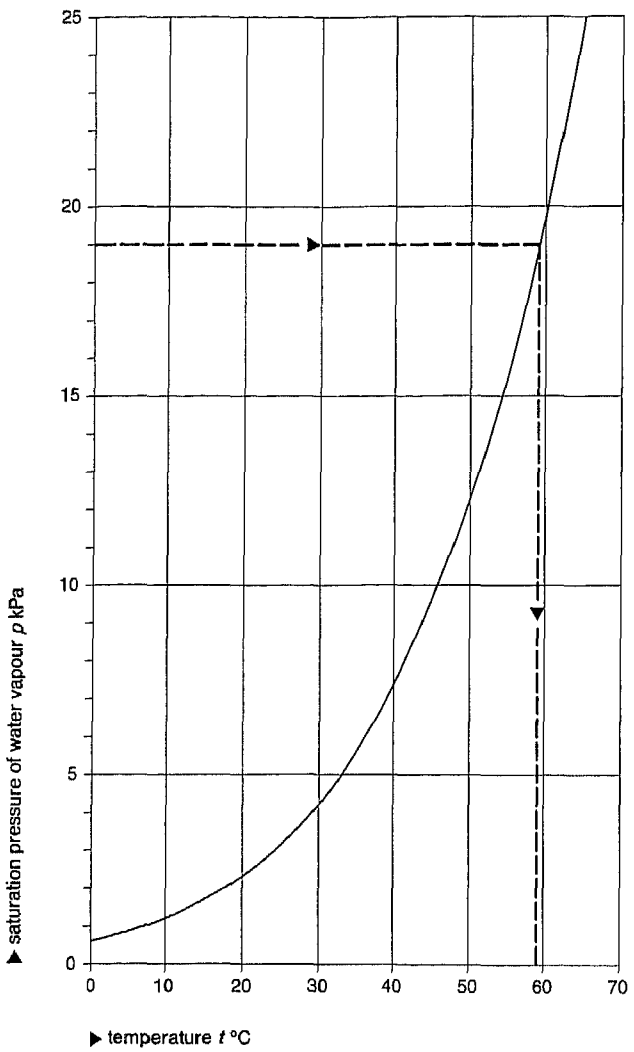


Fig. 3.8.2 The saturation pressure of water vapour p as a function of the temperature t

3.9 Density

Density is calculated as follows:

$$\varrho_{v,o} = \sum_{i=1}^{n} x_i \cdot \varrho_i / 100 \qquad [3.40]$$

where:

$\varrho_{v,o}$	=	density of gas mixture (0 °C; 101.325 kPa)	kg/m^3
x_i	=	concentration of component i	% (vol.)
ϱ_i	=	density of component i (0 °C; 101.325 kPa) (table 1.7)	kg/m^3
n	=	number of components	–

For higher temperatures ϱ_v is calculated as follows:

$$\varrho_{v,T} = \varrho_{v,o} \frac{273.15}{T} \qquad [3.41]$$

where:

T	=	temperature of gas mixture	K
$\varrho_{v,T}$	=	density of flue gases (TK; 101.325 kPa)	kg/m^3

Air factors $a_f > 1$ have little effect on the density of flue gases, since the latter consist predominantly of nitrogen

Fig. 3.9 gives $\varrho_{v,T}$ for the flue gases of Groningen natural gas

The composition of the flue gases of Groningen natural gas is given in tables 3.4.3 and 3.4.4

In addition, fig. 3.9 gives the density $\varrho_{v,T}$ for "wet" air (table 3.4.3)

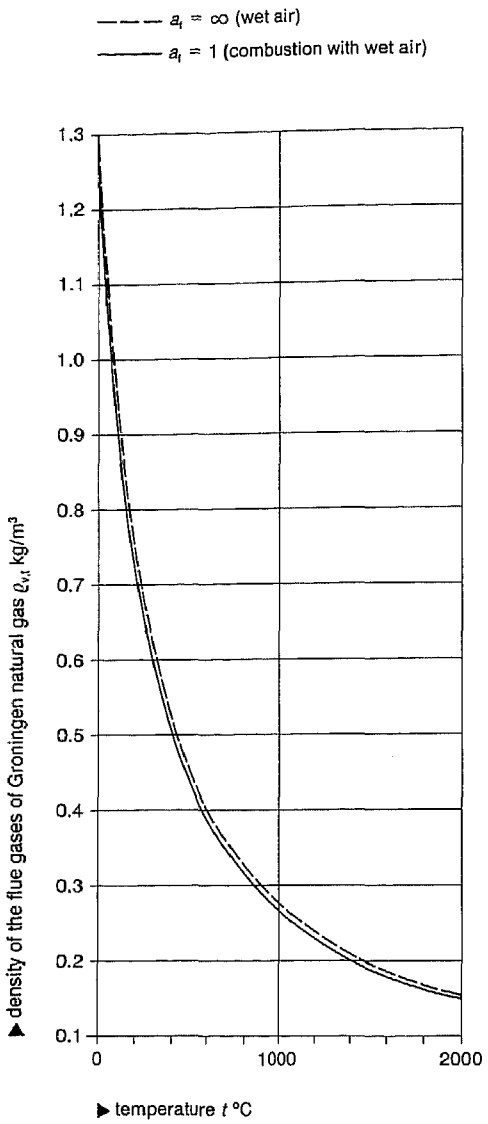


Fig. 3.9 The density $\varrho_{v,T}$ of the flue gases of Groningen natural gas and the density of "wet" air as a function of the flue gas temperature t

3.10 Viscosity

3.10.1 Dynamic viscosity

Table 3.10.1 gives dynamic viscosity μ of pure gases over the temperature range 0 – 1600 °C (lit. 33, 35)

The literature contains a variety of equations for calculating the viscosity of pure gases. A number of these methods are discussed below

3.10.1.1 The Sutherland method (lit. 38)

The simplest equation for viscosity calculations is the Sutherland formula (fig. 3.10.1):

$$\frac{\mu_T}{\mu_o} = \left(\frac{T}{273.15}\right)^{3/2} \frac{273.15 + C_s}{T + C_s} \qquad [3.42]$$

where:

μ_T	=	dynamic viscosity at T K and 101.325 kPa	Pa · s
μ_o	=	dynamic viscosity at 273.15 K and 101.325 kPa (table 3.10.1 and fig. 3.10.1)	Pa · s
C_s	=	Sutherland constant (table 3.10.2)	–
T	=	absolute temperature (= t + 273.15)	K
t	=	temperature	°C

This method provides an accuracy of better than 5 %

3.10.1.2 The Chapman and Cowling method (lit. 5, 12) for pure gases

This method is discussed in 2.5.1.3

3.10.1.3 Viscosity of gas mixtures

The Herning and Zipperer method (lit. 5, 12, 15) is suitable for gas mixtures. This method is described in 2.5.1.1

Where ν and ϱ are known, the dynamic viscosity μ can also be calculated from:

$$\mu = \nu \cdot \varrho \qquad [2.82]$$

Table 3.10.1 Dynamic viscosity μ of pure gases at 101.325 kPa and $0 \leq t \leq 1600\,°C$

Temperature t °C	Dynamic viscosity $\mu \times 10^6$ Pa · s										
	NO**)	NO_2**)	N_2	Ar	CO_2	CO	H_2O	H_2	O_2	SO_2	air
0	17.9	13.7	16.63	20.93	13.80	16.60	8.66	8.41	19.19	11.63	17.16
100	22.7	18.4	20.95	27.00	18.40	20.97	12.13	10.38	24.22	16.06	21.65
200	26.8	22.6	24.82	32.38	22.65	24.89	15.65	12.17	28.73	20.27	25.65
300	31.2	26.5	28.30	37.15	26.57	28.43	19.20	13.85	32.81	24.22	29.26
400	34.7	29.9	31.48	41.41	30.16	31.66	22.77	15.43	36.55	27.91	32.53
500	38.5	33.2	34.38	45.24	33.45	34.64	26.35	16.93	40.00	31.33	35.52
600			37.05	48.74	36.47	37.40	29.92	18.36	43.24	34.53	38.27
700			39.53	51.98	39.24	39.97	33.49	19.74	46.31	37.53	40.82
800			41.86	55.03	41.80	42.44	37.04	21.08	49.26	40.38	43.20
900			44.05	57.99	44.18	44.79	40.56	22.36	52.14	43.11	45.46
1000	52.6***)	45.5	46.14	60.91	46.41	47.06	44.07	23.61	54.99	45.77	47.61
1100			48.15	63.78	48.53	49.2*)	47.54	24.82	57.7*)	48.3*)	49.69
1200			50.11	66.59	50.57	51.3*)	51.00	26.01	60.6*)	50.75*)	51.73
1300			52.04	69.37	52.54	53.3*)	54.37	27.16	63.5*)	53.2*)	53.74
1400			53.96	72.13	54.49	55.3*)	57.78	28.29	66.3*)	55.5*)	55.76
1500			55.89	74.92	56.44	57.2*)	61.10	29.39	69.2*)	57.9*)	57.80
1600	65.8***)		57.84	77.74	58.41	59.2*)	64.39	30.47	71.9*)	60.2*)	59.89

*) Extrapolated (fig. 3.10.1)
**) Lit. 35 – fig. 3.10.1
***) Calculated using Sutherland formula [3.42]

where:

μ	= dynamic viscosity	Pa · s
ν	= kinematic viscosity (3.10.2)	m^2/s
ϱ	= density (3.9)	kg/m^3

3.10.2 Kinematic viscosity

The kinematic viscosity ν of flue gases at temperature t can be calculated from its components using Mann's reciprocal formula (inter alia lit. 38):

$$\frac{1}{\nu_m} = \sum_{i=1}^{n} \frac{x_i}{100 \cdot \nu_i} \qquad [3.43]$$

Table 3.10.2 Sutherland constants

Component	C_s
CH_4	190
C_2H_6	287
C_3H_8	324
C_4H_{10}	349
H_2S	331
SO_2	416
C_2H_4	257
C_3H_6	322
Ar	164
He	78.2
CO_2	266
CO	104
H_2	90
N_2	112
O_2	131
H_2O	673
air	116
NO	139*
NO_2	240*

* Calculated from table 3.10.1

where:

ν_m	=	kinematic viscosity of gas mixture	m^2/s
ν_i	=	kinematic viscosity of component i (table 3.10.3 and fig. 3.10.2)	m^2/s
x_i	=	concentration of component i	% (vol.)
n	=	number of components	–

As mentioned before viscosity can also be calculated using the formula:

$$\nu = \mu/\varrho \qquad [2.82] \qquad m^2/s$$

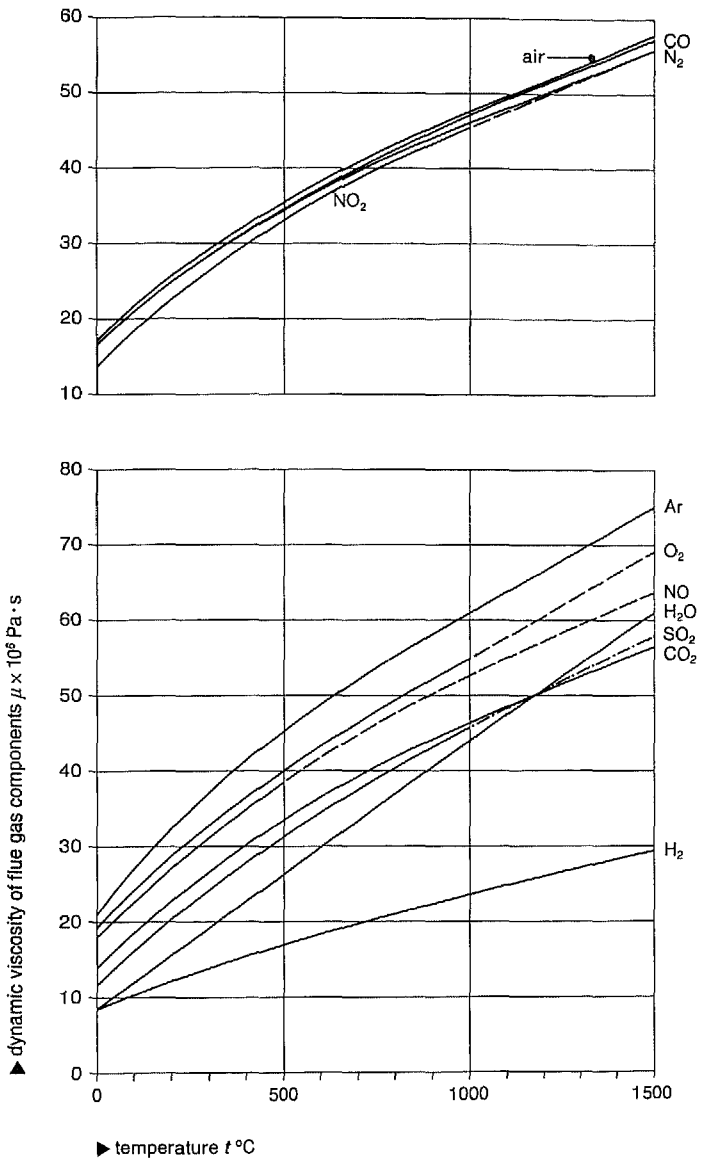


Fig. 3.10.1 The dynamic viscosity μ of pure gases at 101.325 kPa as a function of the flue gas temperature t

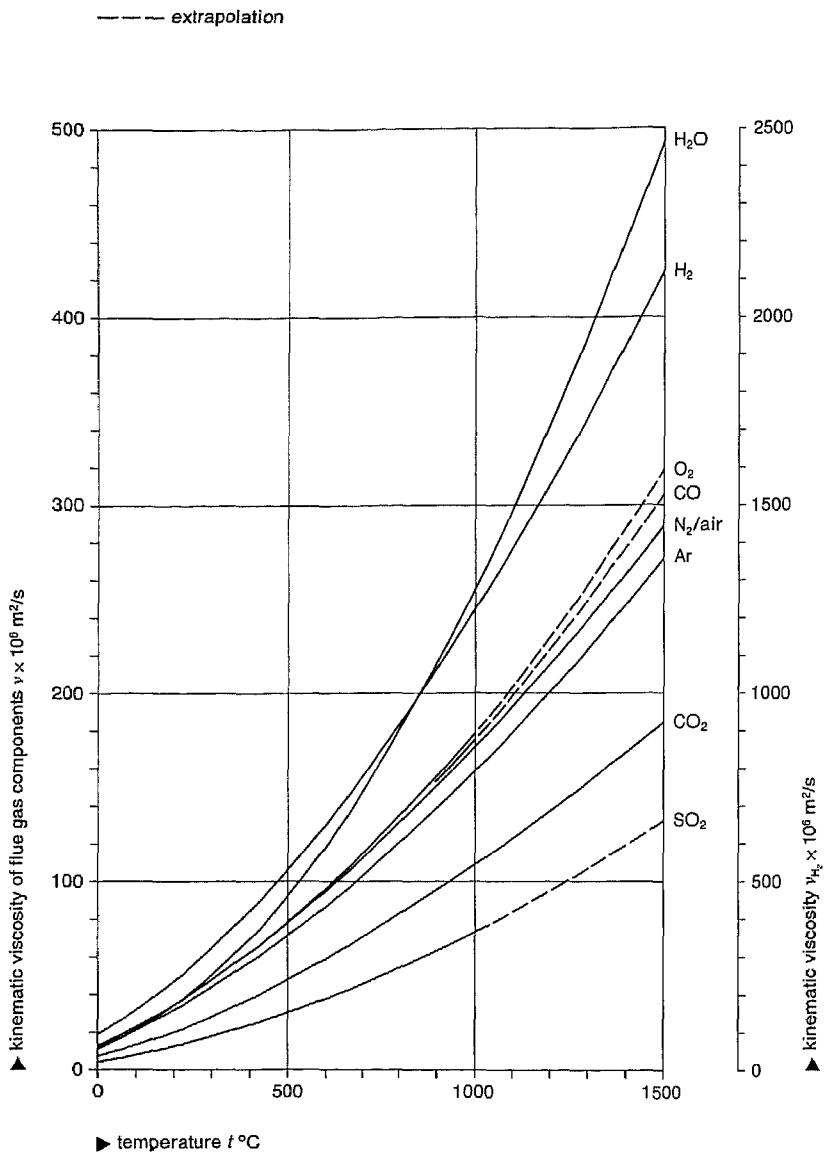


Fig. 3.10.2 The kinematic viscosity ν of pure gases at 101.325 kPa as a function of the temperature t

3.11 Isobaric heat capacity

The isobaric heat capacity c_p represents the quantity of heat which has to be supplied at t °C to raise the temperature of 1 m^3 of gas (0 °C; 101.325 kPa) by 1 K. The isobaric heat capacity c_p is therefore associated with one particular temperature, in contrast to the "average" heat capacity c_{pm} (3.6) which applies to a temperature range of (0 – t) °C

Table 3.11 gives values for the isobaric heat capacity c_p of flue gas components (lit. 34)

In the case of a mixture:

$$c_p = \sum_{i=1}^{n} x_i \cdot c_{p,i}/100 \qquad [3.44]$$

where:

c_p	=	isobaric heat capacity of gas mixture at t °C and 101.325 kPa	kJ/(m^3 · K)
x_i	=	concentration of component i	% (vol.)
$c_{p,i}$	=	isobaric heat capacity of component i at t °C and 101.325 kPa (table 3.11; fig. 3.11; 2.6.1)	kJ/(m^3 · K)
n	=	number of components	–

Note: The isobaric heat capacity c_p of argon (Ar) is constant over the entire temperature range and is 0.926 kJ/(m^3 · K)

Table 3.11 Isobaric heat capacity c_p of pure gases at 101.325 kPa and $0 \leq t \leq 2400$ °C

Temperature t°C			Isobaric heat capacity c_p kJ/(m³ · K)							
	NO***)	NO_2***)	CO_2	O_2	N_2	H_2O	SO_2***)	CO	H_2	air**)
0	1.301	1.669	1.620	1.310	1.302	1.491	1.712	1.302	1.281	1.302
100	1.313	1.810	1.821	1.331	1.306	1.516	1.933	1.310	1.298	1.306
200	1.347	1.960	1.972	1.373	1.315	1.553	2.079	1.327	1.306	1.323
300	1.380	2.076	2.114	1.424	1.336	1.599	2.202	1.352	1.312	1.352
400	1.419	2.182	2.219	1.465	1.365	1.654	2.299	1.382	1.315	1.382
500	1.459	2.279	2.303	1.503	1.398	1.708	2.385	1.415	1.319	1.411
600	1.485*)	2.340*)	2.374	1.532	1.428	1.758	2.436*)	1.449	1.327	1.440
700	1.515*)	2.395*)	2.428	1.557	1.457	1.817	2.481*)	1.478	1.344	1.465
800	1.540*)	2.440*)	2.483	1.574	1.482	1.876	2.518*)	1.503	1.361	1.495
900	1.560*)	2.480*)	2.520	1.591	1.503	1.930	2.550*)	1.524	1.377	1.516
1000	1.576	2.517	2.554	1.608	1.524	1.980	2.581	1.541	1.394	1.532
1200	1.605*)	2.565*)	2.604	1.633	1.557	2.072	2.629*)	1.570	1.436	1.566
1400	1.630*)	2.615*)	2.642	1.654	1.578	2.156	2.669*)	1.595	1.474	1.591
1600	1.645*)	2.645*)	2.675	1.675	1.595	2.223	2.704*)	1.612	1.507	1.608
1800	1.655*)	2.680*)	2.700	1.696	1.612	2.282	2.734*)	1.624	1.541	1.624
2000	1.660	2.703	2.713	1.717	1.629	2.332	2.764	1.637	1.566	1.641
2200	1.670*)	2.725*)	2.726	1.733	1.631	2.374	2.783*)	1.645	1.591	1.654
2400	1.675*)	2.735*)	2.734	1.750	1.645	2.412	2.800*)	1.654	1.612	1.666

*) Interpolated
**) Compare with values for CO
***) Lit. 35

Note: The isobaric heat capacity c_p of argon (Ar) is constant over the entire temperature range and is 0.926 kJ/(m³ · K)

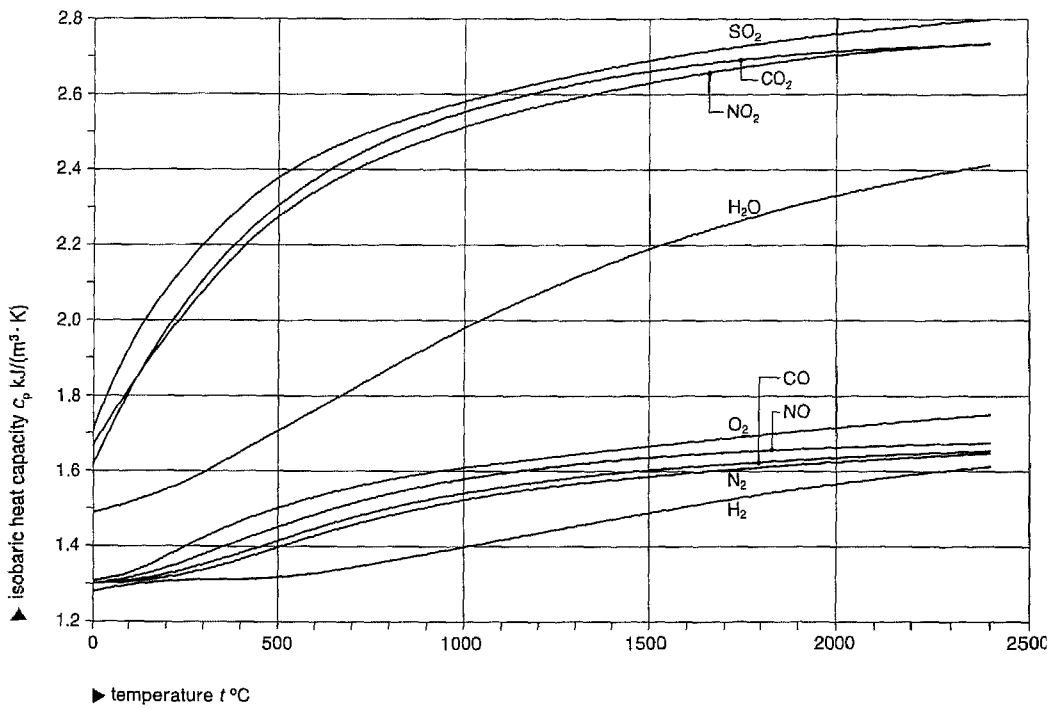


Fig. 3.11 The isobaric heat capacity c_p of pure gases as a function of the temperature t

3.12 Thermal conductivity

The thermal conductivity λ of a number of pure gases is given in table 3.12 a fig. 3.12.1. The values given in the literature vary widely which allows to mal random choice. The values presented here are taken from lit. 36, supplemented with data from lit. 35

Using the basic values given in table 3.12, the thermal conductivity of flue gases can be calculated by means of the empirical formula presented in lit.

$$\lambda = \left[1 + \frac{\left(\frac{x_p}{100}\right) - \left(\frac{x_p}{100}\right)^2}{3.5}\right] \sum_{i=1}^{n} x_i \cdot \lambda_i / 100 \qquad [3.45]$$

where:

λ	=	thermal conductivity of flue gases at t °C and 101.325 kPa	W/(m · K)
x_i	=	concentration of component i	% (vol.)
λ_i	=	thermal conductivity of component i at t °C and 101.325 kPa (table 3.12 and fig. 3.12.1)	W/(m · K)
x_p	=	sum of the concentrations of the "polar" or "non-polar" components	% (vol.)
n	=	number of components	–

The factor $f = \left[1 + \frac{\left(\frac{x_p}{100}\right) - \left(\frac{x_p}{100}\right)^2}{3.5}\right]$ has the function of a "refining factor" (fig. 3.12.2)

Of the components listed in table 3.12, only water is "polar", so that the H content of the flue gases can be used for x_p in equation [3.45]

Table 3.12 Thermal conductivity λ of pure gases at 101.325 kPa and 0 < t < 1200 °C

Temperature	Thermal conductivity λ W/(m · K)								
t °C	CO_2	O_2	N_2	H_2O	CO**)	H_2**)	Ar**)	air	NO**)
0	0.0145	0.0242	0.0242	0.0159	0.023	0.171	0.0163	0.0244	0.024
100	0.0223	0.0315	0.0311	0.0248	0.030	0.211	0.0221	0.0314	0.031
200	0.0301	0.0387	0.0376	0.0328	0.037	0.249	0.0384	0.038	
300	0.0379	0.0456	0.0436	0.0434	0.043	0.285	0.0302	0.0465	–
400	0.0456	0.0523	0.0490	0.0548	0.049	0.321	0.0349	0.0523	–
500	0.0543	0.0586	0.0543	0.0692	0.055	0.357	0.0395	0.0582	–
600	0.0605	0.0644	0.0587	0.0802	–	0.390*)	0.0437	0.0637	–
700	0.0672	0.0700	0.0628	0.0959	–	0.424*)	0.0477	0.0682	–
800	0.0733	0.0756	0.0666	0.1073	–	0.455*)	0.0514	0.0717	–
900	0.0789	0.0808	0.0704	0.1229	–	0.4881*)	0.0550	0.0750	–
1000	0.0835	0.0858	0.0733	0.1372	–	0.519	0.0582	0.0779	–
1200	0.0913	0.0951	0.0791	0.1582	–	0.580*)	0.0647	0.0832	–

For SO_2: λ = 0.0081 W/(m · K) at 0 °C
*) Interpolated (fig. 3.12.1)
**) Lit. 35 b (Co = N_2; NO = O_2)

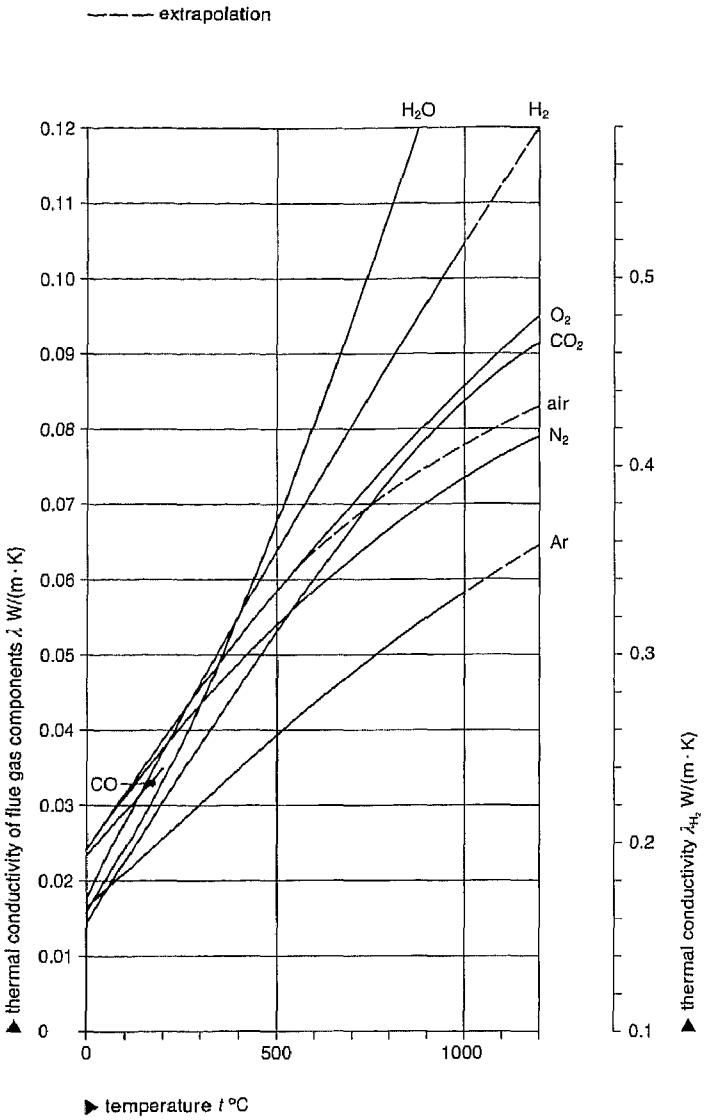


Fig. 3.12.1 The thermal conductivity λ of pure gases at 101.325 kPa as a function of the flue gas temperature t

$$f = \left[1 + \frac{(x_p/100) - (x_p/100)^2}{3.5}\right]$$

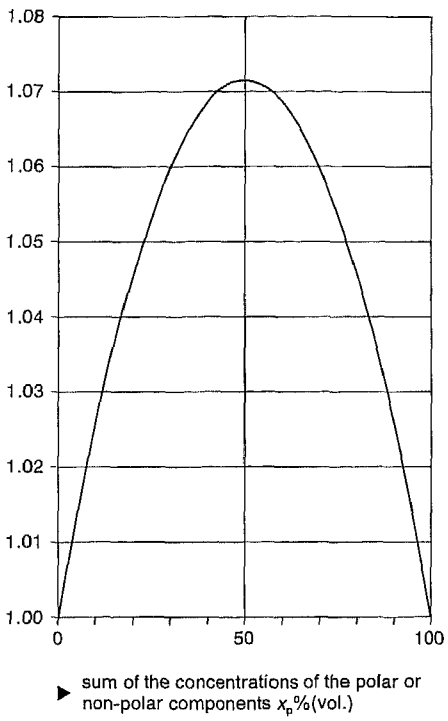


Fig. 3.12.2 The refining factor f as a function of the sum of concentrations of the polar or non-polar components x_p

3.13 Theoretical flame temperature

If no allowance is made for dissociation – the decomposition of a number of gas molecules into other molecules, atomic groups, ions and atoms (so-called "free radicals") at elevated temperatures (> 1500 °C) – the theoretical flame temperature can be calculated by means of:

$$H_i = q_{tot} \cdot c_{pm} \times 10^{-3} \cdot \Delta t - (q_a \cdot c_{pm,a} \times 10^{-3} \cdot \Delta t_{amb} + q_g \cdot c_{pm,g} \times 10^{-3} \cdot \Delta t_g) \quad [3.25\,a]$$

where:

H_i	=	net calorific value of the combustible gas (3.1)	MJ/m³
q_{tot}	=	total quantity of flue gases (3.4)	m³/m³ gas
c_{pm}	=	average isobaric heat capacity of the flue gases over temperature range Δt	kJ/(m³ · K)
Δt	=	temperature range (0 – t)	°C
t	=	temperature of the flue gases (= theoretical flame temperature)	°C
q_a	=	*total quantity of air for complete combustion* (a_f = 1)	m³/m³ gas
a_f	=	air factor (1.4.8)	–
$c_{pm,a}$	=	average isobaric heat capacity of the combustion air over temperature range Δt_{amb}	kJ/(m³ · K)
Δt_{amb}	=	temperature range (0 – t_{amb})	°C
t_{amb}	=	temperature of the ambient air	°C
q_g	=	quantity of combustible gas (= 1)	m³
$c_{pm,g}$	=	average isobaric heat capacity of the combustible gas over temperature range Δt_g	kJ/(m³ · K)
Δt_g	=	temperature range (0 – t_g)	°C
t_g	=	temperature of the combustible gas	°C

For natural gases formula [3.25a] may well be replaced by:

$$\frac{H_i}{q_{tot}} = c_{pm,t} \times 10^{-3} (t - t_{amb}) \quad [3.46]$$

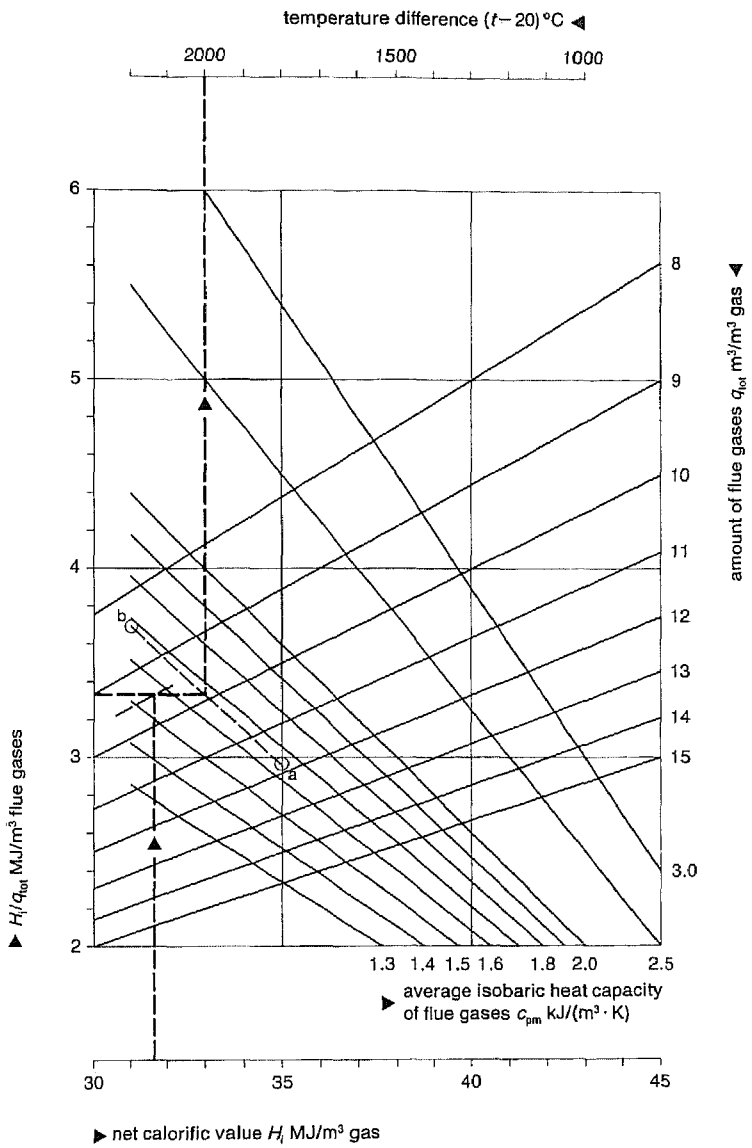


Fig. 3.13 The theoretical flame temperature t as a function of the net calorific value H_i, the average isobaric heat capacity of the flue gases c_{pm} and the total amount of flue gases q_{tot}

where:

t	=	theoretical flame temperature	°C
H_i	=	net calorific value (3.1)	MJ/m³ gas
q_{tot}	=	total quantity of flue gases (3.4)	m³/m³ gas
$c_{pm,t}$	=	average isobaric heat capacity of the flue gases at temperature t	kJ/(m³ · K)
t_{amb}	=	temperature of the ambient air	°C

Since c_{pm} is a function of t, the above equation can only be resolved by trial and error, using fig. 3.13 as a guide.

Example: Groningen natural gas (table 1.9)

H_i = 31.669 MJ/m³ gas (table 3.1.2)
q_{tot} = 9.4874 m³/m³ gas (table 3.4.3)
t_{amb} = 20 °C

The value of H_i/q_{tot} [3.46] is 3.34 MJ/m³ (fig. 3.13)

For $a_f = 1$ it follows from tables 3.43 and 3.6:

a. c_{pm} = 1.642 kJ/m³ at $(t - 20)$ = 1800 °C
b. c_{pm} = 1.680 kJ/m³ at $(t - 20)$ = 2200 °C

The point where the straight line through a – b intersects the line H_i/q_{tot} = 3.34 gives a value of $(t - 20)$ = 2000 °C. This results in a value of 2020 °C for the theoretical flame temperature t

3.14 Heat transfer coefficient

Heat transfer coefficient α_{tot} is given by:

$$\alpha_{tot} = \alpha_c + \alpha_r \qquad [3.47]$$

The heat transfer coefficient for convection α_c can usually be calculated using a number of formulas which are valid only in certain conditions and require no further elucidation here. The heat transfer coefficient for radiation can be calculated using simple empirical formulas. One method of determining the heat transfer coefficient for radiation α_r (an apparent coefficient of heat transfer by radiation) is described below.

Gases radiate selectively, in other words they radiate or absorb only within given wavelength bands. There are only two principal gases which need to be considered in relation to certain radiation phenomena, H_2O and CO_2, both of which occur in flue gases. Figs. 3.14.1 and 3.14.2 (lit. 33) give values for α_r for CO_2 and H_2O, respectively, as a function of t_g, t_w, p and s, where:

α_r	=	radiation coefficient for CO_2 or H_2O	$W/(m^2 \cdot K)$
t_g	=	temperature of combustion products	°C
t_w	=	wall temperature	°C
p	=	partial pressure of CO_2 or H_2O	kPa
s	=	thickness of radiating layer	m

The partial pressure p of CO_2 and H_2O in the combustion products can be calculated using:

$$\frac{p}{p_{tot}} = \frac{q}{q_{st} + (a_f - 1)\,a} \qquad [3.48]$$

where:

p	=	partial pressure of CO_2 or H_2O	[3.48]	kPa
p_{tot}	=	total pressure of flue gases (generally 101.325)		kPa
q	=	quantity of CO_2 or H_2O produced (3.4)		m^3/m^3 gas
q_{st}	=	quantity of flue gases generated by stoichiometric combustion ($a_f = 1$) (3.4)		m^3/m^3 gas
a_f	=	air factor; $(a_f - 1)$ = excess air (1.4.8)		–
a	=	theoretical air requirement (3.3)		m^3/m^3 gas

For a_r:

$$\alpha_r = \alpha_{r(CO_2)} + \alpha_{r(H_2O)} \qquad [3.49]$$

For thickness of radiating layer s (lit. 40):

$$s = f \cdot D \qquad [3.50]$$

where:

f	= a factor expressing the shape of the "gas body"	–
D	= diameter of pipe or combustion chamber	m

Table 3.14 gives a number of values for factor f (for pipes $f = 0.9$). In the case of "gas bodies" of arbitrary shape, the following equation may be used for s (lit. 41):

$$s = 3.25 \frac{V}{F} \qquad [3.51]$$

where:

V	= volume	m^3
F	= total wall area	m^2

Table 3.14 Shape constants for a number of "gas bodies"

Shape of "gas body"	f
cylinder of infinite length and diameter D (radiation on wall)	0.9
cylinder of infinite length and diameter D (radiation on centre of base plane)	0.9
cylinder of which $h = D$ (radiation on surrounding surface)	0.6
cylinder of which $h = D$ (radiation on centre of base plane)	0.77

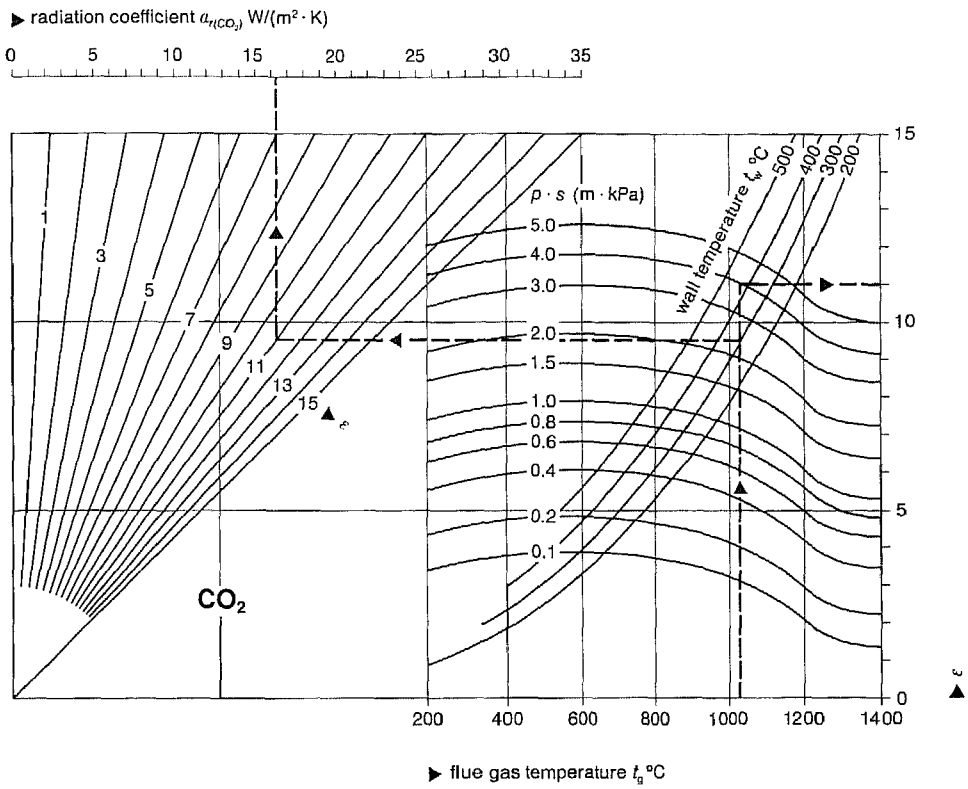


Fig. 3.14.1 The CO_2 radiation coefficient $\alpha_{r(CO_2)}$ as a function of the flue gas temperatuur t_g, the wall temperature t_w, the partial CO_2 pressure p and the thickness of the radiating layer s

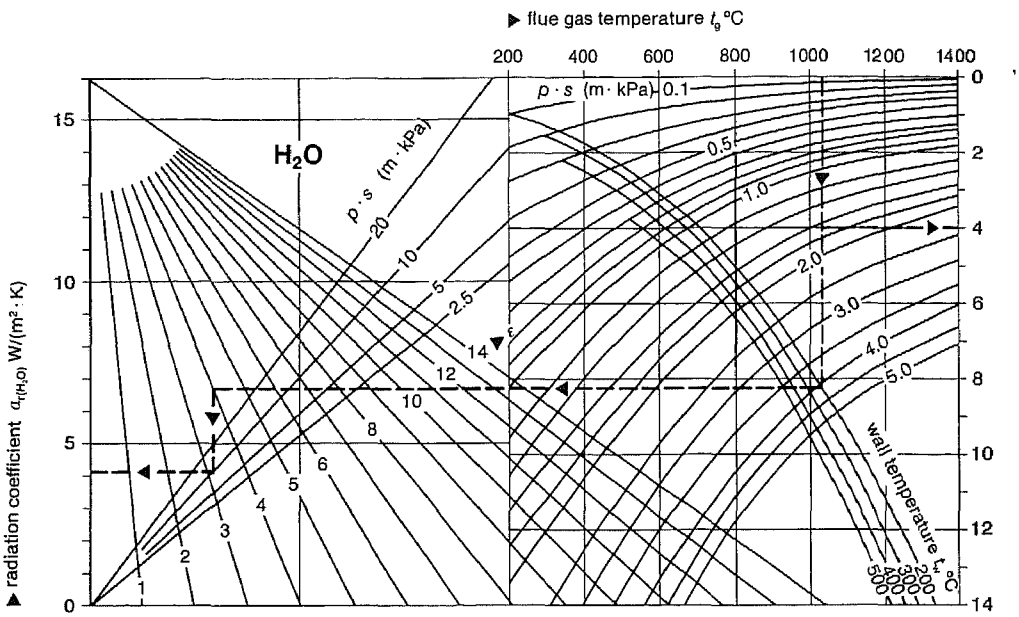


Fig. 3.14.2 The H_2O radiation coefficient $\alpha_{r(H_2O)}$ as a function of the flue gas temperature t_g, the wall temperature t_w, the partial H_2O pressure p and the thickness of the radiating layer s

3.15 Flammability limits and autoignition temperatures of gases and gas mixtures

3.15.1 General

Fig. 3.15.1, which has been compiled using data from various sources in the literature, presents a temperature-composition diagram for methane-air mixtures, divided in regions based on flammability behaviour. In the area between "upper flammability limit" (*UL*) and "lower flammability limit" (*LL*) (1.4.12) and below the "autoignition temperature" (1.4.22), the gas mixture will explode if it is ignited in any way. In the area between "upper flammability limit" and "lower flammability limit" and above the "autoignition temperature", autoignition will occur.

Table 3.15.1 gives the flammability limits in air and oxygen and the autoignition temperatures for pure gases (lit. 43 and 46). The highest temperature occurring during combustion (the theoretical flame temperature) – disregarding any dissociation of the combustible gas – is indicated by the lines above "autoignition temperature" (fig. 3.15.1)

As a general rule, when a combustible gas is combined with air or oxygen in an enclosed space, an exothermic reaction will take place between the combustible gas and the oxygen present. The speed of the reaction is a function of the temperature of the mixture.

At room temperature this reaction – refferred to as "slow combustion" – is almost imperceptible. The speed of the reaction increases with increasing temperature.

When the "autoignition temperature" is reached, the gas mixture will ignite spontaneously provided the gas/air ratio is within certain limits (fig. 3.15.1)

If the temperature of the gas mixture is below the autoignition temperature, the mixture has to be ignited in some way in order to cause an "explosion". Once again, the gas/air ratio has to lie within certain limits (fig. 3.15.1). "Explosion" here means "deflagration" (1.4.13), an exothermic reaction which proceeds at a speed below the prevailing velocity of sound.

In addition to deflagration, another type of reaction is "detonation" (1.4.14); this is an exothermic reaction which creates shock waves and in which the flame front propagates at a velocity equal to or greater than the prevailing

Table 3.15.1 Flammability limits in air and oxygen at 20 °C and 101.325 kPa and autoignition temperatures

No.	Component	Formula	Flammability limits (20 °C; 101.325 kPa)				Autoignition temperature
			Concentration of gas in air % (vol.)		Concentration of gas in oxygen % (vol.)		K
			LL	*UL*	*LL*	*UL*	
1	methane	CH_4	4.4	16.5	5.1	61.0	903
2	ethane	C_2H_6	3.0	12.5	3.0	66.0	788
3	propane	C_3H_8	2.2	9.5	2.3	55.0	723
4	2-methylpropane (isobutane)	C_4H_{10}	1.8	8.4	1.8	48.0	733
5	butane	C_4H_{10}	1.9	8.5	1.8	49.0	678
6	2,2-dimethylpropane	C_5H_{12}	1.4	7.5			723
7	2-methylbutane (isopentane)	C_5H_{12}	1.4	7.7			
8	pentane	C_5H_{12}	1.5	7.8			582
9	2,2-dimethylbutane	C_6H_{14}	1.2	7.0			
10	2,3-dimethylbutane	C_6H_{14}	1.2	7.0			
11	3-methylpentane	C_6H_{14}	1.2	7.0			
12	2-methylpentane (isohexane)	C_6H_{14}	1.2	7.0			
13	hexane	C_6H_{14}	1.2	7.5			498
14	2-methylhexane (isoheptane)	C_7H_{16}	1.1	6.7			
15	heptane	C_7H_{16}	1.2	6.7			488
16	octane	C_8H_{18}	1.0				493
17	nonane	C_9H_{20}	0.85				478
18	decane	$C_{10}H_{22}$	0.75	5.6			483
19	undecane	$C_{11}H_{24}$					
20	dodecane	$C_{12}H_{26}$	0.6				478
21	tridecane	$C_{13}H_{28}$					
22	tetradecane	$C_{14}H_{30}$	0.5				473

23	cyclohexane	C_6H_{12}	1.3	8.0			518
24	methylcyclohexane	C_7H_{14}	1.1	6.7			523
25	benzene	C_6H_6	1.4	7.1			833
26	toluene	C_7H_8	1.2	7.1			753
27	xylene (o)	C_8H_{10}	1.0	6.7			703
28	methyl mercaptan	CH_3SH	4.1				
29	ethyl mercaptan	C_2H_5SH	2.8	18.0			573
30	propyl mercaptan	C_3H_7SH					
31	carbonyl sulphide	COS					
32	hydrogen sulphide	H_2S	4.0	44.0			
33	sulphur dioxide	SO_2	–	–	–	–	–
34	ethene	C_2H_4	2.4	32.5	3.0	80.0	763
35	propene	C_3H_6	2.4	10.3	2.1	53.0	733
36	1-butene	C_4H_8	1.6	9.3	1.8	58.0	658
37	1-pentene	C_5H_{10}	1.4				
38	1,2-butadiene	C_4H_6					
39	1-butyne	C_4H_6					
40	methanol	CH_3OH	6.7	36.0			658
41	ethanol	C_2H_5OH	3.3	19.0			638
42	argon	Ar	–	–	–	–	–
43	helium	He	–	–	–	–	–
44	carbon dioxide	CO_2	–	–	–	–	–
45	carbon monoxide	CO	12.5	74.0	15.5	94.0	
46	hydrogen	H_2	4.0	75.0	4.0	94.0	673
47	nitrogen	N_2	–	–	–	–	–
48	oxygen	O_2	–	–	–	–	–
49	nitric oxide	NO	–	–	–	–	–
50	nitrogen dioxide	NO_2	–	–	–	–	–
51	water vapour	H_2O	–	–	–	–	–
52	air (dry)	–	–	–	–	–	–

velocity of sound. The explosive pressures generated by detonation are significantly higher than those produced by deflagration (lit. 42 and 44)

A number of gases and vapours react – before reaching autoignition temperature – by producing a "cold flame" (a barely visible flame)

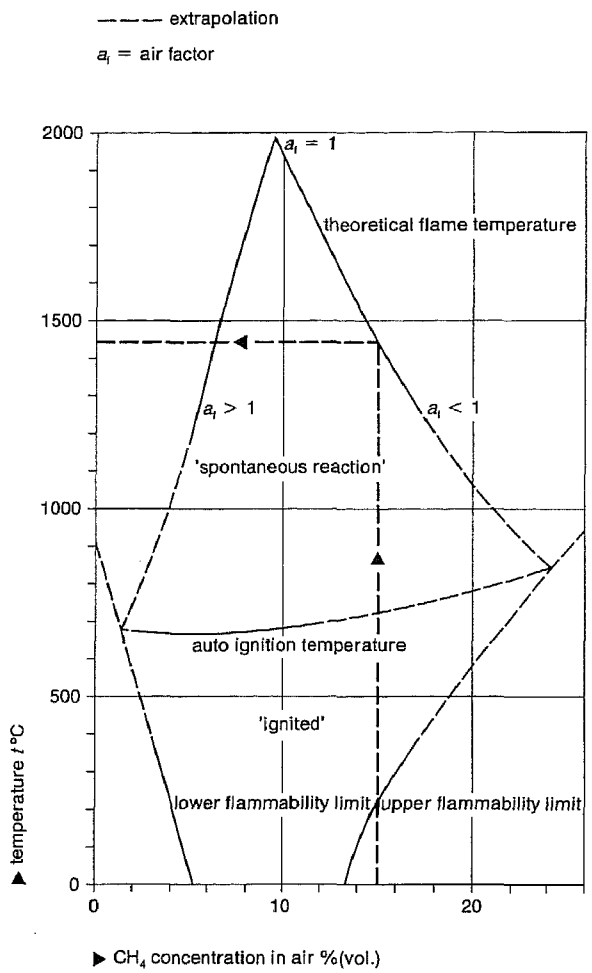


Fig. 3.15.1 General flammability diagram for combustible gases

Every combustible gas has two flammability limits, upper and lower (1.4.12), generally expressed in percentage by volume of the combustible gas in air or oxygen (table 3.15.1). While the gas/air ratio remains between these limits, sufficient heat will be developed after ignition to enable the gas/air mixture to continue to support combustion (lit. 43)

The flammability limits of a gas mixture are dictated by several factors and can be measured or calculated using empirically developed formulas.

The speed at which the flame front propagates – the burning velocity – depends among other things on the temperature and the composition of the gas mixture. Various measurement methods and empirical formulas are available for measuring the burning velocity of a gas mixture.

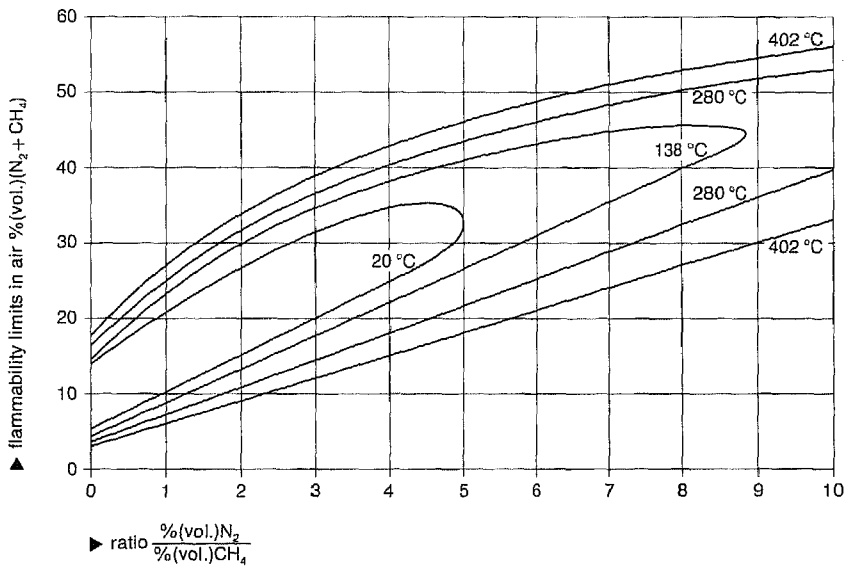


Fig. 3.15.2 Flammability limits LL and UL of a (N_2 + CH_4) gas mixture in air at 101.325 kPa as a function of the N_2/CH_4 ratio and the mixture temperature

3.15.2 Factors affecting flammability limits of gas/air mixtures

There are a number of factors which determine whether a gas/air mixture will be explosive:

1. Composition
Inert components reduce the flammability range (the area between the upper and lower flammability limits – fig. 3.15.1)

2. Temperature
The flammability range increases with increasing temperature. When the autoignition temperature is reached, the gas/air mixture will ignite spontaneously, i.e. with no energy supplied from outside.

3. Pressure
Changes in barometric pressure within the normal range have no significant effect on the flammability limits. At low pressures ($\ll$101.325 kPa) however, the flammability limits are brought closer together and at higher pressures they are further apart (except in the case of CO/air mixtures, where the gap between the flammability limits becomes narrower at higher pressures – (lit. 43)

4. Humidity
The upper and lower flammability limits are brought closer together as moisture content (humidity) increases, the upper flammability limit being shifted more than the lower. Here, too, CO/air mixtures are affected most (lit. 43)

5. Ignition energy
The amount of ignition energy supplied has an effect on the flammability limits. There is little information in the literature on this point.

6. Turbulence
The effect of turbulence on the flammability limits is only mentioned in passing in the literature and is generally disregarded.

7. Shape of combustion space
The flammability limits are generally determined in a cylindrical combustion space, by varying its diameter and attitude. Many experiments are currently being performed in spherical combustion chambers. These have the advantage of reduced heat loss to the surroundings and reduced wall effects on flame propagation.

3.15.3 Calculation of flammability limits

Measurement of the flammability limits of a gas mixture is a time-consuming and expensive process. In practice, therefore, empirical formulas are used to calculate the flammability limits from the composition of the gas mixture. The accuracy achieved is amply sufficient, since wide safety margins are generally used in practice.

Le Chatelier (lit. 43) gives the following equation for the flammability limits of a gas mixture at atmospheric pressure:

$$L_m = \frac{100}{\Sigma x_i / L_i} \text{ \% (vol.)} \qquad [3.52]$$

where:

L_m	=	upper/lower flammability limit of gas mixture	% (vol.) gas in air
L_i	=	upper/lower flammability limit of component i (table 3.15.1)	% (vol.) gas in air
x_i	=	concentration of component i in gas mixture	% (vol.)

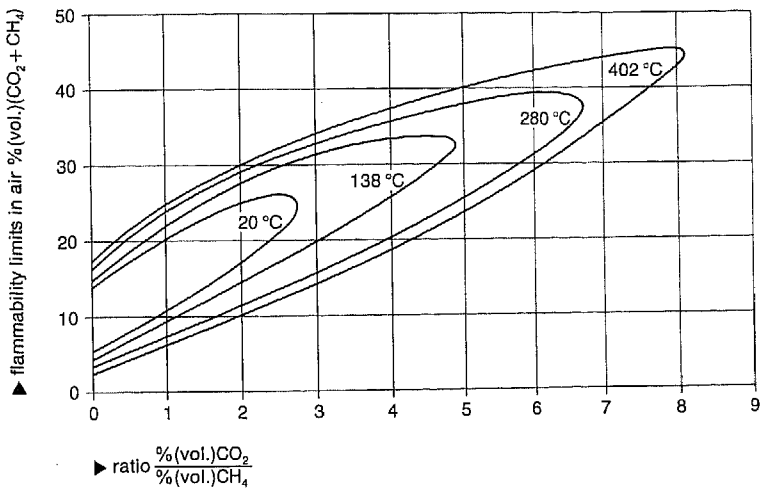


Fig. 3.15.3 Flammability limits LL and UL of a (CO_2 + CH_4) gas mixture in air at 101.325 kPa as a function of the CO_2/CH_4 ratio and the mixture temperature

The above formula cannot be applied to any desired gas mixture. In particular the presence of certain flammable vapours – for example acetone (C_3H_6O) – will have a significant effect on the result (3.15.1 – cool flame)

This formula generally gives good results when applied to natural gases. It can also be used for natural gases containing inert gases (CO_2 and N_2) and even oxygen (O_2)

The procedure in this case is as follows (see example):
- if oxygen (O_2) is present, the composition of the gas has to be corrected to render it "airless";
- the combustible components are linked arbitrarily to the inert components present. Lit. 43, 45 and 46 give the flammability limits in air for a number of combinations of combustible and inert gases (figs. 3.15.2 and 3.15.3);
- Le Chatelier's formula is then used to calculate the flammability limits in air of these combinations (combustible and inert gases) and the other components.

Table 3.15.2 Calculation of flammability limits in air of Groningen natural gas

Component	Formula	x_i % (vol.)	Air-free composition (vol.)
methane	CH_4	81.30	81.34
ethane	C_2H_6	2.85	2.85
propane	C_3H_8	0.37	0.37
butane	C_4H_{10}	0.14	0.14
pentane	C_5H_{12}	0.04	0.04
hexane	C_6H_{14}	0.05	0.05
nitrogen	N_2	14.35	14.32
oxygen	O_2	0.01	–
carbon dioxide	CO_2	0.89	0.89
		100	100

Example:
The quantity of air ($O_2 + N_2$) represented by 0.01 % (vol.) oxygen (O_2) is 0.05 % (vol.) i.e.
0.01 % (vol.) O_2
0.04 % (vol.) N_2

The corrected volume of the gas mixture is thus 99.95 % (vol.) of the original volume. The N_2 concentration is corrected as follows:
remaining in gas mixture – (14.35 – 0.04) = 14.31 % (vol.).

Making the corrected volume up to 100 %, the corrected "air-free" composition of the gas mixture is shown in table 3.15.2

Table 3.15.3 lists the combinations of combustible and inert gases and the other combustible components and gives their flammability limits in air.

Table 3.15.3 Calculation of flammability limits of Groningen natural gas in air

Combustible	x_i	Inerts % (vol.)		Σx_i	Ratio inert/ combustible	Flammability limits % (vol.)*)	
Component	% (vol.)	N_2	CO_2	% (vol.)		UL_i	LL_i
CH_4	80	14.32		94.32	0,18	15.0**)	6.1**)
CH_4	1.34		0.89	2.23	0.66	18.1***)	8.9***)
C_2H_6	2.85			2.85		12.5	3.0
C_3H_8	0.37			0.37		9.5	2.2
C_4H_{10}	0.14			0.14		8.5	1.9
C_5H_{12}	0.04			0.04		7.8	1.5
C_6H_{14}	0.05			0.05		7.5	1.2
				100			

*) Table 3.15.1
**) Fig. 3.15.2 (lit. 45)
***) Fig. 3.15.3 (lit. 45)

For Groningen natural gas the lower explosion limit (*LL*) and the upper explosion limit (*UL*) can be calculated from table 3.15.3:

$$LL = \frac{100}{\Sigma x_i/LL_i} = 5.9\ \%\ \text{(vol.) gas in air} \qquad [3.52]$$

$$UL = \frac{100}{\Sigma x_i/UL_i} = 14.9\ \%\ \text{(vol.) gas in air} \qquad [3.52]$$

This calculated result still has to be corrected for the presence of 0.01 (vol.) % oxygen (O_2) in the original gas mixture. The corrected values are:

$LL = 5.9 \cdot 100/99.95$****) = 5.9 % (vol.) gas in air
$UL = 14.9 \cdot 100/99.95$****) = 14.9 % (vol.) gas in air

****) Corrected "air-free" gas mixture

The effect of the 0.01 % (vol.) O_2 in the gas mixture can thus be disregarded

N.B.

1. If it is not possible to link the combustible components to the inert components in such a way that flammable mixtures are created in turn (see example), then the original gas mixture is not explosive

2. If the "air-free" gas mixture is explosive but the flammability limits after correction for the oxygen present are over 100 %, then the original mixture is not explosive because it already contains too much air

3. If the lower flammability limit of the original gas mixture is "below" 100 % but the upper flammability limit is "above" 100 %, the gas mixture is definitely explosive

3.15.4 Effect of pressure and temperature on flammability limits

Empirical formulas have been developed for a number of combustible gases which make it possible to calculate the flammability limits as a function of pressure or temperature. No formulas are to be found in the literature which take account of the effects of pressure and temperature simultaneously.

In lit. 45 it is demonstrated that it is possible to apply Le Chatelier's rule for the calculation of the flammability limits of gas mixtures as a function of temperature (20 – 400 °C) at 101.325 kPa (table 3.15.4)

Table 3.15.4 Flammability limits in air (lit. 45) at 101.325 kPa and 20 ≤ t ≤ 402 °C

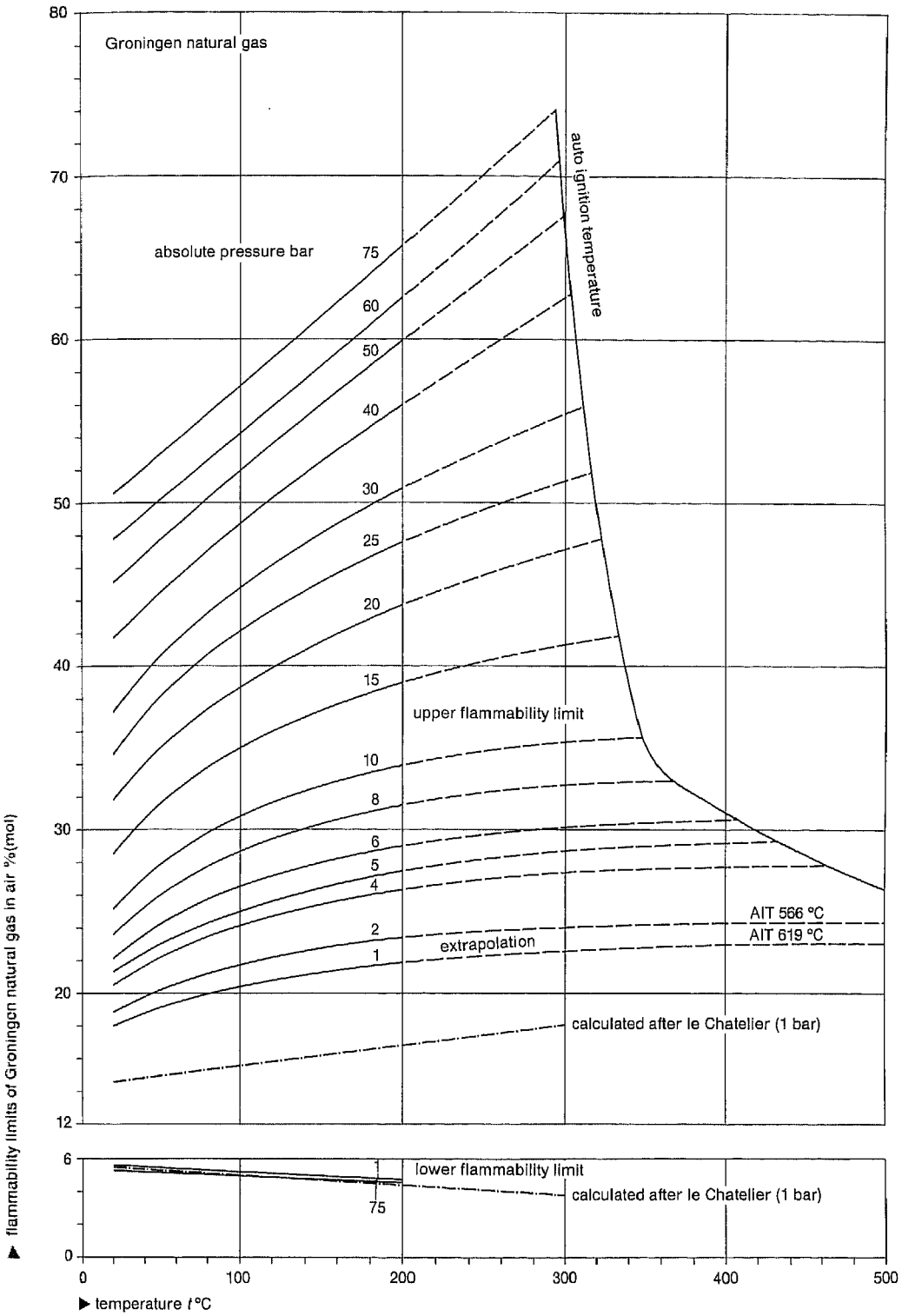
Component	Formula	20 °C		138 °C		280 °C		402 °C	
		LL	*UL*	*LL*	*UL*	*LL*	*UL*	*LL*	*UL*
methane	CH_4	5.1	13.5	4.4	14.1	3.6	15.7	3.0	17.3
ethane	C_2H_6	3.0	11.7	2.5	12.3	2.1	14.1	1.7	16.0
propane	C_3H_8	2.4	9.3	2.1	9.3	1.8	9.7	1.3	11.1
butane	C_4H_{10}	2.0	7.6	1.6	7.9	1.4	7.8	1.2	7.5
ethylene	C_2H_4	2.9	17.7	2.5	20.8	2.0	27.3	1.5	34.7
propylene	C_3H_6	2.5	10.0	2.1	10.7	1.6	11.4	1.4	12.8
carbon monoxide	CO	19.5	72.9	16.2	77.0	12.7	81.3	10.8	85.2
hydrogen	H_2	4.1	72.5	3.6	75.4	3.1	82.3	2.7	86.5

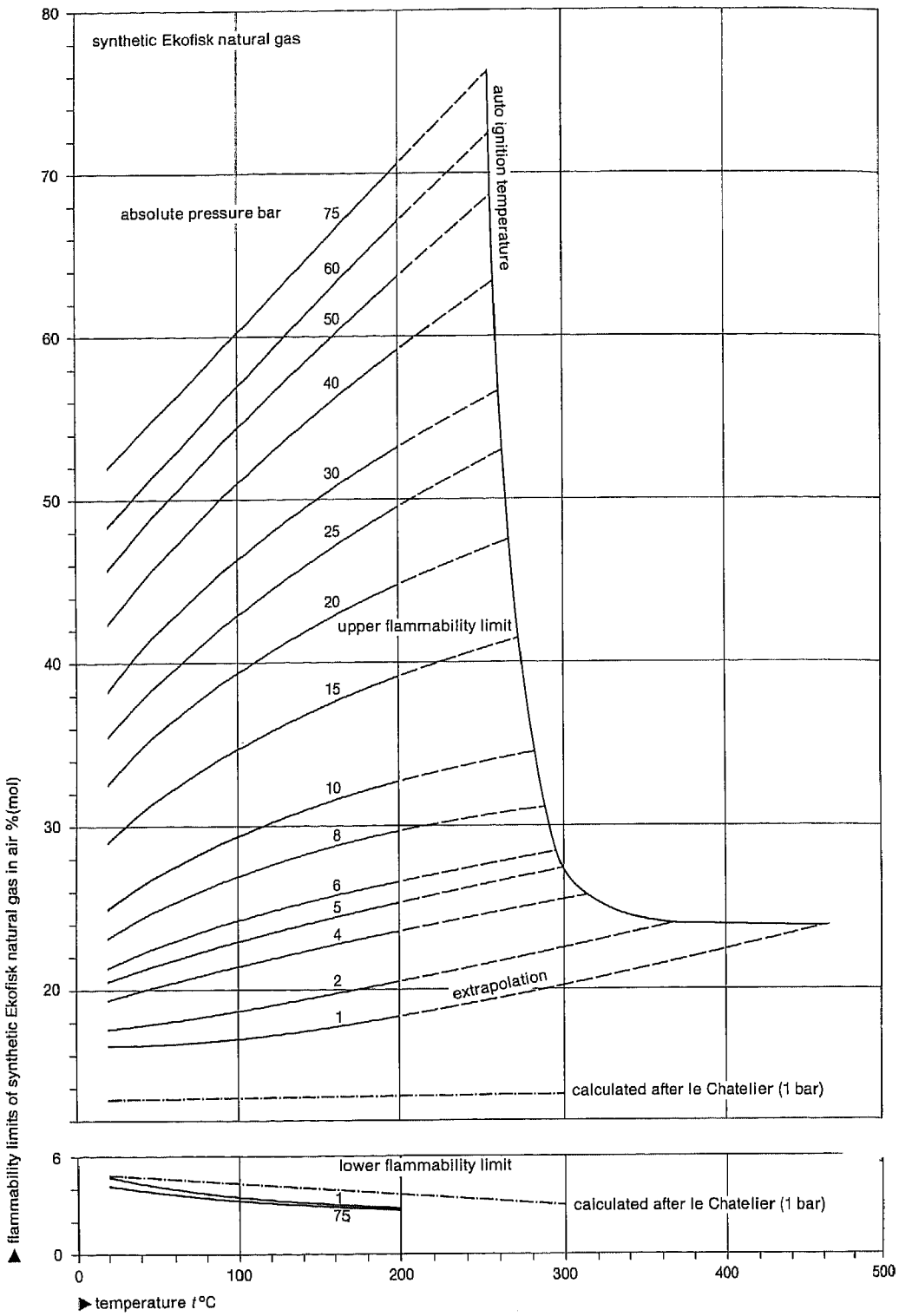
Note: Since the flammability limits at higher temperatures are known only up to C_4H_{10}, all components heavier than C_4H_{10} are counted as C_4H_{10}

In a number of applications – including the injection of air in high calorific gases and the use of natural gas in gas engines – it is necessary to know the flammability limits as a function of pressure and temperature.
In 1972, DSM were commissioned by Gasunie to carry out tests on two natural gases, namely:
Groningen natural gas – the most common natural gas of "relatively" low calorific value H_s = 35.17 MJ/m^3 (fig. 3.15.4) and
Ekofisk natural gas – the gas having the highest calorific value H_s = 44.16 MJ/m^3 (fig. 3.15.5)
The maximum limits of initial pressure and temperature – 45 bar and 400 °C respectively – were imposed by the test equipment.
During the tests carried out by DSM on the flammability limits of both Groningen and Ekofisk gases, the research team was surprised on several occasions by autoignition behaviour of gas/air mixtures. Further study of this problem yielded only a limited amount of information on the occurrence of autoignition as a function of the gas/air ratio and the conditions of pressure and temperature.
After the 1977 tests DSM improved and extended the test equipment and Gasunie commissioned DSM in 1984 to develop formulas on the basis of the data already collected, where necessary supplemented with new test data and information from literature, which would make it possible to calculate the flammability limits and autoignition temperatures of any given natural gas from composition, pressure and temperature. The terms of reference are that the formulae must be valid up to a pressure of 75 bar and a temperature of 400 °C. These test results are given in figs. 3.15.4 and 3.15.5. For further information contact N.V. Nederlandse Gasunie.

Fig. 3.15.4 gives the results for Groningen natural gas (table 3.15.3), which are again based on figs. 3.15.2 and 3.15.3 and table 3.15.4

Fig. 3.15.5 (page 212) gives the results for synthetic Ekofisk natural gas, which are again based on figs. 3.15.2 and 3.15.3 and table 3.15.4


Groningen natural gas
absolute pressure bar
75
60
50
40
30
25
20
15
10
8
6
5
4
2
1
auto ignition temperature
upper flammability limit
AIT 566 °C
AIT 619 °C
extrapolation
calculated after le Chatelier (1 bar)
lower flammability limit
calculated after le Chatelier (1 bar)
75
80
70
60
50
40
30
20
12
6
0
0
100
200
300
400
500
▶ temperature t °C
▲ flammability limits of Groningen natural gas in air %(mol)


synthetic Ekofisk natural gas
absolute pressure bar
75
60
50
40
30
25
20
15
10
8
6
5
4
2
1
auto ignition temperature
upper flammability limit
extrapolation
calculated after le Chatelier (1 bar)
lower flammability limit
1
75
calculated after le Chatelier (1 bar)
80
70
60
50
40
30
20
6
0
0
100
200
300
400
500
▲ flammability limits of synthetic Ekofisk natural gas in air %(mol)
▶ temperature t °C

Section 4

General information

4.1 Multilingual glossary of common gas industry terms

4.2 Commonly used abbreviations

4.3 Temperature conversion

4.4 Commonly used dimensionless numbers

4.1 Multilingual glossary of common gas industry terms

4.1.1	Gross heating value; Gross calorific value; Gross heat of combustion	Oberer Heizwert; Brennwert Pouvoir calorifique supérieure Calorische bovenwaarde; Verbrandingswaarde
	Net heating value; Net calorific value; Net heat of combustion	Heizwert Pouvoir calorifique inférieure; Chaleur de combustion Calorische onderwaarde; Stookwaarde
4.1.2	Density	Dichte Masse spécifique; Masse volumique Volumieke massa; Dichtheid
4.1.3	Relative density; Specific gravity	Relative Dichte Densité Dichtheid t.o.v. lucht
4.1.4	Explosive limits; Flammability limits	Zündgrenzen Limites d'inflammabilité Explosiegrenzen
4.1.5	Autoignition temperature	Selbstzündungstemperatur Température d'inflammation spontanée; Température d'auto-inflammation Zelfontbrandingstemperatuur
4.1.6	Dew-point	Taupunkt Point de rosée Dauwpunt
4.1.7	Heat capacity; Specific heat	Spezifische Wärme Chaleur spécifique Soortelijke warmte

4.1.8	Viscosity	Zähigkeit Viscosité Viscositeit
4.1.9	Boiling point	Siedepunkt Point d'ébullition Kookpunt
4.1.10	Air requirement	Luftbedarf Air comburant Luchtbehoefte
4.1.11	Sweet gas	Süssgas Gaz naturel non corrosif Zwavelvrij gas
4.1.12	Sour gas	Saures Gas Gaz naturel corrosif Zwavelrijk gas
4.1.13	Heat transfer: Conduction	Wärmeleitung Conductibilité thermique Geleiding
	Convection	Wärmekonvektion Convection de chaleur Convectie
	Radiation	Wärmestrahlung Radiation de chaleur Straling
4.1.14	Standing losses; Holding losses	Betriebsbereitschaftverluste Mise en veilleuse Stilstandsverliezen

4.2 Commonly used abbreviations

ACI	Algemene Vereniging Centrale Verwarmingsindustrie
ACQ	Annual Contract Quantity
AEGPL	Association Européenne des Gaz de Petrole Liquéfiés
AER	Algemene Energie Raad
AG	Aktiengesellschaft
AGA	American Gas Association
AIChE	American Institute of Chemical Engineers
ANG	Associated Natural Gas
ANSI	American National Standards Institute
API	American Petroleum Institute
ASA	American Standards Association
ASME	American Society for Mechanical Engineers
ASTM	American Society for Testing and Materials
BAGS	Beleids-Advies Groep Stadsverwarming
BCGW	Beleids-Commissie Gas en Water NNI
BEB	Gewerkschaften Brigitta und Elwerath Betriebsführungs GmbH
BGC	British Gas Corporation
BIPM	Bureau International des Poids et Mesures
BNOC	British National Oil Corporation
BSI	British Standards Institute
Btu	British thermal unit
BTW	Belasting Toegevoegde Waarde
CBS	Centraal Bureau voor de Statistiek
CECA	Commission Européenne de Charbon et Acier
CEDIGAZ	Centre International d'Information sur le Gaz Naturel et tous Hydrocarbures Gazeux
CEE	Communauté Economique Européenne
CEN	Comité Européenne de Normalisation
CERN	Commission Européenne des Recherches Nucléaires
CET	Central European Time
CFP	Compagnie Française des Petroles
CGPM	Conférence Générale des Poids et Mesures
CNG	Compressed Natural Gas
CODATA	Committee on Data for Science and Technology
CPB	Centraal Planbureau
CTI	Centraal Technisch Instituut (TNO)
DCQ	Daily Contract Quantity
DETG	Deutsche Erdgas Transport GmbH
DFTG	Deutsche Flüssigerdgas Terminal Gesellschaft
DIN	Deutsches Institut für Normung e.V.

DOE	Department of Energy
DSM	Dutch State Mines (Staatsmijnen DSM)
DTZ	Distrigaz
DVGW	Deutscher Verein des Gas- und Wasserfaches
DVM	Deutscher Verband für Materialprüfung
ECCC	European Communities Chemistry Committee
ECE	Economic Commission for Europe
ECN	Energieonderzoekcentrum Nederland
ECSC	European Coal and Steel Community
EEC	European Economic Community
EEG	Europese Economische Gemeenschap
EFB	European Federation of Biotechnology
EFC	European Federation of Corrosion
EFChE	European Federation of Chemical Engineering
EFTA	European Free Trade Association
EG	Europese Gemeenschap
EGKS	Europese Gemeenschap voor Kolen en Staal
ENI	Ente Nazionale Idrocarburi
ERDA	Energy Research and Development Administration
ERR	Economically Recoverable Reserves
ESC	Energie Studie Centrum
EUCHEM	European Commission for Chemistry
EWE	Energieversorgung Weser-Ems AG
FEA	Federal Energy Administration
FECS	Federation of European Chemical Societies
FERC	Federal Energy Regulatory Commission
FIGO	Fabrikanten en Importeurs van en Groothandelaars in gas- en oliebranders
FOM	Stichting Fundamenteel Onderzoek van de Materie
FPC	Federal Power Commission
FRIF	Fondation de Recherches Internationales sur les Flammes
GAVO	Gasinstallatievoorschriften
GDF	Gaz de France
GERG	Groupe Européen des Recherches Gazières
GIVEG	Gasinstituut van de Vereniging van Exploitanten van Gasbedrijven
GNL	Gaz Naturel Liquéfié
GPL	Gaz Propane Liquide
GRI	Gas Research Institute
GU	N.V. Nederlandse Gasunie
HLO	Hoger Laboratorium Onderwijs
HTO	Hoger Technisch Onderwijs
IBMG	Internationaal Bureau voor Maten en Gewichten

ICONA	Interdepartementale Coördinatiecommissie voor Noordzee Aangelegenheden
IFRF	International Flame Research Institute
IGT	Institute of Gas Technology
IGU	International Gas Union
INFAC	Informatiecentrum Airconditioning
IOI	Internationaal Octrooi Instituut
IP	Institute of Petroleum
ISO	International Organization for Standardization
IUPAC	International Union of Pure and Applied Chemistry
KDI	Stichting Kwaliteitsdienst
KEMA	Keuringsinstituut Elektrische Materialen
KIVI	Koninklijk Instituut van Ingenieurs
KOVI	Keuringsinstituut voor Onderdelen voor de Verwarmings- en luchtbehandelings-Industrie
KSLA	Koninklijke Shell Laboratorium Amsterdam
KVGN	Koninklijke Vereniging van Gasfabrikanten in Nederland
LCF	Liquid Chemical Fuel
LGN	Liquide de Gaz Naturel
LNG	Liquefied Natural Gas
LPG	Liquefied Petroleum Gas
LSEO	Landelijke Stuurgroep Energie Onderzoek
LTD	Limited Liability Company
MAC	Maximum Allowable Concentration
MAK	Maximale Arbeitsplatz-Konzentration
MARCO-GAZ	Union des Industries Gazières des Pays du Marché Commune
MBO	Middelbaar Beroepsonderwijs
MCN	Methanol Chemie Nederland
METG	Mittelrheinische Erdgas Transport Gesellschaft
MIC	Maximum Immission Concentration
MIK	Maximale Immissions-Konzentration
MWS	Mehrwertsteuer
NACA	National Advisory Committee for Aeronautics
NAM	Nederlandse Aardolie Maatschappij
NBS	National Bureau of Standards
NCB	National Coal Board
NEL	National Engineering Laboratory
NEN	Nederlandse Norm
NEOM	Nederlandse Energie Ontwikkelings Maatschappij
NETG	Nordrheinische Erdgas Transport Gesellschaft
NGL	Natural Gas Liquids
NGPA	Natural Gas Processors Association

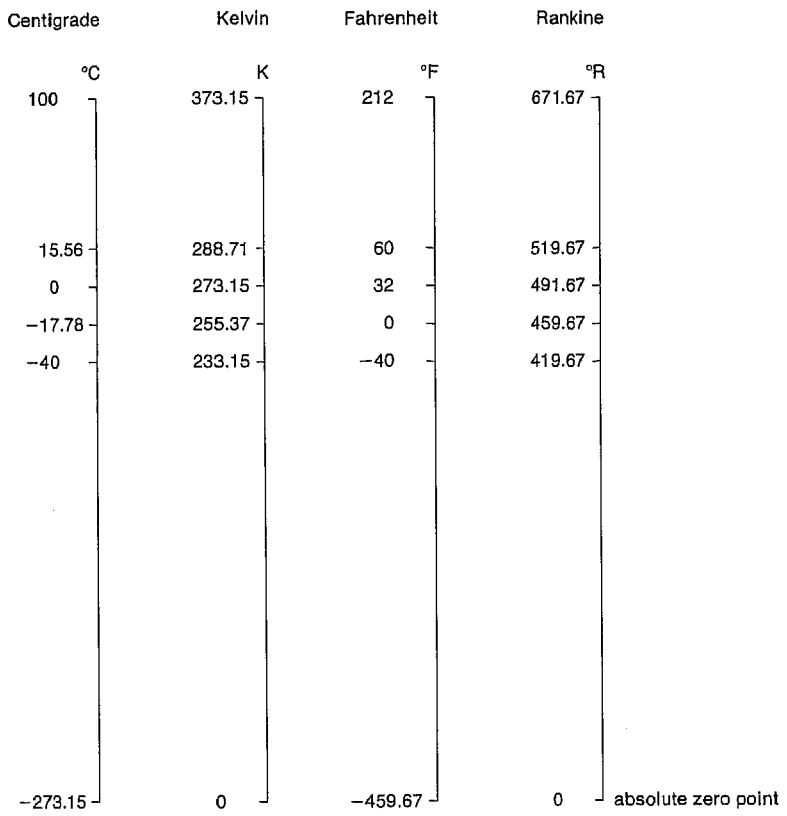
NGPSA	Natural Gas Processors Suppliers Association
NIL	Nederlands Instituut voor Lastechniek
NNI	Nederlands Normalisatie Instituut
NPT	Normal Pressure and Temperature
OAPEC	Organization of Arabic Petroleum Exporting Countries
OE	Olie Equivalent
OECD	Organization for Economic Co-operation and Development
OPEC	Organization of Petroleum Exporting Countries
PTB	Physikalisch Technische Bundesanstalt
RCN	Reactorcentrum Nederland
RG	Ruhrgas AG
RWE	Rheinisch-Westfälisches Elektrizitätswerk AG
SA	Société Anonyme
SEGEO	Société Européenne de Gaz Est-Ouest
SEP	Samenwerkende Elektriciteits Produktiebedrijven
SETG	Süddeutsche Erdgas Transport Gesellschaft
SI	International System of Units
SI	Système International d'Unités
SIPM	Shell Internationale Petroleum Maatschappij
SKE	Steenkool Equivalent
SNAM	Societa Nazionale Azienda Metanodotti SPA
SNEA	Société Nationale Elf d'Aquitane
SNG	Substitute Natural Gas
SRG	Sommers Ruhrgas Methode
STUNET	Stuurgroep Studie Noordzee-eiland en Terminal
TAG	Trans Austrian Gas Pipeline
TCTD	Technische Commissie voor Toestellen onder Druk
TENP	Trans Europa Naturgas Pipeline
TNO	Stichting Toegepast Natuurwetenschappelijk Onderzoek
TÜV	Technischer Überwachungsverein
TVA	Tax Valeur Ajoutée
UCN	Ultra-Centrifuge Nederland
ULCC	Ultra-Large Crude Carriers
UT	Universal Time (Greenwich Mean Time)
VAT	Value-Added Tax
VDI	Verein Deutscher Ingenieure
VEGIN	Vereniging van Exploitanten van Gasbedrijven in Nederland
VEW	Vereinigte Elektrizitätswerke Westfalen AG
VISA	Veiligheid Industriële Stookinstallaties Aardgas
VLCC	Very Large Crude Carriers
VWO	Voorbereidend Wetenschappelijk Onderwijs
WO	Wetenschappelijk Onderwijs

4.3 Temperature conversion

°C degrees Celsius
K kelvin (thermodynamic temperature)
°F degrees Fahrenheit
°R degrees Rankine

$$t\,°C = (273.15 + t)\,K = (1.8 \cdot t + 32)\,°F = 1.8\,(273.15 + t)\,°R$$

$$t\,°F = (459.67 + t)\,°R = \left(\frac{t-32}{1.8}\right)°C = \left(\frac{459.67+t}{1.8}\right)K$$



4.4 Table 4.4 Commonly used dimensionless numbers

Constant	Abbreviation	Formula	Application
Archimedes	*Ar*	$\frac{g \cdot l \cdot \Delta\varrho}{w^2 \cdot \varrho}$	thermosyphoning/ stack effect
Damköhler	*Da* I	$\frac{U \cdot l}{w \cdot c}$	heat and material transfer in chemical reactions
	Da II	$\frac{U \cdot l^2}{w \cdot c}$	
	Da III	$\frac{H \cdot U \cdot l}{c_p \cdot w \cdot T \cdot \varrho}$	
	Da IV	$\frac{H \cdot U \cdot l^2}{\lambda \cdot T}$	
Fourier	*Fo*	$\frac{\lambda \cdot t}{\varrho \cdot c_p \cdot l^2}$	heat transfer
Froude	*Fr*	$\frac{w^2}{g \cdot l}$	buoyancy, pneumatic transfer
Grashof	*Gr*	$\frac{l^3 \cdot g \cdot \Delta T}{\nu^2 \cdot T}$	natural convection
Lewis	$Le = Sc/Pr$	$\frac{\lambda}{\varrho \cdot c_p \cdot D}$	coupling of heat and material transfer
Mach	*M*	$\frac{w}{v_k}$	compressible flow
Nusselt	*Nu*	$\frac{h \cdot l}{\lambda}$	forced convection
Peclet	$Pe = Re \cdot Pr$	$\frac{w \cdot l \cdot \varrho \cdot c_p}{\lambda}$	forced convection, flame stabilisation
Prandtl	*Pr*	$\frac{c_p \cdot \varrho \cdot \nu}{\lambda}$	natural and forced convection
Reynolds	*Re*	$\frac{w \cdot d}{\nu}$	frictional resistance
Schmidt	*Sc*	$\frac{\nu}{D}$	material transfer
Sherwood	*Sh*	$\frac{k \cdot l}{D}$	material transfer
Stanton	$St = \frac{Nu}{Re \cdot Pr}$	$\frac{h}{c_p \cdot \varrho \cdot w}$	forced convection
Thring		$\frac{\varrho \cdot c_p \cdot w}{\varepsilon \cdot \sigma \cdot T^3}$	heat transfer by radiation
Weber	*We*	$\frac{w^2 \cdot \varrho \cdot l}{\gamma}$	liquid atomisation

Symbols used in table 4.4 (lit. 7)

v_k	=	velocity of sound	m/s
c_p	=	isobaric heat capacity	J/(kg · K)
g	=	acceleration due to gravity	m/s^2
l	=	length	m
t	=	time	s
σ	=	Stefan-Boltzmann constant	$W/(m^2 \cdot K^4)$
w	=	flow velocity	m/s
γ	=	surface tension	N/m
c	=	molar concentration	mol/m^3
D	=	molar diffusion coefficient	m^2/s
H	=	enthalpy	J/mol
T	=	temperature	K
ϱ	=	density	kg/m^3
U	=	molar reaction rate	$mol/(m^3 \cdot s)$
h	=	heat transfer coefficient	$W/(m^2 \cdot K)$
k	=	material transfer coefficient	m/s
ε	=	emissivity	–
λ	=	thermal conductivity	W/(m · K)
ν	=	kinematic viscosity	m^2/s
ΔT	=	temperature difference	K
d	=	diameter	m

Section 15

Index

A

abbreviations – commonly used –, 4.2
acceleration – – due to standard gravity, 1.1.6
acentric – – factor, 1.9, 2.2.1.5, 2.2.2.1, Table 2.2.5
adiabatic – – efficiency, 2.8.7
– – expansion, 2.8.4, 2.8.5
air – composition of dry –, Table 3.3.1
– composition of wet –, Table 3.3.2
– – deficiency, 1.4.8
– excess –, 1.4.8
– – factor, 1.4.8, 3.8
– flammability limits in –, 1.9
– – free mixtures, 3.15.3
– – requirement for combustion, 1.9, Table 3.2.1, Table 3.2.2, 3.3, 3.8, 4.1.10
– theoretical – requirement, 1.4.7, 4.1.10
alcohols – hydrocarbon classification of –, 1.5.6
alkyl – – group, 1.5.5, 1.5.6
amount – – of substance, 1.3.6
ampere – SI base unit for electric current –, 1.2.4
annual – – efficiency, 1.4.18
API – – compressibility calculation method, 2.2.2.1
area – SI units and prefixes for –, 1.3.3
argon – atomic mass of –, 1.1.7
aromatics – hydrocarbon classification of –, 1.5.4
associated – – units, 1.3.13
atomic – – mass, 1.1.7
autoignition – – temperature, 1.4.21, 1.9, 3.15.1, 4.1.5
average – – isobaric heat capacity, 3.6
– – overall efficiency, 1.4.18
– weighted –, 2.1.1

B

base – SI – units, 1.2
bends – friction factor for –, 2.10
– pressure loss in –, 2.10
Blasius – – friction factor, 2.10
body – gas – shape, 3.14
boiling – – point of gases, Table 1.7, 1.10, 4.1.9

burning – laminar – velocity, 1.4.11, 3.15.1
burnout – – flame length, 3.5.2
BWR – – compressibility calculation method, 2.2.1.2

C calorie – international –, 1.1.1
– thermochemical –, 1.1.1
calorific – – value, 1.4.2, 1.6, Table 1.9, 3.1, 4.1.1
– high – natural gas, 3.15.3
candela – SI base unit for luminous intensity –, 1.2.7
capacity – average isobaric heat – for flue gases, 3.6, 4.1.7
– isobaric heat –, 2.6.1, 3.11, 4.1.7
– isochoric heat –, 2.6.2, 4.1.7
carbon – atomic mass of –, 1.1.7
carbon dioxide – effect – on water content of natural gases, 2.11
Carr – dynamic viscosity by –, 2.5.1.2
change – isobaric enthalpy –, 2.8.6.2
– isothermal enthalpy –, 2.8.6.1
– isentropic exponent for temperature/pressure –, 2.7.2.2
– isentropic exponent for volume/pressure –, 2.7.2.1
Chapman – dynamic viscosity by –, 2.5.1.3, 3.10.1.2
le Chatelier – flammability limits by –, 1.4.12, 3.15.3
classification – – of hydrocarbons, 1.5
chemically – water vapour formed –, 3.2, 3.8
coefficient(s) – heat transfer –, 3.14
– – for BWR equation, Table 2.2.2
– virial – for DIN equation, 2.2.2.2
Colebrook – – transition zone, 2.10
cold – – flame, 3.15.1
collision – Lennard Jones – diameter and integral, 2.5.1.3
combustion – Delbourg's – potential, 1.4.9
– – efficiency, 1.4.18, 3.7
– incomplete –, 3.5
– natural gas –, 3.2
– – process, 3.5.2

– – products, 3.4
– quantity of – products, 3.4
– – space shape, 3.15.2
– stoichiometric –, Table 3.2.1, Table 3.2.2, Table 3.2.3

components – non polar –, 3.12
– properties of 52 –, Table 1.7

composition – – of dry air, Table 3.3.1
– – of flue gases, 3.4, Table 3.4.1, Table 3.4.2, Table 3.4.3, Table 3.4.4
– – of liquid natural gas, 1.10.1
– – of wet air, Table 3.3.2

compressibility – – by API method, 2.2.2.1
– – by BWR method, 2.2.1.2
– – by DIN method, 2.2.2.2
– – by Edmister, 2.2.1.5
– – by GERG method, 2.2.1.4
– – by ISO method, 2.2.1.3
– – by NX19 method, 2.2.1.1
– – factor, Table 1.9, 2.2
– – for gas mixtures, 2.2.1
– – for high calorific value gases by extended NX19 method, 2.2.1.1
– – for pure gases, 2.2.2, Table 2.2.5
– super – factor by NX19, 2.2

compression – isentropic –, 2.8.7
– – ratio, 2.8.7
– temperature rise due to –, 2.8.7

concentration – – of water vapour in air, 3.3

condensation – heat of –, 3.7
– retrograde –, 1.4.16

condition – normal –, 2.4
– operating –, 2.4

conduction – heat transfer by –, 4.1.13

conductivity – thermal – for flue gases, 3.12
– thermal – for gases, 2.3

constant(s) – equilibrium –, 3.5.1
– fundamental –, 1.1
– gas –, 1.1.5, 1.4.19

		– gas shape –, Table 3.14
		– Sutherland –, Table 3.10.2
		– Universal gas –, 1.1.5, 1.4.19
	content	– heat – of flue gases, 3.13
		– water vapour – of air, 3.3
		– water vapour – of flue gases, 3.8
		– water vapour – of natural gas, 2.11
	convection	– heat transfer by –, 3.14, 4.1.13
		– – losses, 1.4.18
	conversion	– – % (mol) to % (mass) vv, 1.8.2
		– – % (mol) to % (vol.) vv, 1.8.1
		– – tables, 1.6
		– temperature –, 4.3
	critical	– – pressure, Table 1.7
		– pseudo – pressure, 1.9, 2.1
		– pseudo – temperature, 1.9, 2.1
		– – Reynolds number, 2.10
		– – temperature, 1.4.15, Table 1.7
		– – volume, Table 1.7
	current	– electric –, 1.3.12
D	Darcy	– – friction factor, 2.10
	deficiency	– oxygen –, 3.5.1
	definition	– – of air deficiency, 1.4.8
		– – of air factor, 1.4.8
		– – of annual efficiency, 1.4.18
		– – of average overall efficiency, 1.4.18
		– – of autoignition temperature, 1.4.21
		– – of calorific value, 1.4.2
		– – of le Chateliers rule, 1.4.12
		– – of convection losses, 1.4.18
		– – of critical flow, 1.4.20
		– – of critical temperature, 1.4.15
		– – of cubic metre, 1.1.8
		– – of deflagration, 1.4.13
		– – of Delbourg's combustion potential, 1.4.9
		– – of detonation, 1.4.14
		– – of direct efficiency, 1.4.18
		– – of excess air, 1.4.8
		– – of flammability limits, 1.4.12
		– – of flue efficiency, 1.4.18

– – of flue losses, 1.4.18
– – of gas constant, 1.4.19
– – of gas hydrates, 1.4.17
– – of gas modulus, 1.4.5
– – of heating efficiency, 1.4.18
– – of indirect efficiency, 1.4.18
– – of laminar burning velocity, 1.4.11
– – of litre, 1.4.22
– – of natural gas, 1.4.1
– – of radiation losses, 1.4.18
– – of relative density, 1.4.3
– – of retrograde condensation, 1.4.16
– – of sooting number, 1.4.10
– – of SRG method, 1.4.6
– – of standing losses, 1.4.18
– – of stoichiometric air requirement, 1.4.7, 1.4.8
– – of theoretical air requirement, 1.4.7
– – of Universal gas constant, 1.4.19
– – of useful energy, 1.4.18
– – of Wobbe index, 1.4.4
deflagration – – of gases, 1.4.13, 3.15.1
Delbourg – – combustion potential, 1.4.9
density – – of flue gases, 3.9, 4.1.2
– – of gases, Table 1.7, 1.9, 2.4, 4.1.2
– – of liquid natural gas, 1.10.1, 4.1.2
– – of liquid nitrogen, 1.10.2, 4.1.2
– relative – of gases, Table 1.7, 4.1.3
derivatives – partial –, 2.6.2
detonation – – of gases, 1.4.14, 3.15.1
dew point – water – of gases, 2.11, 4.1.6
– water – of flue gases, 3.7, 3.8, 4.1.6
diagram – enthalpy / entropy –, 2.8.3
diameter – Lennard Jones collision –, 2.5.1.3
difference – isobaric heat capacity –, 2.6.1
dimensionless – – numbers, Table 4.4
DIN – compressibility by – method, 2.2.2.2
dissociation – – of gases, 3.13
dry – – air composition, Table 3.3.1
– – air requirement, 3.3

dynamic – – viscosity of flue gases, 3.10.1, Table 3.10.1, 4.1.8
– – viscosity of gases, 1.6.9, 2.5.1, 4.1.8

E

Edmister – compressibility calculation method by –, 2.2.1.5

effect – – of hydrogen sulphide and carbon dioxide on water content of natural gases, 2.11
– Pointing – on water content of natural gases, 2.11
– pressure/temperature – on flammability limits, 3.15.4
– solubility – on water content of natural gases, 2.11

efficiency – adiabatic –, 2.8.7
– annual –, 1.4.18
– average overall –, 1.4.18
– direct –, 1.4.18
– flue –, 1.4.18
– heating –, 1.4.18
– indirect –, 1.4.18, 3.7
– – ratio, 3.7

electric – – current, 1.3.12
– – resistance, 1.3.12
– – voltage, 1.3.12

EMR – – critical temperature and pressure calculation method, 2.1.2
– – values, Table 2.1.4

energy – SI – units and prefixes for –, 1.3.9

enthalpy – – of gases, 2.8.1

entropy – – of gases, 2.8.1

equation – chemical reaction –, 3.2

equilibrium – – constants for incomplete combustion equations, 3.5.1

excess – – air, 1.4.8

exothermic – – reaction, 3.15.1

expansion – isenthalpic –, 2.8.5
– isentropic –, 2.8.4

explosive – – limits, 4.1.4

F

factor
- acentric –, 1.9, 2.2.1.5, 2.2.2.1
- air –, 1.4.8
- equilibrium – for combustion processes, 3.5.2
- summation – for ISO compressibility, 2.2.1.3

Fanning
- – friction factor, 2.10

flame
- – speed, 1.4.11
- – temperature, 3.13

flammability
- calculation of – limits in air, 3.15.3
- – limits in air, 1.9, Table 3.15.1, 3.15
- – limits in oxygen, Table 3.15.1
- – limits of Ekofisk natural gas in air, Fig. 3.15.5
- – limits of Groningen natural gas in air, Fig. 3.15.4

flow
- critical –, 1.4.20
- heat – conversion table, 1.6.5

flue
- average isobaric heat capacity of – gases, 3.6
- density of – gases, 3.9, 4.1.2
- dynamic viscosity of – gases by Chapman, 3.10.1.2
- dynamic viscosity of – gases by Herning and Zipperer, 3.10.1.3
- dynamic viscosity of – gases by Sutherland, 3.10.1.1
- dynamic viscosity of – gases, 3.10.1, Table 3.10.1
- – efficiency, 1.4.18, 3.7
- heat transfer of – gases, 3.14
- isobaric heat capacity of – gases, 3.11
- kinematic viscosity of – gases by
- Mann, 3.10.2
- – losses, 1.4.18, 3.7
- sensible heat of – gases, 3.6
- thermal conductivity of – gases, 3.12
- viscosity of – gases, 3.10
- water content of – gases, 3.8
- water dew point of – gases, 3.7, 3.8

force
- conversion tables for –, 1.6.2
- SI units and prefixes for –, 1.3.7

formation
- heat of –, 3.1
- homogeneous methane – reaction, 3.5.1

freezing
- – point of water, 1.1.4

friction
- – factor for pipes and bends, 2.10

fundamental
- – constants, 1.1

G gas(es)
- acentric factor of –, 2.2.1.1, 2.2.1.5, Table 2.2.5
- air requirement of –, 1.4.7, 1.9, 3.3
- autoignition temperature of –, 1.4.21, 1.9, 3.15, Table 3.15.1
- average isobaric heat capacity of flue –, 3.6
- boiling point of –, Table 1.7
- calorific values of –, 1.4.2, 1.9, 3.1, Table 3.1.1
- combustion of –, 3.2, 3.5
- composition of flue –, 3.4
- compressibility of –, 2.2, Table 2.2.5
- – constant, 1.1.5, 1.4.19
- critical flow of –, 1.4.20
- critical pressure of –, Table 1.7, 1.9, 2.1
- critical temperature of –, 1.4.15, Table 1.7, 1.9, 2.1
- critical volume of –, Table 1.7
- definition of –, 1.4
- Delbourg's combustion potential of –, 1.4.9
- density of flue –, 3.9, 4.1.2
- density of –, Table 1.7, 1.9, 2.4, 4.1.2
- dew point of flue –, 3.7, 3.8
- dew point of –, 2.11
- EMR values of –, Table 2.1.4
- enthalpy of –, 2.8.1
- entropy of –, 2.8.2
- expansion of –, 2.8.4, 2.8.5
- flame speed of –, 1.4.11
- flame temperature of –, 3.13
- flammability limits in air of –, 1.4.12, 1.9, 3.15, Table 3.15.1
- flammability limits in oxygen of –, Table 3.15.1

- Groningen natural –, 1.9
- heat capacity of flue –, 3.6, 3.11
- heat capacity of –, 2.6
- heat transfer of flue –, 3.14
- H-S diagram of –, 2.8.3
- – hydrates, 1.4.17
- ideal molar volume of –, 1.1.3
- incomplete combustion of –, 3.5
- inert –, 3.5.1
- isenthalpic expansion of –, 2.8.5
- isentropic compression of –, 2.8.7
- isentropic expansion of –, 2.8.4
- isentropic exponents of –, 2.7
- isobaric heat capacity of flue –, 3.6, 3.11
- isobaric heat capacity of –, 2.6
- isochoric heat capacity of –, 2.6
- laminar burning velocity of –, 1.4.11
- – modulus, 1.4.5
- molar mass of –, Table 1.7, 1.9
- molar volume of –, 1.1.3, Table 1.7, 1.9
- natural –, 1.4.1, 1.9, 3.15
- normal molar volume of –, 1.1.3
- pressure loss in pipes and bends for –, 2.10
- production of inert –, 3.5.1
- production of shield –, 3.5.1
- properties of –, Table 1.7
- properties of Groningen natural –, 1.9
- real density of –, Table 1.7, 1.9, 2.4
- real molar volume of –, Table 1.7
- reduced pressure of –, 2.2.1.5
- reduced temperature of –, 2.2.1.5
- refractive index of –, Table 2.1.4
- relative density of –, 1.4.3, Table 1.7, 1.9, 4.13
- retrograde condensation of –, 1.4.16
- Reynolds number of –, 2.9
- sensible heat of flue –, 3.6
- shield –, 3.5.1
- sooting number of –, 1.4.10

– sound velocity of –, 2.7.3
– sour –, 4.1.12
– supercompressibility of –, 2.2
– sweet –, 4.1.11
– theoretical flame temperature of –, 3.13
– thermal conductivity of flue –, 3.12
– thermal conductivity of –, 2.3
– true isobaric heat capacity of flue –, 3.11
– Universal gas constant of –, 1.1.5
– velocity of sound of –, 2.7.3
– virial coefficient of –, 2.2.2.2
– viscosity of flue –, 3.10
– viscosity of –, 1.3.11, 2.5
– water content of flue –, 3.3, 3.8
– water content of –, 2.11
– water dew point of flue –, 3.7, 3.8
– water dew point of –, 2.11
– water vapour content of flue –, 3.3, 3.8
– water vapour content of –, 2.11
– Wobbe index of –, 1.4.4, 1.9

GERG – – compressibility calculation method, 2.2.1.4

glossary – multilingual –, 4.1
gravity – standard acceleration due to –, 1.1.6
gross – – calorific value, 1.6.6, 1.9, 3.1, 4.1.1
Gupta – – friction factor for bends, 2.10.2

H

Hagen – – friction factor, 2.10
heat – – capacity, 2.6, 3.6, 3.11, 4.1.7
– – content, 3.13
– – flow, 1.6.5
– isobaric – capacity of flue gases, 3.6, 3.11, 4.1.7
– isobaric – capacity of gases, 2.6.1, 4.1.7
– isochoric – capacity of gases, 2.6.2, 4.1.7
– latent – of vaporization, 1.10, 3.7
– – of condensation, 3.7
– – of formation, 3.1

	–	quantity of –, 1.6.4
	–	sensible –, 3.6
	–	– transfer, 1.6.8, 4.1.13
	–	– transfer coefficient, 3.14
heating	–	– efficiency, 1.4.18, 3.7
helium	–	atomic mass of –, 1.1.7
Hermann von	–	– friction factor, 2.10
Herning	–	– dynamic viscosity, 2.5.1.1, 3.10.1.3
Hoffmann	–	– friction factor, 2.10
holding	–	– losses, 4.1.14, 1.4.18
homogeneous	–	– methane formation reaction, 3.5.1
	–	– water gas reaction, 3.5.1
H-S	–	– diagram, 2.8.3
humidity	–	relative – of air, 3.3
hydrates	–	gas –, 1.4.17
hydrocarbons	–	classification of –, 1.5
hydrogen	–	atomic mass of –, 1.1.7
hydrogen sulphide	–	effect of – on watercontent, 2.11
I		
ideal	–	– gas law, 2.2
	–	– molar volume, 1.1.3
ignition	–	auto – temperature, 1.4.21
	–	– energy, 3.15.2
	–	spontaneous –, 3.15.1
incomplete	–	– combustion, 3.5
indirect	–	– efficiency, 1.4.18, 3.7
inert	–	– gas production, 3.5.1
integral	–	collision –, 2.5.1.3
international	–	– calorie, 1.1.1
isenthalpic	–	– expansion, 2.8.5
isentropic	–	– compression, 2.8.7
	–	– expansion, 2.8.4
	–	– exponent, 2.7
ISO	–	– compressibility calculation method, 2.2.1.3
isobaric	–	– enthalpy change, 2.8.6.2
	–	– heat capacity, 2.6.1, 3.6, 3.11, 4.1.7
isothermal	–	– enthalpy change, 2.8.6.1

J	Jones	–	Lennard – collision diameter, 2.5.1.3
		–	Lennard – potential parameter, 2.5.1.3
	Joule	–	– conversion, 1.1.1, 1.6
		–	– Thomson effect, 2.8.5
K	Kay	–	rule of –, 2.1.1
	Kelvin	–	absolute temperature in –, 1.1.4
		–	SI base unit for temperature –, 1.2.5
	kinematic	–	– viscosity of flue gases, 3.10.2, 4.1.8
		–	– viscosity of gases, 2.5.1.3, 4.1.8
L	laminar	–	– burning velocity, 1.4.11
		–	– flow, 2.9
	latent	–	– heat of vaporization, 3.7
	layer	–	radiating thickness –, 3.14
	le Chatelier	–	formula of –, 3.15.3
		–	rule of –, 1.4.12
	length	–	burn out –, 3.5.2
		–	SI units and prefixes for –, 1.3.3
	Lennard	–	– Jones collision diameter, 2.5.1.3
		–	– Jones potential parameter, 2.5.1.3
	light	–	speed of – in vacuum, 1.1.2
	limits	–	flammability –, 1.4.12, 3.15, 4.1.4
	liquid	–	– Groningen natural gas, 1.10.1
		–	– nitrogen, 1.10.2
	litre	–	definition of –, 1.4.22
	loss(es)	–	holding –, 1.4.18, 4.1.14
		–	pressure – in pipes and bends, 2.10
		–	standing –, 1.4.18, 4.1.14
	lower	–	– flammability limits, Table 1.9, 3.15
M	Mann	–	– kinematic viscosity, 3.10.2
	mass	–	atomic –, 1.1.7
		–	molar –, Table 1.7, 1.9
		–	SI units and prefixes for –, 1.3.5
		–	– /volume conversion, 1.8.2
	matter	–	SI base unit for quantity of –, 1.2.6
	measures	–	Imperial weights and –, 1.6.1
	mercaptans	–	hydrocarbon classification of –, 1.5.5
	methane	–	– formation reaction, 3.5.1
	methanol	–	– calorific value from heat of formation, 3.1
	method	–	SRG interchangeability –, 1.4.6

	metre	–	definition of cubic –, 1.1.8
		–	SI base unit for length –, 1.2.1
	Mishra	–	– friction factor for bends, 2.10
	mixing	–	– rules for BWR formule, 2.2.1.2
	modulus	–	gas –, 1.4.5
	molar	–	ideal-volume, 1.1.3
		–	– mass, Table 1.7
		–	real – volume, Table 1.7, 1.9
	mole	–	SI base unit for quantity of matter –, 1.2.6
	multilingual	–	– glossary, 4.1
	multiples	–	– of SI units, 1.3.1
N	naphtenes	–	hydrocarbon classification of –, 1.5.3
	natural	–	combustion of – gas, 3.2
		–	definition of – gas, 1.4.2
		–	explosion limits of – gas, 3.15.3
		–	water content of – gas, 2.11
		–	water vapour content of – gas, 2.11
	net	–	– calorific value, 1.9, 3.1, 4.1.1
		–	definition of – calorific value, 1.6.6
	nitrogen	–	atomic mass of –, 1.1.7
		–	liquid –, 1.10.2
	normal	–	– condition, 2.4
		–	molar volume, 1.1.3
	non-ideal	–	isentropic exponents for – gases, 2.7.2
	non-polar	–	– components, 3.12
	NO_x	–	– in flue gases, 3.4
	number(s)	–	dimensionless –, 4.4
		–	Reynolds –, 2.9
		–	sooting –, 1.4.10
	NX19	–	– compressibility calculation method, 2.2.1.1
O	obsolete	–	– units, 1.3.14
	olefins	–	hydrocarbon classification of –, 1.5.2
	operating	–	– conditions, 2.4
	Ostwald	–	– triangle, 3.5.2
	oxygen	–	atomic mass of –, 1.1.7
		–	– deficiency, 3.5.1
		–	– requirement for combustion, 3.2

P

paraffins – hydrocarbon classification of –, 1.5.1
parameter – Lennard-Jones potential –, 2.5.1.3
partial – – derivatives, 2.6
– – water vapour pressure, 3.8
point – boiling – gases, Table 1.7
– boiling – of liquid natural gas, 1.10.1
– boiling – of liquid nitrogen, 1.10.2
– freezing – of water, 1.1.4
Pointing – – effect on water vapour content of gases, 2.11
Poiseuille – – laminar friction factor, 2.10
polar – – components, 3.12
potential – Delbourg's combustion –, 1.4.9
– Lennard-Jones – parameter, 2.5.1.3
power – compression –, 2.8.7
– SI units and prefixes for –, 1.3.10
Prandtl – – friction factor, 2.10
pressure – – conversion tables, 1.6.3
– critical – of gases, Table 1.7, 2.1
– – effect on flammability limits, 3.15.4
– – effect on heat capacity, 2.6.1
– – effect on viscosity, 2.5.1.3
– – loss in pipes and bends, 2.10
– pseudo critical –, 2.1
– – ratio, 2.8.7
– reduced –, 2.2.2.1
– saturation – of water vapour, 3.3, 3.7, 3.8
process – combustion – factor, 3.5.2
production – inert gas –, 3.5.1
– shield gas –, 3.5.1
products – combustion –, 3.4
properties – – of pure gases, Table 1.7
– – of liquid Groningen natural gas, 1.10.1
– – of liquid nitrogen, 1.10.2

	pure	–	compressibility of – gases, 2.2.2, Table 2.2.5
		–	heat capacity of – gases, 2.6, 3.6, 3.11
		–	thermal conductivity of – gases, 2.3, 3.12
		–	viscosity of – gases, 2.5, 3.10
Q	quantity	–	combustion products –, 3.4
		–	conversion tables for heat –, 1.6.4
R	radian	–	SI unit for a plane angle –, 1.2.8
	radiating	–	– layer thickness, 3.14
	radiation	–	– heat transfer coefficient, 3.14, 4.1.13
		–	– losses, 1.4.18
		–	selective –, 3.14
	radicals	–	free –, 3.13
	ratio	–	compression –, 2.8.7
		–	efficiency –, 3.7
		–	pressure –, 2.8.7
	reaction	–	combustion – equation, 3.2
		–	exothermic –, 3.15.1
		–	homogeneous methane formation –, 3.5.1
		–	homogeneous water gas –, 3.5.1
	real	–	– molar volume, Table 1.7, 1.9
	reciprocal	–	Mann's – formula for kinematic viscosity, 3.10.2
	reduced	–	– pressure, 2.2.1.5, 2.2.2.1
		–	– temperature, 2.2.1.5, 2.2.2.1
	reference	–	– fluid, Table 2.2.4
	refining	–	– factor on thermal conductivity, 3.12
	refractive	–	– index, Table 2.1.4
	relative	–	definition of – density, 1.4.3, 4.1.3
		–	– density, Table 1.7, 1.9, 4.1.3
		–	– humidity of air, 3.3
		–	– surface roughness, 2.10
	requirement	–	air – for combustion, 1.9, 3.3, 3.8, 4.1.10
		–	definition of air –, 1.4.7
		–	oxygen –, 3.2
	resistance	–	SI units and prefixes for electrical –, 1.3.12

	retrograde	–	definition of – condensation, 1.4.16
	Reynolds	–	critical – number, 2.10
		–	– number, 2.9, Table 4.4
	rise	–	temperature – due to compression, 2.8.7
	roughness	–	relative surface –, 2.10
	rule	–	definition of le Chateliers –, 1.4.12
		–	Kay's –, 2.1.1
S	saturation	–	– pressure of water vapour, 3.3
	second	–	SI unit for time –, 1.2.3
	sensible	–	– heat, 3.6, 3.13
	selective	–	– radiation, 3.14
	shape	–	combustion space –, 3.15.2
		–	gas body –, 3.14
	shield	–	– gas, 3.5
	shock	–	– waves, 3.15.1
	SI	–	– units and prefixes, 1.2, 1.3.1
	solubility	–	– effect on water content, 2.11
	sooting	–	– number, 1.4.10
	sound	–	– velocity, 2.7.3, 3.15.1
	sour	–	– gas, 4.1.12
	space	–	combustion – shape, 3.15.2
	speed	–	– of light, 1.1.2
	spontaneous	–	– ignition, 3.15.1
	SRG	–	– method, 1.4.6
	standard	–	– losses, 1.4.18, 4.1.14
	steradian	–	SI unit for a solid angle –, 1.2.9
	stoichiometric	–	– air requirement, 1.4.8, 3.3
		–	– combustion, 3.2
		–	– combustion products, 3.4
	sulphur	–	atomic mass of –, 1.1.7
	summation	–	ISO – factors for compressibility, 2.2.1.3
	supercompressibility	–	NX19 –, 2.2
	Sutherland	–	– dynamic viscosity of flue gases, 3.10.1.1
	sweet	–	– gas, 4.1.11

T

tables
– conversion –, 1.6
Techo
– – friction factor, 2.10
temperature
– autoignition –, 1.4.21, 1.9, 3.15.1, 4.1.5
– – conversion, 4.3
– critical –, 1.4.15, Table 1.7, 1.9, 2.1
– – effect on flammability limits, 3.15.4
– reduced –, 2.2.1.5, 2.2.2.1
– pseudo critical –, 1.9, 2.1
– – rise due to compression, 2.8.7
– SI units and prefixes for –, 1.2, 1.3.4
– wall –, 3.14
theoretical
– – air requirement, 1.4.7, Table 3.2.1, Table 3.2.2, 3.3
– – flame temperature, 3.13
thermal
– – conductivity of flue gases, 3.12
– – conductivity of gases, 1.6.7, 2.3
thermochemical
– – calorie, 1.1.1
thickness
– – of radiating layer, 3.14
time
– SI units and prefixes for –, 1.2, 1.3.2
transfer
– heat –, 1.6.8, 4.1.13
– heat – coefficient, 3.14
transition
– – zone, 2.9, 2.10
triangle
– Ostwald –, 3.5.2
turbulence
– – influence on flammability limits, 3.15.2
turbulent
– – flow, 2.9

U

units
– associated SI –, 1.3.13
– obsolete –, 1.3.14
– SI –, 1.3
Universal
– – gas constant, 1.1.5
upper
– – flammability limits, Table 1.9, 3.15.1
US
– – weights and measures, 1.6.1
useful
– – energy, 1.4.18

V

vaporization
– latent heat of –, 3.7
vapour
– partial – pressure, 3.8
– water – concentration, 3.3
– water – content, 3.3
– water – saturation pressure, 3.3
velocity
– burning – 3.15.1
– laminar burning –, 1.4.11

		–	sound –, 2.7.3, 3.15.1
	virial	–	DIN – coefficients, 2.2.2.2
	viscosity	–	– conversion tables, 1.6.9
		–	dynamic –, 2.5.1, 3.10.1, 4.1.8
		–	kinematic –, 2.5.2, 3.10.2, 4.1.8
		–	– of flue gases, 3.10, 4.1.8
		–	– of gases, 2.5, 4.1.8
		–	SI units and prefixes for –, 1.3.11
	voltage	–	electric –, 1.3.12
	volume	–	critical –, Table 1.7
		–	normal molar –, 1.1.3
		–	real molar –, Table 1.7, Table 1.9
		–	SI units and prefixes for –, 1.3.3
W	Wasielewski	–	– friction factor, 2.10
	water	–	– dew point of flue gases, 3.8
		–	– dew point of natural gases, 2.11
		–	freezing point of –, 1.1.4
		–	– gas reaction, 3.5.1
		–	partial pressure of – vapour, 3.8
		–	– vapour concentration in air, 3.3, Table 3.3.2
		–	– vapour content of air, 3.3
		–	– vapour content of flue gases, 3.8
		–	– vapour content of natural gases, 2.11
		–	– vapour formed by combustion, 3.8
		–	– vapour heat of condensation, 3.7
		–	saturation pressure of – vapour, 3.7, 3.8
	waves	–	shock –, 3.15.1
	weighted	–	– average method, 2.1.1
	weights	–	– and measures (US), 1.6.1
	Weisbach	–	– friction factor, 2.10
	wet	–	– air composition, 3.3, Table 3.3.2
		–	– air requirement, 1.9, 3.3
	White	–	– friction factor, 2.10
	Wobbe index	–	definition of –, 1.4.4, 1.9
Z	Zipperer	–	dynamic viscosity by –, 2.5.1.1, 3.10.1.3

Section 6

References

Section 6 References

Lit. 1 Thermodynamics Research Center Hydrocarbon Project (TRCHP); **Selected values of properties of hydrocarbons and related compounds.** College Station, Texas A & M University, April 1984.

Lit. 2 **Natural Gas – Calculation of calorific value, density and relative density.** International standard ISO 6976–1983 (E). Geneva, International Organization for Standardization, 1983.

Lit. 3 Perry R.H., Green D.W.; **Perry's Chemical Engineers Handbook.** New York, Mc Graw – Hill Inc., 6th edition, 1984.

Lit. 4 Weast R.C.; **CRC Handbook of Chemistry and Physics.** Boca Raton, CRC Press Inc., 63rd edition, 1982.

Lit. 5 API; **Technical Data Book – Petroleum Refining, metric edition,** vol 1 and 2. Washington, American Petroleum Institute, 1977 – 1981.

Lit. 6 Lorenz I.M.; **Numerical Values of Properties of Combustible Gases and Related Materials.**
Paper IGU/E17–73, 12th World Gas Conference, Nice, 1973. International Gas Union, London.

Lit. 7 Kremer H.; **Wichtige dimensionslose Kennzahlen der Wärmeübertragung und Verbrennung (in German).** Arbeitsblatt nr. 151 (Juli 1966). Gaswärme Institut, Essen.

Lit. 8 Campbell J.M.; **Gasconditioning and processing,** 4th edition, vol. 1 and 2. Norman, Oklahoma, Campbell Petroleum Series, 1978.

Lit. 9 McLeod W.R., Campbell J.M.; **Simple method permits prediction of natural gas critical properties.** The Oil and Gas Journal (USA), July 7, 1969, pp 115–118.

Lit. 10 Herning F., Wolowski E.; **Kompressibilitätszahlen und Realgasfaktoren von Erdgasen nach neuen Amerikanischen Berechnungsunterlagen (in German).** Essen, FRG, Gas Berichte Ruhrgas AG, A66 pp 7–14.

Lit. 11 Bishnoi P.R., Miranda R.D., Robinson D.B.; **BWR applied to NG/SNG needs.** Hydrocarbon Processing (USA), November, 1974, p 197–201.

Lit. 12 Reid A.C., Prausnitz J.M., Sherwood T.K.; **The properties of gases and liquids, their estimation and correlation.** New York, McGraw-Hill, 3rd edition, 1977.

Lit. 13 Snijder R.; **Onderzoek toepassing NX-19 (in Dutch).** Groningen, Gasunie, report TP/IO 8009, January 1978.

Lit. 14 **Gaseous fuels and other gases; density and relative density under standard condition.** DIN standard 1871, Februari, 1978, Beuth, Berlin.

Lit. 15 Katz D.L., Cornell D., Kobayashi R., Poettman F.H., Vary J.A., Elenbaas J.R., Weinaug C.F.; **Handbook of natural gas engineering.** New York, McGraw-Hill Book Company, 1959.

Lit. 16 IUPAC; **Helium: International thermodynamic tables of the fluid state** – 4. Oxford, Pergamon Press, 1977.

Lit. 17 Hilsenrath J., Beckett C.W., Benedict W.S., Fano L., Hoge H.J., Masi J.F., Nuttall R.L., Touloukian Y.S.; **Tables of thermodynamic and transport properties.** Oxford, Pergamon Press, 1960.

Lit. 18a Edmister W.C.; **Applied Hydrocarbon Thermodynamics.** Houston, Gulf Publishing Company, vol 1 – 1961, vol 2 – 1974.

Lit. 18b Edmister W.C., Lee B.I.; **Applied Hydrocarbon Thermodynamics.** Houston, Gulf Publishing Company, vol. 1, 1984.

Lit. 19 Kronig R.; **Leerboek der Natuurkunde (in Dutch).** Amsterdam, Scheltema & Holkema, 1966.

Lit. 20 Geerssen T.M.; **De soortelijke warmte en de constante van Poisson k van Gronings aardgas (in Dutch).** Groningen, Gasunie, report 353 CT/'69, 31st October, 1969.

Lit. 21 Antonelli A.; **Geluidssnelheid in gassen (in Dutch).** Proces Techniek (Neth.) 16,2,1972 pp 122–127.

Lit. 22 Thomas L.K., Hankinson R.W., Phillips K.A.; **Determination of acoustic velocities for natural gas.** J. of Petr. Techn. (USA), July 1970, pp 889–895.

Lit. 23 Andsager R.L., Knapp R.M.; **Acoustic measurement of distance in natural gas systems.** Symposium Society of Petroleum Engineers AIME. Omaha, September 15–16, 1966. Paper SPE 1640.

Lit. 24 Oranje L.; **Gastemperatuur en transportcapaciteit (in Dutch).** Groningen, Gasunie, report TP/OF 7275, 12th December 1977.

Lit. 25 Techo R., Tickner R.R., James R.E.; **An accurate equation for the computation of the friction factor for smooth pipes from the Reynolds number.** Journal of Applied Mechanics, June 1965, p. 443.

Lit. 26 Geerssen T.M.; **Het watergehalte van verzadigd aardgas als functie van druk en temperatuur (in Dutch).** Groningen, Gasunie, memo 1603 (CT/'69, 22nd May, 1969.

Lit. 27 Robinson J.N., Wiekert E., Moore R.G., Heidemann R.A.; **Charts help estimate H_2O content of sour gases.** The Oil and Gas Journal (USA), February 6, 1978, pp 77–78.

Lit. 28 Jaeschke M., Harbrink B.; **Korrektur des AGA NX-19-mod-Rechenverfahrens für Realgasfaktoren von Erdgas H (in German).** GWF-Gas/Erdgas (Germany) 123,1,(1982), pp 20–27.

Lit. 29 Withdrawn.

Lit. 30 Bonner J.A., Snijder R.; **Compressibility factors for gas measurement in Europe.** Arlington. American Gas Association Operating Section, proceedings paper T 410 – T 413, 1978.

Lit. 31 Par Research Project NX-19; **Manual for the determination of supercompressibility factors for natural gas.** New York, American Gas Association, 1962.

Lit. 32 Spiers H.M.; **Technical Data on Fuel.** London, British National Committee World Power Conference, 6th edition, 1962.

Lit. 33 Gumz W.; **Kurzes Handbuch der Brennstoff- und Feuerungstechnik (in German).** Berlin, Springer, 3rd edition, 1962.

Lit. 34 Heiligenstaedt W.; **Wärmetechnische Rechnungen für Industrieöfen (in German).** Düsseldorf, Verlag Stahleisen, 4th edition, 1966.

Lit. 35a **VDI-Wärmeatlas (in German).** Düsseldorf, VDI-Verlag, 1st edition, 1963.

Lit. 35b **VDI-Wärmeatlas (in German).** Düsseldorf, VDI-Verlag, 4th edition, 1984.

Lit. 36 **Basisgegevens over Gronings aardgas (in Dutch).** Groningen, Gasunie, July, 1968.

Lit. 37 Geerssen T.M.; **De theoretische hoeveelheid condensatiewarmte, die vrijkomt wanneer natte verbrandingsgassen worden gekoeld beneden het waterdauwpunt en de invloed hiervan op het indirecte rendement van een stookinstallatie (in Dutch).** Groningen, Gasunie, report TP/SP 83.R.515, July 1983.

Lit. 38 Brückner H.; **Gastafeln (in German).** München, Verlag von R. Oldenbourg, 2nd edition, 1952.

Lit. 39 Lehman H.; **Wärmeleitfähigkeit von Gasgemischen (in German).** Chem. Techn. (Germany) 9,9, (September 1957) pp 530–637.

Lit. 40 Schack A.; **Der industrielle Wärmeübergang für Praxis und Studium mit grundlegenden Zahlenbeispielen (in German).** Düsseldorf, Stahleisen, 6th edition, 1962.

Lit. 41 Claus J.; **Warmteoverdracht door straling in met gas gestookte vuurhaarden (in Dutch).** Verwarming en Ventilatie (Neth.), December 1964, nr. 12, pp 543–551.

Lit. 42 Maas W.; **Explosies (in Dutch).** De Veiligheid (Neth.), 46,5,1970, pp 179–185.

Lit. 43 Coward H.F., Jones G.W.; **Limits of flammability of gases and vapors,** Bulletin 503 Bureau of Mines. Washington, US Government Printing Office, 1952.

Lit. 44 Lewis B., Elbe G. von; **Combustion, flames and explosions of gases.** New York, Academic Press, 1961.

Lit. 45 Kwiatkowski K. von; **Über den Einfluss höherer Temperaturen auf die Gültigkeit der Regel von Le Chatelier zur Berechnung der Grenzen der Flammenausbreitung von Brenngas-Luftgemischen (in German).** Dissertation, Technical University, Aachen, 27 July, 1966.

Lit. 46 Zabetakis M.G.; **Flammability characteristics of combustible gases and vapors** Bulletin 627, Bureau of Mines. Washington, US Government Printing Office, 1965.

Lit. 47 Schmidt E.; **Properties of water and steam in SI-units.** Berlin, Springer, 1969.

Notes

Notes

Notes

Published by
N.V. Nederlandse Gasunie
P.O.Box 19
9700 MA Groningen
The Netherlands
Phone ++31 50 21 23 21

Working drawings: Jan van Beusekom, Boskoop
Design: Jan van Beusekom, Boskoop

June 1988

BF 885/10 D