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ISO 12213-3

Second edition
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Natural gas — Calculation of compression factor —

Part 3:
Calculation using physical properties

Gaz naturel — Calcul du facteur de compression —

Partie 3: Calcul à partir des caractéristiques physiques

Reference number
ISO 12213-3:2006(E)

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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

International Standards are drafted in accordance with the rules given in the ISO/IEC Directives, Part 2.

The main task of technical committees is to prepare International Standards. Draft International Standards adopted by the technical committees are circulated to the member bodies for voting. Publication as an International Standard requires approval by at least 75 % of the member bodies casting a vote.

Attention is drawn to the possibility that some of the elements of this document may be the subject of patent rights. ISO shall not be held responsible for identifying any or all such patent rights.

ISO 12213-3 was prepared by Technical Committee ISO/TC 193, *Natural gas*, Subcommittee SC 1, *Analysis of natural gas*.

This second edition cancels and replaces the first edition (ISO 12213-3:1997), which has been technically revised. The revision includes changes to Subclause 4.4.1 and the addition of a new annex, Annex E.

ISO 12213 consists of the following parts, under the general title *Natural gas — Calculation of compression factor*:

- *Part 1: Introduction and guidelines*
- *Part 2: Calculation using molar-composition analysis*
- *Part 3: Calculation using physical properties*

Natural gas — Calculation of compression factor —

Part 3:
Calculation using physical properties

1 Scope

ISO 12213 specifies methods for the calculation of compression factors of natural gases, natural gases containing a synthetic admixture and similar mixtures at conditions under which the mixture can exist only as a gas.

This part of ISO 12213 specifies a method for the calculation of compression factors when the superior calorific value, relative density and carbon dioxide content are known, together with the relevant pressures and temperatures. If hydrogen is present, as is often the case for gases with a synthetic admixture, the hydrogen content also needs to be known.

NOTE In principle, it is possible to calculate the compression factor when any three of the parameters superior calorific value, relative density, carbon dioxide content (the usual three) and nitrogen content are known, but subsets including nitrogen content are not recommended.

The method is primarily applicable to pipeline quality gases within the ranges of pressure p and temperature T at which transmission and distribution operations normally take place, with an uncertainty of about ± 0,1 %. For wider-ranging applications the uncertainty of the results increases (see Annex F).

More detail concerning the scope and field of application of the method is given in ISO 12213-1.

2 Normative references

The following referenced documents are indispensable for the application of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 6976:1995, *Natural gas — Calculation of calorific values, density, relative density and Wobbe index from composition*

ISO 12213-1, *Natural gas — Calculation of compression factor — Part 1: Introduction and guidelines*

ISO 80000-4, *Quantities and units — Part 4: Mechanics*

ISO 80000-5, *Quantities and units — Part 5: Thermodynamics*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 12213-1 apply.

4 Method of calculation

4.1 Principle

The method recommended uses equations which are based on the concept that pipeline quality natural gas may be uniquely characterized for calculation of its volumetric properties by an appropriate and distinctive set of measurable physical properties. These characteristics, together with the pressure and temperature, are used as input data for the method.

The method uses the following physical properties: superior calorific value, relative density and carbon dioxide content. The method is particularly useful in the common situation where a complete molar composition is not available, but may also be preferred for its relative simplicity. For gases with a synthetic admixture, the hydrogen content needs to be known.

4.2 The SGERG-88 equation

The calculation method using physical properties is based on the standard GERG 88 (SGERG-88) virial equation for natural gases [1], [2], [3]. The standard GERG 88 virial equation is derived from the master GERG 88 (MGERG-88) virial equation, which is a method of calculation based on a molar-composition analysis [4].

The SGERG-88 virial equation from which the compression factor Z is calculated may be written as

$$Z = 1 + B\rho_\mathrm{m} + C\rho_\mathrm{m}^2 \tag{1}$$

where

B and C are functions of the input data comprising the superior calorific value H_S, the relative density d, the contents of both inert and combustible non-hydrocarbon components of the gas mixture ($\mathrm{CO_2}$ and $\mathrm{H_2}$) and the temperature T;

ρ_m is the molar density given by

$$\rho_\mathrm{m} = p/(ZRT) \tag{2}$$

where

$$Z = f_1(p, T, H_\mathrm{S}, d, x_{\mathrm{CO_2}}, x_{\mathrm{H_2}}) \tag{3}$$

However, the SGERG-88 method treats the natural-gas mixture internally as a five-component mixture consisting of an equivalent hydrocarbon gas (with the same thermodynamic properties as the sum of the hydrocarbons present), nitrogen, carbon dioxide, hydrogen and carbon monoxide. To characterize the thermodynamic properties of the hydrocarbon gas adequately, the hydrocarbon heating value H_CH is also needed. Therefore, the calculation of Z uses

$$Z = f_2\,(p, T, H_\mathrm{CH}, x_\mathrm{CH}, x_{\mathrm{N_2}}, x_{\mathrm{CO_2}}, x_{\mathrm{H_2}}, x_\mathrm{CO}) \tag{4}$$

In order to be able to model coke oven gas mixtures, the mole fraction of carbon monoxide is taken to have a fixed relation to the hydrogen content. If hydrogen is not present ($x_{\mathrm{H_2}} < 0{,}001$), then set $x_{\mathrm{H_2}} = 0$. The natural-gas mixture is then treated in the calculation method as a three-component mixture (see Annex B).

The calculation is performed in three steps:

First, the five-component composition from which both the known superior calorific value and the known relative density can be calculated satisfactorily may be found from the input data by an iterative procedure described in detail in Annex B.

Secondly, once this composition is known, B and C may be found using relationships also given in Annex B.

In the third step, Equations (1) and (2) are solved simultaneously for ρ_m and Z by a suitable numerical method.

A flow diagram of the procedure for calculating Z from the input data is shown in Figure B.1.

4.3 Input variables

4.3.1 Preferred input data set

The input variables required for use with the SGERG-88 equation are the absolute pressure, temperature and superior calorific value (volumetric basis), the relative density, the carbon dioxide content and the hydrogen content. Thus the physical properties used in the input data set (set A) are

H_S, d, x_{CO_2} and x_{H_2}

Relative density is referred to normal conditions (101,325 kPa and 0 °C) and superior calorific value is referred to normal conditions (101,325 kPa and 0 °C) and a combustion temperature of 25 °C.

4.3.2 Alternative input data sets

Three alternatives to the preferred input data set (see 4.3.1) may be used with the standard GERG 88 virial equation:

x_{N_2}, H_S, d and x_{H_2} (set B)

x_{N_2}, x_{CO_2}, d and x_{H_2} (set C)

x_{N_2}, x_{CO_2}, H_S and x_{H_2} (set D)

The alternative input data sets are considered fully in GERG Technical Monograph TM5[3]. Use of the alternative input data sets gives results which may differ at the fourth decimal place. This part of ISO 12213 recommends the use of input data set A.

4.4 Ranges of application

4.4.1 Pipeline quality gas

The ranges of application for pipeline quality gas are as defined below:

absolute pressure $0\ \text{MPa} \leqslant p \leqslant 12\ \text{MPa}$

temperature $263\ \text{K} \leqslant T \leqslant 338\ \text{K}$

mole fraction of carbon dioxide $0 \leqslant x_{CO_2} \leqslant 0{,}20$

mole fraction of hydrogen $0 \leqslant x_{H_2} \leqslant 0{,}10$

superior calorific value $30\ \text{MJ·m}^{-3} \leqslant H_S \leqslant 45\ \text{MJ·m}^{-3}$

relative density $0{,}55 \leqslant d \leqslant 0{,}80$

The mole fractions of other natural-gas components are not required as input. These mole fractions shall, however, lie within the following ranges (the ratio of successive mole fractions in the alkane homologous series is typically 3:1 — see Annex E):

methane $0{,}7 \leqslant x_{CH_4} \leqslant 1{,}0$

nitrogen $0 \leqslant x_{N_2} \leqslant 0{,}20$

ethane $0 \leqslant x_{\mathrm{C_2H_6}} \leqslant 0{,}10$

propane $0 \leqslant x_{\mathrm{C_3H_8}} \leqslant 0{,}035$

butanes $0 \leqslant x_{\mathrm{C_4H_{10}}} \leqslant 0{,}015$

pentanes $0 \leqslant x_{\mathrm{C_5H_{12}}} \leqslant 0{,}005$

hexanes $0 \leqslant x_{\mathrm{C_6}} \leqslant 0{,}001$

heptanes $0 \leqslant x_{\mathrm{C_7}} \leqslant 0{,}000\,5$

octanes plus higher hydrocarbons $0 \leqslant x_{\mathrm{C_{8+}}} \leqslant 0{,}000\,5$

carbon monoxide $0 \leqslant x_{\mathrm{CO}} \leqslant 0{,}03$

helium $0 \leqslant x_{\mathrm{He}} \leqslant 0{,}005$

water $0 \leqslant x_{\mathrm{H_2O}} \leqslant 0{,}000\,15$

The method applies only to mixtures in the single-phase gaseous state (above the dew point) at the conditions of temperature and pressure of interest. For pipeline quality gas, the method is applicable over wider ranges of temperature and pressure but with increased uncertainty (see Figure 1). In the computer implementation, the lower temperature limit is set at 250 K.

4.4.2 Wider ranges of application

The ranges of application tested beyond the limits given in 4.4.1 are:

absolute pressure $0\ \mathrm{MPa} \leqslant p \leqslant 12\ \mathrm{MPa}$

temperature $263\ \mathrm{K} \leqslant T \leqslant 338\ \mathrm{K}$

mole fraction of carbon dioxide $0 \leqslant x_{\mathrm{CO_2}} \leqslant 0{,}30$

mole fraction of hydrogen $0 \leqslant x_{\mathrm{H_2}} \leqslant 0{,}10$

superior calorific value $20\ \mathrm{MJ \cdot m^{-3}} \leqslant H_{\mathrm{S}} \leqslant 48\ \mathrm{MJ \cdot m^{-3}}$

relative density $0{,}55 \leqslant d \leqslant 0{,}90$

The allowable mole fractions of other major natural-gas components are extended to:

methane $0{,}5 \leqslant x_{\mathrm{CH_4}} \leqslant 1{,}0$

nitrogen $0 \leqslant x_{\mathrm{N_2}} \leqslant 0{,}50$

ethane $0 \leqslant x_{\mathrm{C_2H_6}} \leqslant 0{,}20$

propane $0 \leqslant x_{\mathrm{C_3H_8}} \leqslant 0{,}05$

The limits for other minor natural-gas components remain as given in 4.4.1 for pipeline quality gas.

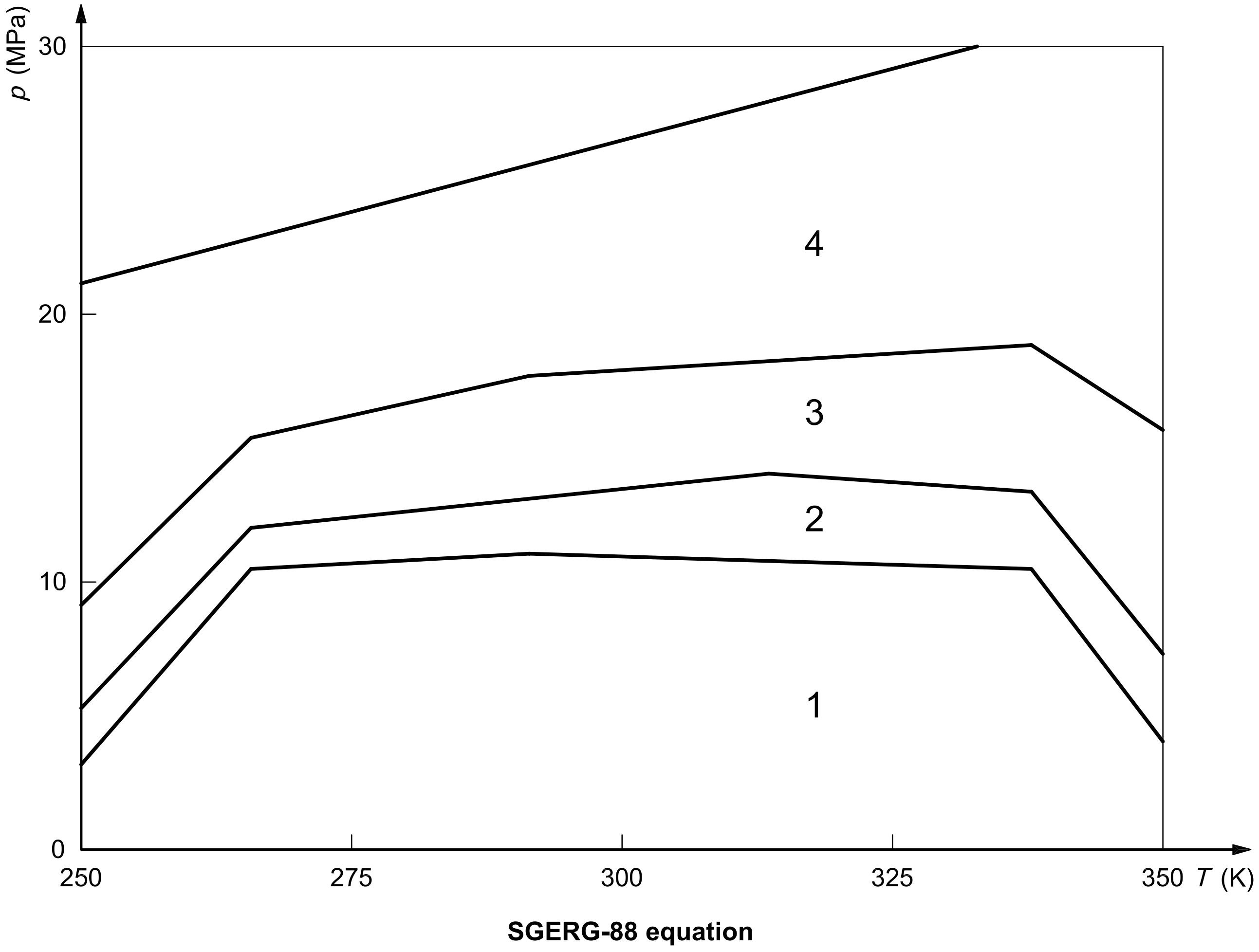
The method is not applicable outside these ranges; the computer implementation described in Annex B will not allow violation of the limits of composition quoted here.

4.5 Uncertainty

4.5.1 Uncertainty for pipeline quality gas

The uncertainty in the prediction of the compression factor ΔZ (for the temperature range 263 K to 338 K) is ± 0,1 % at pressures up to 10 MPa and ± 0,2 % between 10 MPa and 12 MPa for natural gases with $x_{\mathrm{N_2}} \leqslant 0{,}20$, $x_{\mathrm{CO_2}} \leqslant 0{,}09$, $x_{\mathrm{C_2H_6}} \leqslant 0{,}10$ and $x_{\mathrm{H_2}} \leqslant 0{,}10$, and for $30\ \mathrm{MJ \cdot m^{-3}} \leqslant H_\mathrm{S} \leqslant 45\ \mathrm{MJ \cdot m^{-3}}$ and $0{,}55 \leqslant d \leqslant 0{,}80$ (see Figure 1).

For gases with a CO_2 content exceeding a mole fraction of 0,09, the uncertainty of ± 0,1 % is maintained for pressures up to 6 MPa and for temperatures between 263 K and 338 K. This uncertainty level is determined by comparison with the GERG databank on measurements of the compression factor for natural gases [5], [6] and with the Gas Research Institute data [9].



Key

p	pressure
T	temperature

1	ΔZ	⩽ ± 0,1 %
2	ΔZ	± 0,1 % to ± 0,2 %
3	ΔZ	± 0,2 % to ± 0,5 %
4	ΔZ	± 0,5 % to ± 3,0 %

Figure 1 — Uncertainty limits for the calculation of compression factors

(The uncertainty limits given are expected to be valid for natural gases and similar gases with $x_{\mathrm{N_2}} \leqslant 0{,}20$; $x_{\mathrm{CO_2}} \leqslant 0{,}09$; $x_{\mathrm{C_2H_6}} \leqslant 0{,}10$ and $x_{\mathrm{H_2}} \leqslant 0{,}10$, and for $30\ \mathrm{MJ \cdot m^{-3}} \leqslant H_\mathrm{S} \leqslant 45\ \mathrm{MJ \cdot m^{-3}}$ and $0{,}55 \leqslant d \leqslant 0{,}80$)

4.5.2 Uncertainty for wider ranges of application

The estimated uncertainties involved in calculations of compression factors beyond the limits of quality given in 4.5.1 are discussed in Annex F.

4.5.3 Impact of uncertainties of input variables

Listed in Table 1 are typical values for the uncertainties of the relevant input variables. These values may be achieved under optimum operating conditions.

As a general guideline only, an error propagation analysis using the above uncertainties in the input variables produces an additional uncertainty of about ± 0,1 % in the result at 6 MPa and within the temperature range 263 K to 338 K. Above 6 MPa, the additional uncertainties are greater and increase roughly in direct proportion to the pressure (see Reference [3]).

4.5.4 Reporting of results

Results for the compression factor shall be reported to four places of decimals, together with the pressure and temperature values and the calculation method used (ISO 12213-3, SGERG-88 equation). For verification of calculation procedures, it is useful to carry extra digits.

Table 1 — Uncertainties of input variables

Input variable	Absolute uncertainty
Absolute pressure	± 0,02 MPa
Temperature	± 0,15 K
Mole fraction of carbon dioxide	± 0,002
Mole fraction of hydrogen	± 0,005
Relative density	± 0,001 3
Superior calorific value	± 0,06 $\text{MJ}\cdot\text{m}^{-3}$

5 Computer program

Software which implements this International Standard has been prepared. Users of this part of ISO 12213 are invited to contact ISO/TC 193/SC 1, either directly or through their ISO member body, to enquire about the availability of this software.

Annex A
(normative)

Symbols and units

The symbols specified in this annex are those which are used in both the main text and in Annex B. The units specified here are those which give consistency with the values of the coefficients given in Annex B.

Symbol	Meaning	Units
b_{H0}	Zero-order (constant) term in the molar heating value (H_{CH}) expansion of B_{11} [Equation (B.20)]	$\mathrm{m^3 \cdot kmol^{-1}}$
b_{H1}	First-order (linear) term in the molar heating value (H_{CH}) expansion of B_{11} [Equation (B.20)]	$\mathrm{m^3 \cdot MJ^{-1}}$
b_{H2}	Second-order (quadratic) term in the molar heating value (H_{CH}) expansion of B_{11} [Equation (B.20)]	$\mathrm{m^3 \cdot kmol \cdot MJ^{-2}}$
$b_{H0}(0)$	Terms in the temperature expansion of b_{H0} [Equation (B.21)]	$\mathrm{m^3 \cdot kmol^{-1}}$
$b_{H0}(1)$		$\mathrm{m^3 \cdot kmol^{-1} \cdot K^{-1}}$
$b_{H0}(2)$		$\mathrm{m^3 \cdot kmol^{-1} \cdot K^{-2}}$
$b_{H1}(0)$	Terms in the temperature expansion of b_{H1} [Equation (B.21)]	$\mathrm{m^3 \cdot MJ^{-1}}$
$b_{H1}(1)$		$\mathrm{m^3 \cdot MJ^{-1} \cdot K^{-1}}$
$b_{H1}(2)$		$\mathrm{m^3 \cdot MJ^{-1} \cdot K^{-2}}$
$b_{H2}(0)$	Terms in the temperature expansion of b_{H2} [Equation (B.21)]	$\mathrm{m^3 \cdot kmol \cdot MJ^{-2}}$
$b_{H2}(1)$		$\mathrm{m^3 \cdot kmol \cdot MJ^{-2} \cdot K^{-1}}$
$b_{H2}(2)$		$\mathrm{m^3 \cdot kmol \cdot MJ^{-2} \cdot K^{-2}}$
$b_{ij}(0)$	Terms in the temperature expansion of b_{ij} [Equation (B.22)]	$\mathrm{m^3 \cdot kmol^{-1}}$
$b_{ij}(1)$		$\mathrm{m^3 \cdot kmol^{-1} \cdot K^{-1}}$
$b_{ij}(2)$		$\mathrm{m^3 \cdot kmol^{-1} \cdot K^{-2}}$
B	Second virial coefficient [Equation (1)]	$\mathrm{m^3 \cdot kmol^{-1}}$
B_{ij}	Second virial coefficient for binary interaction between component i and component j [Equation (B.22)]	$\mathrm{m^3 \cdot kmol^{-1}}$
c_{H0}	Zero-order (constant) term in the molar heating value (H_{CH}) expansion of C_{111} [Equation (B.29)]	$\mathrm{m^6 \cdot kmol^{-2}}$
c_{H1}	First-order (linear) term in the molar heating value (H_{CH}) expansion of C_{111} [Equation (B.29)]	$\mathrm{m^6 \cdot kmol^{-1} \cdot MJ^{-1}}$
c_{H2}	Second-order (quadratic) term in the molar heating value (H_{CH}) expansion of C_{111} [Equation (B.29)]	$\mathrm{m^6 \cdot MJ^{-2}}$

Symbol	**Meaning**	**Units**
$c_{H0}(0)$ $c_{H0}(1)$ $c_{H0}(2)$	Terms in the temperature expansion of c_{H0} [Equation (B.30)]	$m^6 \cdot kmol^{-2}$ $m^6 \cdot kmol^{-2} \cdot K^{-1}$ $m^6 \cdot kmol^{-2} \cdot K^{-2}$
$c_{H1}(0)$ $c_{H1}(1)$ $c_{H1}(2)$	Terms in the temperature expansion of c_{H1} [Equation (B.30)]	$m^6 \cdot kmol^{-1} \cdot MJ^{-1}$ $m^6 \cdot kmol^{-1} \cdot MJ^{-1} \cdot K^{-1}$ $m^6 \cdot kmol^{-1} \cdot MJ^{-1} \cdot K^{-2}$
$c_{H2}(0)$ $c_{H2}(1)$ $c_{H2}(2)$	Terms in the temperature expansion of c_{H2} [Equation (B.30)]	$m^6 \cdot MJ^{-2}$ $m^6 \cdot MJ^{-2} \cdot K^{-1}$ $m^6 \cdot MJ^{-2} \cdot K^{-2}$
$c_{ijk}(0)$ $c_{ijk}(1)$ $c_{ijk}(2)$	Terms in the temperature expansion of c_{ijk} [Equation (B.31)]	$m^6 \cdot kmol^{-2}$ $m^6 \cdot kmol^{-2} \cdot K^{-1}$ $m^6 \cdot kmol^{-2} \cdot K^{-2}$
C	Third virial coefficient [Equation (1)]	$m^6 \cdot kmol^{-2}$
C_{ijk}	Third virial coefficient for ternary interaction between components i, j and k [Equation (B.31)]	$m^6 \cdot kmol^{-2}$
d	Relative density [d(air) = 1; Equation (B.1)]	—
DH_{CH}	Change in the molar heating value H_{CH} during iteration [Equations (B.10) and (B.11)]	$MJ \cdot kmol^{-1}$
H_{S}	Superior calorific value [gas at normal conditions (0 °C, 1,013 25 bar), combustion temperature 25 °C]	$MJ \cdot m^{-3}$
H	Molar heating value (combustion temperature 25 °C)	$MJ \cdot kmol^{-1}$
M	Molar mass [Equations (B.5) and (B.8)]	$kg \cdot kmol^{-1}$
p	Absolute pressure	bar
R	(Universal) gas constant	$m^3 \cdot bar \cdot kmol^{-1} \cdot K^{-1}$
T	Absolute temperature	K
t	Celsius temperature [= T – 273,15; Equation (B.27)]	°C
V_{m}	Molar volume (= $1/\rho_{\mathrm{m}}$)	$m^3 \cdot kmol^{-1}$
x	Mole fraction of a component	—
y	Combination rule parameters for the binary unlike-interaction virial coefficients B_{12} and B_{13} (Table B.2) and the ternary unlike-interaction virial coefficient C_{ijk} [Equation (B.32)]	—
Z	Compression factor	—
ρ	Mass density [Equations (B.8) and (B.42)]	$kg \cdot m^{-3}$
ρ_{m}	Molar density (= V_{m}^{-1})	$kmol \cdot m^{-3}$

Additional subscripts

n	Value at normal conditions ($T_n = 273{,}15$ K, $p_n = 1{,}013\ 25$ bar)
CH	For the equivalent hydrocarbon
CO	For carbon monoxide
CO_2	For carbon dioxide
H_2	For hydrogen
N_2	For nitrogen

Additional qualifiers

(air)	For dry air of standard composition [Equation (B.1)]
(D)	For special value of ρ used in Equation (B.11)
1	For the equivalent hydrocarbon [Equations (B.12) and (B.15)]
2	For nitrogen [Equations (B.12) and (B.16)]
3	For carbon dioxide [Equations (B.12) and (B.17)]
4	For hydrogen [Equations (B.12) and (B.18)]
5	For carbon monoxide [Equations (B.12) and (B.19)]
(id)	Ideal gas state
(u)	Iteration counter (B.2.1)
(v)	Iteration counter (B.2.2)
(w)	Iteration counter (B.4)

Annex B
(normative)

Description of the SGERG-88 method

This annex gives the equations for, and numerical values of, coefficients which together specify completely the SGERG method for calculation of compression factors.

It also describes iteration procedures adopted by GERG [3] for implementing the method in the verified Fortran 77 subroutine SGERG.FOR. This subroutine provides the correct solution; other computational procedures are acceptable provided that they can be demonstrated to yield identical numerical results. The calculated results shall agree to at least the fourth place of decimals with the examples given in Annex C.

Other implementations which are known to produce identical results are as follows:

a) A BASIC version, described in GERG TM5 [3], which may be used with a variety of metric reference conditions. This programme was designed mainly for PC applications.

b) A version in C, described in German DVGW Directives, sheet G486 [8].

c) A version in Turbo Pascal.

All these programmes have been verified to give the same results to within 10^{-5}. The availability of the programmes and the conditions which apply to their use are discussed in Part 1 of this International Standard.

B.1 Basic structure of the calculation method

As described in 4.2, the calculation proceeds in three steps, which are shown schematically in Figure B.1.

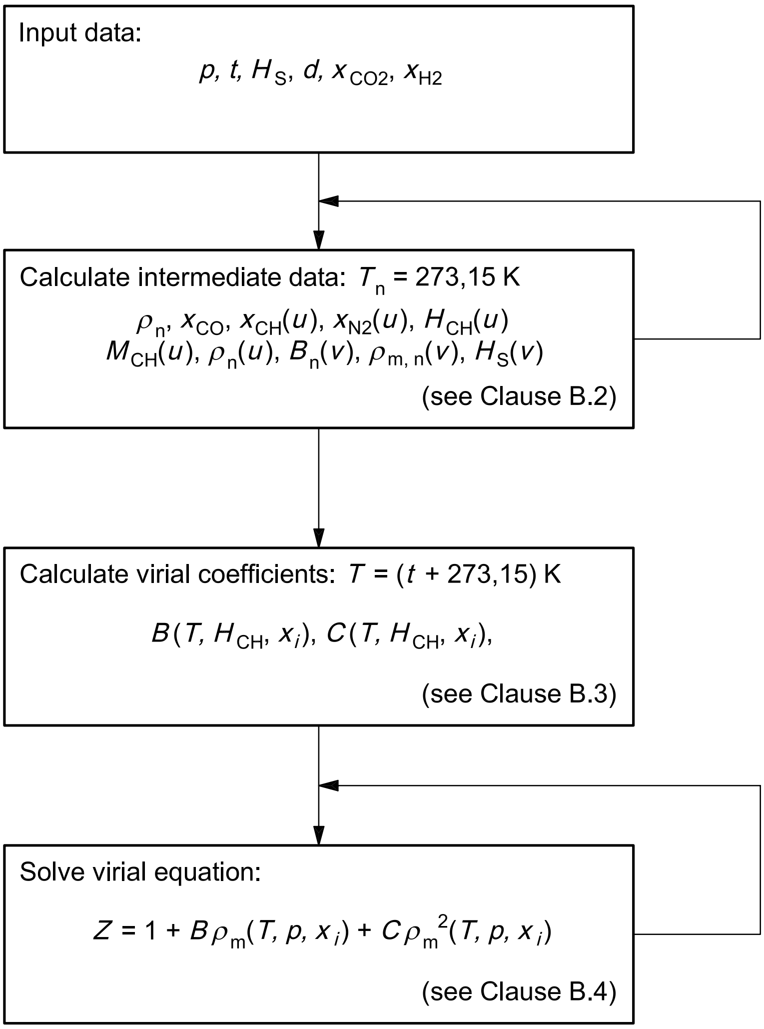


Figure B.1 — Flow diagram for standard GERG-88 calculation method
(x_i = mole fraction of component i)

The calculation is described below in the order in which these three steps are carried out.

Step I

The input data are pressure, temperature, gross calorific value, relative density and the mole fractions of carbon dioxide and hydrogen. If the values of the first three parameters are in any units other than bar, °C and MJ/m^3, they shall first be converted precisely to values in bar, °C and MJ/m^3, respectively, using the guidelines set out in Annex D.

The input data are then used to calculate the following intermediate data:

Mole fraction of:	
hydrocarbon gas	x_{CH}
nitrogen	x_{N_2}
carbon monoxide	x_{CO}
Molar heating value of the equivalent hydrocarbon	H_{CH}

Molar mass of the equivalent hydrocarbon	M_{CH}
Second virial coefficient ($T_{\mathrm{n}} = 273{,}15$ K)	B_{n}
Molar density at normal conditions	$\rho_{\mathrm{m,n}}$
Mass density at normal conditions	ρ_{n}
Superior calorific value of the gas	H_{S}

In Equations (B.1) to (B.46), each symbol represents a physical quantity divided by its selected unit (see Annex A), such that their quotient is the dimensionless value of the quantity.

Step II

The intermediate data are used to calculate the second and third virial coefficients for the natural gas at the required temperature, $B(T,H_{\mathrm{CH}},x_i)$ and $C(T,H_{\mathrm{CH}},x_i)$.

Step III

The second and third virial coefficients determined in the second step are inserted in the virial equation, and the compression factor Z is calculated for a given pressure and temperature.

The symbols used are defined in Annex A.

B.2 Calculation of intermediate data

The eight intermediate-data values (x_{CH}, $x_{\mathrm{N_2}}$, x_{CO}, H_{CH}, M_{CH}, B_{n}, $\rho_{\mathrm{m,n}}$, ρ_{n}) are determined from Equations (B.1) to (B.8) using the iterative method presented in Figure B.2. Values of the constants used in these equations are given in Table B.1.

$$\rho_{\mathrm{n}} = d\rho_{\mathrm{n}}(\mathrm{air}) \tag{B.1}$$

$$x_{\mathrm{CO}} = 0{,}096\,4\,x_{\mathrm{H2}} \tag{B.2}$$

$$V_{\mathrm{m,n}}(\mathrm{id}) = RT_{\mathrm{n}}/p_{\mathrm{n}} \tag{B.3}$$

$$\rho_{\mathrm{m,n}}(v) = \left[V_{\mathrm{m,n}}(\mathrm{id}) + B_{\mathrm{n}}(v)\right]^{-1} \tag{B.4}$$

$$M_{\mathrm{CH}}(u) = -\,2{,}709\,328 + 0{,}021\,062\,199\,H_{\mathrm{CH}}(u-1) \tag{B.5}$$

$$x_{\mathrm{CH}}(u) = H_{\mathrm{S}}\Big/\left[H_{\mathrm{CH}}(u-1)\rho_{\mathrm{m,n}}(v)\right] - \left[\left(x_{\mathrm{H_2}}H_{\mathrm{H_2}} + x_{\mathrm{CO}}H_{\mathrm{CO}}\right)\Big/H_{\mathrm{CH}}(u-1)\right] \tag{B.6}$$

$$x_{\mathrm{N_2}}(u) = 1 - x_{\mathrm{CH}}(u) - x_{\mathrm{CO_2}} - x_{\mathrm{H_2}} - x_{\mathrm{CO}} \tag{B.7}$$

$$\rho_{\mathrm{n}}(u) = \left[x_{\mathrm{CH}}(u)M_{\mathrm{CH}}(u) + x_{\mathrm{N_2}}(u)M_{\mathrm{N_2}}\right]\rho_{\mathrm{m,n}}(v) + \left(x_{\mathrm{CO_2}}M_{\mathrm{CO_2}} + x_{\mathrm{H_2}}M_{\mathrm{H_2}} + x_{\mathrm{CO}}M_{\mathrm{CO}}\right)\rho_{\mathrm{m,n}}(v) \tag{B.8}$$

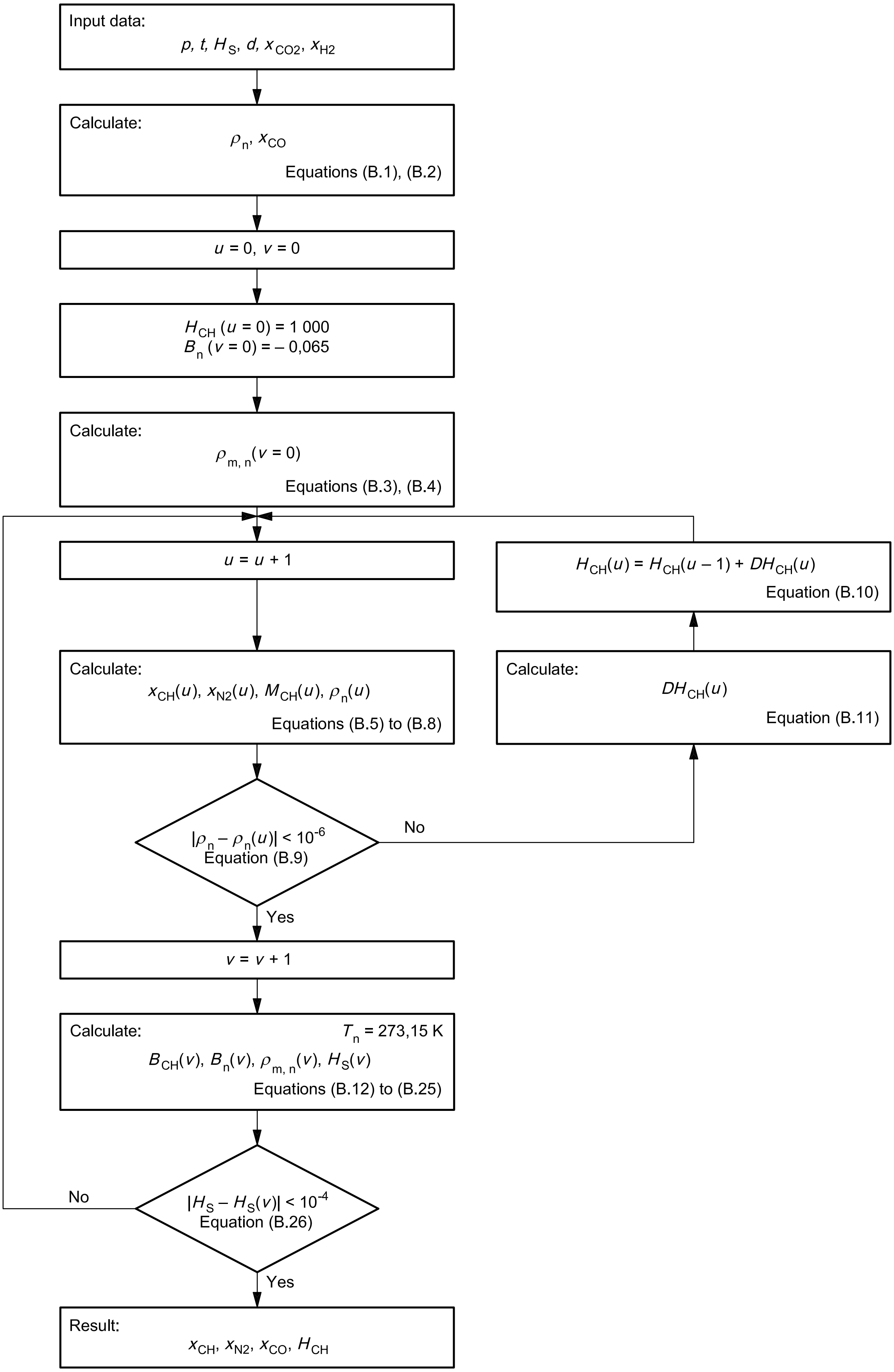


Figure B.2 — Flow diagram for computing intermediate data by iteration

Table B.1 — Values of the constants used in Equations (B.1) to (B.8)
(adjusted to conform with the molar masses and molar calorific values in ISO 6976:1995)

$H_{\mathrm{H_2}}$	= 285,83	$\mathrm{MJ \cdot kmol^{-1}}$
H_{CO}	= 282,98	$\mathrm{MJ \cdot kmol^{-1}}$
$M_{\mathrm{N_2}}$	= 28,013 5	$\mathrm{kg \cdot kmol^{-1}}$
$M_{\mathrm{CO_2}}$	= 44,010	$\mathrm{kg \cdot kmol^{-1}}$
$M_{\mathrm{H_2}}$	= 2,015 9	$\mathrm{kg \cdot kmol^{-1}}$
M_{CO}	= 28,010	$\mathrm{kg \cdot kmol^{-1}}$
R	= 0,083 145 1	$\mathrm{m^3 \cdot bar \cdot kmol^{-1} \cdot K^{-1}}$
$V_{\mathrm{m,n}}(\mathrm{id})$	= 22,414 097	$\mathrm{m^3 \cdot kmol^{-1}}$
$\rho_{\mathrm{n}}(\mathrm{air})$	= 1,292 923	$\mathrm{kg \cdot m^{-3}}$

B.2.1 Iteration with the molar heating value H_{CH} (inner loop)

Equations (B.1) to (B.8) are applied in sequence so as to obtain the first approximation in the uth iteration step. The starting values are:

$H_{\mathrm{CH}}(u = 0) = 1\,000\ \mathrm{MJ \cdot kmol^{-1}}$

$B_{\mathrm{n}}(v = 0) = -\,0{,}065\ \mathrm{m^3 \cdot kmol^{-1}}$

The values of the other constants used in Equations (B.1) to (B.8) are given in Table B.1.

The convergence criterion for this inner iteration loop is that the absolute difference between the calculated density of the gas at normal conditions $\rho_{\mathrm{n}}(u)$ and the known density (either measured directly or determined from the relative density) of the gas at normal conditions ρ_{n} is less than 10^{-6}, i.e.

$$\left|\rho_{\mathrm{n}} - \rho_{\mathrm{n}}(u)\right| < 10^{-6} \tag{B.9}$$

If this condition is not satisfied, then an improved value of the molar heating value $H_{\mathrm{CH}}(u)$, for use in Equations (B.5) to (B.8), is calculated using Equation (B.10) as follows:

$$H_{\mathrm{CH}}(u) = H_{\mathrm{CH}}(u-1) + DH_{\mathrm{CH}}(u) \tag{B.10}$$

where

$$DH_{\mathrm{CH}}(u) = \left[\rho_{\mathrm{n}} - \rho_{\mathrm{n}}(u)\right]\left[\rho(D) - \rho_{\mathrm{n}}(u)\right]^{-1} \tag{B.11}$$

$\rho_{\mathrm{n}}(u)$ being the density value for the current iteration step [commencing with $H_{\mathrm{CH}}(u - 1)$],

$\rho(D)$ being the density determined by Equations (B.4) to (B.8) using $[H_{\mathrm{CH}}(u - 1) + 1]$ as input for the molar heating value.

When the left-hand side of Equation (B.9) is less than 10^{-6}, this iteration loop is terminated and iteration with the second virial coefficient begins.

B.2.2 Iteration with the second virial coefficient B_n (outer loop)

The intermediate values $x_\mathrm{CH}(u)$, $x_{\mathrm{N}_2}(u)$, x_CO and $H_\mathrm{CH}(u)$ from the preceding iteration and the input data x_{CO_2} and x_{H_2} are used to determine an improved value for the second virial coefficient $B_\mathrm{n}(v)$ for the whole gas at normal conditions.

The second virial coefficient for the natural gas is given by the following equation:

$$B(T) = x_1^2 B_{11} + 2x_1x_2B_{12} + 2x_1x_3B_{13} + 2x_1x_4B_{14} + 2x_1x_5B_{15} + x_2^2B_{22} + 2x_2x_3B_{23} + 2x_2x_4B_{24} +$$

$$+ x_3^2B_{33} + x_4^2B_{44} + x_5^2B_{55} \tag{B.12}$$

Some of the terms that are missing in Equation (B.12), i.e. B_{25}, B_{34}, etc., have been found not to improve the accuracy of the calculation if included and are therefore set at zero.

$$B_\mathrm{n}(v) = B\left(T_\mathrm{n}\right) \tag{B.13}$$

where

$$T = T_\mathrm{n} = 273{,}15 \tag{B.14}$$

$$x_1 = x_\mathrm{CH}(u) \tag{B.15}$$

$$x_2 = x_{\mathrm{N}_2}(u) \tag{B.16}$$

$$x_3 = x_{\mathrm{CO}_2} \tag{B.17}$$

$$x_4 = x_{\mathrm{H}_2} \tag{B.18}$$

$$x_5 = x_\mathrm{CO} \tag{B.19}$$

$$B_{11} = b_{H0} + b_{H1}H_\mathrm{CH}(u) + b_{H2}H_\mathrm{CH}^2(u) \tag{B.20}$$

where the coefficients b_{H0}, b_{H1} and b_{H2} are second-degree polynomials as a function of temperature

$$B_{11} = b_{H0}(0) + b_{H0}(1)T + b_{H0}(2)T^2 + \left[b_{H1}(0) + b_{H1}(1)T + b_{H1}(2)T^2\right]H_\mathrm{CH}(u) +$$

$$+\left[b_{H2}(0) + b_{H2}(1)T + b_{H2}(2)T^2\right]H_\mathrm{CH}^2(u) \tag{B.21}$$

and the second virial coefficients B_{14}, B_{15}, B_{22}, B_{23}, B_{24}, B_{33}, B_{34}, B_{44} and B_{55} are also second-degree polynomials as a function of temperature, in the general form

$$B_{ij} = b_{ij}(0) + b_{ij}(1)T + b_{ij}(2)T^2 \tag{B.22}$$

The unlike-interaction virial coefficients B_{12} and B_{13} are given by

$$B_{12} = \left[0{,}72 + 1{,}875 \times 10^{-5}(320 - T)^2\right]\left(B_{11} + B_{22}\right)/2 \tag{B.23}$$

$$B_{13} = -\,0{,}865\left(B_{11}B_{33}\right)^{1/2} \tag{B.24}$$

The coefficients in Equations (B.21) to (B.24) are given in Table B.2.

Table B.2 — Numerical values for the coefficients $b(0)$, $b(1)$ and $b(2)$ in the temperature expansion of the second virial coefficient for pure gases and of the unlike-interaction virial coefficients
(The units of B are $\mathrm{m^3 \cdot kmol^{-1}}$ when the temperature is in kelvins.)

	ij	$b(0)$	$b(1)$	$b(2)$
CH	$H0$	$-4{,}254\,68 \times 10^{-1}$	$2{,}865\,00 \times 10^{-3}$	$-4{,}620\,73 \times 10^{-6}$
CH	$H1$	$8{,}771\,18 \times 10^{-4}$	$-5{,}562\,81 \times 10^{-6}$	$8{,}815\,10 \times 10^{-9}$
CH	$H2$	$-8{,}247\,47 \times 10^{-7}$	$4{,}314\,36 \times 10^{-9}$	$-6{,}083\,19 \times 10^{-12}$
N_2	22	$-1{,}446\,00 \times 10^{-1}$	$7{,}409\,10 \times 10^{-4}$	$-9{,}119\,50 \times 10^{-7}$
CO_2	33	$-8{,}683\,40 \times 10^{-1}$	$4{,}037\,60 \times 10^{-3}$	$-5{,}165\,70 \times 10^{-6}$
H_2	44	$-1{,}105\,96 \times 10^{-3}$	$8{,}133\,85 \times 10^{-5}$	$-9{,}872\,20 \times 10^{-8}$
CO	55	$-1{,}308\,20 \times 10^{-1}$	$6{,}025\,40 \times 10^{-4}$	$-6{,}443\,00 \times 10^{-7}$
CH + N_2	12	$y = 0{,}72 + 1{,}875 \times 10^{-5}(320 - T)^2$		
CH + CO_2	13	$y = -0{,}865$		
CH + H_2	14	$-5{,}212\,80 \times 10^{-2}$	$2{,}715\,70 \times 10^{-4}$	$-2{,}500\,00 \times 10^{-7}$
CH + CO	15	$-6{,}872\,90 \times 10^{-2}$	$-2{,}393\,81 \times 10^{-6}$	$5{,}181\,95 \times 10^{-7}$
N_2 + CO_2	23	$-3{,}396\,93 \times 10^{-1}$	$1{,}611\,76 \times 10^{-3}$	$-2{,}044\,29 \times 10^{-6}$
N_2 + H_2	24	$1{,}200\,00 \times 10^{-2}$	0,000 00	0,000 00

The value of $B_\mathrm{n}(v)$ obtained from Equation (B.13) is used to calculate the vth approximation of $\rho_\mathrm{m,n}$ using Equation (B.4).

Equation (B.6) is then used, in the inverse way to that in which it was used previously, to obtain a value for $H_\mathrm{S}(v)$, i.e.

$$H_\mathrm{S}(v) = \left[x_1(u) H_\mathrm{CH}(u-1) + x_4 H_4 + x_5 H_5\right] \rho_\mathrm{m,n}(v) \tag{B.25}$$

where H_4 $(= H_{\mathrm{H_2}})$ and H_5 $(= H_\mathrm{CO})$ are the molar heating values at 298,15 K of hydrogen and carbon monoxide, respectively. The convergence criterion for the outer iteration loop (iteration counter v) is that the absolute difference between the measured superior calorific value H_S and the calculated calorific value $H_\mathrm{S}(v)$ is less than 10^{-4}, i.e.

$$\left|H_\mathrm{S} - H_\mathrm{S}(v)\right| < 10^{-4} \tag{B.26}$$

If this criterion is not satisfied, then the value for $B_\mathrm{n}(v)$ determined from Equation (B.13) is used as a new input value for Equation (B.4) and the whole iteration procedure, i.e. the inner iteration loop (iteration counter u), is restarted from Equation (B.5) using the current values of $H_\mathrm{CH}(u-1)$ and $\rho_\mathrm{m,n}(v)$.

When both convergence criterion (B.9) and convergence criterion (B.26) are satisfied simultaneously, the final intermediate data for the mole fractions x_CH and $x_{\mathrm{N_2}}$ and for the molar heating value H_CH have been determined.

B.3 Calculation of virial coefficients

The second and third virial coefficients $B(T)$ and $C(T)$ of a natural gas are now determined from the mole fractions $x_{\mathrm{CO_2}}$ and $x_{\mathrm{H_2}}$ (input data) and x_CH, $x_{\mathrm{N_2}}$ and x_CO (intermediate data) and the molar heating value H_CH (see Figures B.1 and B.3).

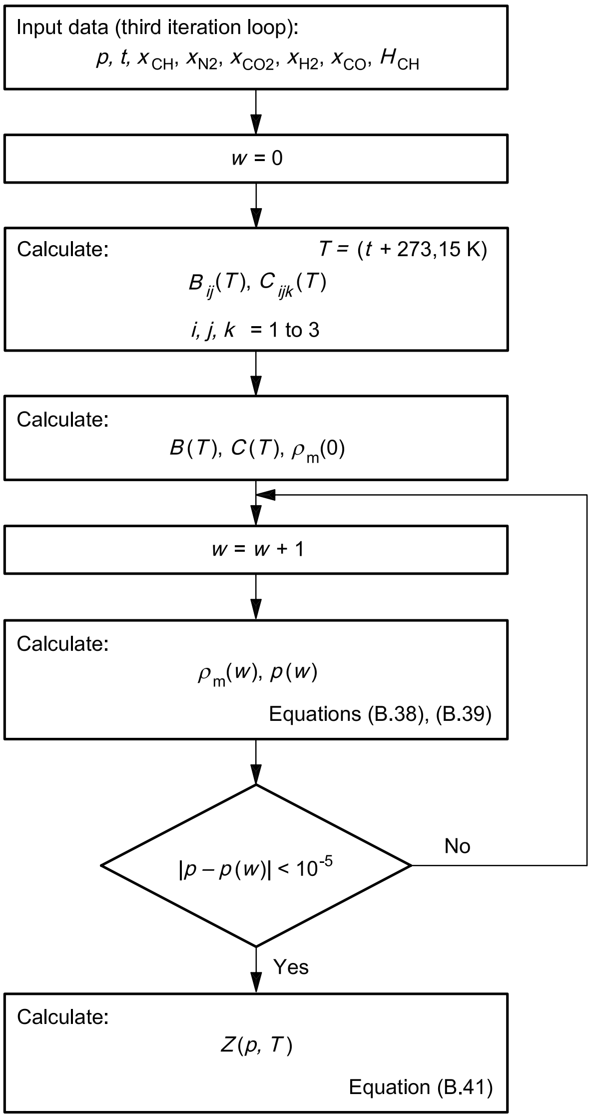


Figure B.3 — Flow diagram for compression factor calculation

B.3.1 Calculation of $B(T)$

The second virial coefficient $B(T)$ is calculated from Equation (B.12) by the procedure described in B.2.2 for a temperature

$$T = t + 273{,}15 \tag{B.27}$$

B.3.2 Calculation of $C(T)$

The third virial coefficient for a natural gas at a temperature T is determined using the following equation:

$$C(T) = x_1^3 C_{111} + 3x_1^2 x_2 C_{112} + 3x_1^2 x_3 C_{113} + 3x_1^2 x_4 C_{114} + 3x_1^2 x_5 C_{115} + 3x_1 x_2^2 C_{122} + 6x_1 x_2 x_3 C_{123} + \\ + 3x_1 x_3^2 C_{133} + x_2^3 C_{222} + 3x_2^2 x_3 C_{223} + 3x_2 x_3^2 C_{233} + x_3^3 C_{333} + x_4^3 C_{444} \tag{B.28}$$

The possible additional terms that are missing in Equation (B.28) have been found not to improve the accuracy of the calculation if included and have therefore been set at zero.

Furthermore, in Equation (B.28):

$$C_{111} = c_{\mathrm{H0}} + c_{\mathrm{H1}} H_{\mathrm{CH}} + c_{\mathrm{H2}} H_{\mathrm{CH}}^2 \tag{B.29}$$

where c_{H0}, c_{H1} and c_{H2} are second-degree polynomials as a function of temperature, viz:

$$C_{111} = c_{\mathrm{H0}}(0) + c_{\mathrm{H0}}(1)T + c_{\mathrm{H0}}(2)T^2 + \left[c_{\mathrm{H1}}(0) + c_{\mathrm{H1}}(1)T + c_{\mathrm{H1}}(2)T^2\right] H_{\mathrm{CH}} + \\ + \left[c_{\mathrm{H2}}(0) + c_{\mathrm{H2}}(1)T + c_{\mathrm{H2}}(2)T^2\right] H_{\mathrm{CH}}^2 \tag{B.30}$$

as are C_{222}, C_{333}, C_{444}, C_{115}, C_{223} and C_{233}, viz:

$$C_{ijk} = c_{ijk}(0) + c_{ijk}(1)T + c_{ijk}(2)T^2 \tag{B.31}$$

The coefficients in Equations (B.30) and (B.31) are given in Table B.3.

Table B.3 — Numerical values of the coefficients $c(0)$, $c(1)$ and $c(2)$ in the temperature expansion of the third virial coefficient for pure gases and of the unlike-interaction virial coefficients
(The units of C are m^6·kmol^{-2} when the temperature is in kelvins.)

	ijk	$c(0)$	$c(1)$	$c(2)$
CH	$H0$	$-3{,}024\,88 \times 10^{-1}$	$1{,}958\,61 \times 10^{-3}$	$-3{,}163\,02 \times 10^{-6}$
CH	$H1$	$6{,}464\,22 \times 10^{-4}$	$-4{,}228\,76 \times 10^{-6}$	$6{,}881\,57 \times 10^{-9}$
CH	$H2$	$-3{,}328\,05 \times 10^{-7}$	$2{,}231\,60 \times 10^{-9}$	$-3{,}677\,13 \times 10^{-12}$
N_2	222	$7{,}849\,80 \times 10^{-3}$	$-3{,}989\,50 \times 10^{-5}$	$6{,}118\,70 \times 10^{-8}$
CO_2	333	$2{,}051\,30 \times 10^{-3}$	$3{,}488\,80 \times 10^{-5}$	$-8{,}370\,30 \times 10^{-8}$
H_2	444	$1{,}047\,11 \times 10^{-3}$	$-3{,}648\,87 \times 10^{-6}$	$4{,}670\,95 \times 10^{-9}$
CH + CH + N_2	112	$y = 0{,}92 + 0{,}001\,3\,(T - 270)$		
CH + CH + CO_2	113	$y = 0{,}92$		
CH + CH + H_2	114	$y = 1{,}20$		
CH + CH + CO	115	$7{,}367\,48 \times 10^{-3}$	$-2{,}765\,78 \times 10^{-5}$	$3{,}430\,51 \times 10^{-8}$
CH + N_2 + N_2	122	$y = 0{,}92 + 0{,}001\,3\,(T - 270)$		
CH + N_2 + CO_2	123	$y = 1{,}10$		
CH + CO_2 + CO_2	133	$y = 0{,}92$		
N_2 + N_2 + CO_2	223	$5{,}520\,66 \times 10^{-3}$	$-1{,}686\,09 \times 10^{-5}$	$1{,}571\,69 \times 10^{-8}$
N_2 + CO_2 + CO_2	233	$3{,}587\,83 \times 10^{-3}$	$8{,}066\,74 \times 10^{-6}$	$-3{,}257\,98 \times 10^{-8}$

The other unlike-interaction virial coefficients used are given by

$$C_{ijk} = y_{ijk}\left(C_{iii} C_{jjj} C_{kkk}\right)^{1/3} \tag{B.32}$$

where y_{ijk} is given by

$$y_{112} = y_{122} = 0{,}92 + 0{,}001\,3(T - 270) \tag{B.33}$$

$$y_{113} = y_{133} = 0{,}92 \tag{B.34}$$

$$y_{114} = 1{,}20 \tag{B.35}$$

$$y_{123} = 1{,}10 \tag{B.36}$$

Equation (B.32) shows that the temperature dependence of the unlike-interaction virial coefficients is determined essentially by the temperature dependence of the third virial coefficients for the pure components.

B.4 Calculation of the compression factor and molar density

The very last stage in the calculation of the compression factor and the molar density is to solve Equations (1) and (2) simultaneously for the given value of the pressure p. For the first approximation in the iteration using w, ρ_m is given by

$$\rho_\mathrm{m}^{-1}(w = 0) = RT/p + B \tag{B.37}$$

where the second virial coefficient B is defined by Equation (B.12) for a temperature T (see Figure B.3). An improved value $\rho_\mathrm{m}(w)$ is then given by

$$\rho_\mathrm{m}^{-1}(w) = \left(RT/p\right)\left[1 + B\rho_\mathrm{m}(w-1) + C\rho_\mathrm{m}^2(w-1)\right] \tag{B.38}$$

where the third virial coefficient C for the mixture is defined by Equation (B.28) for a given temperature T. The convergence criterion for the iteration using w is that the absolute difference between the calculated pressure $p(w)$ given by Equation (B.39) and the given pressure p is less than 10^{-5} [see Equation (B.40)].

$$p(w) = RT\rho_\mathrm{m}(w)\left[1 + B\rho_\mathrm{m}(w) + C\rho_\mathrm{m}^2(w)\right] \tag{B.39}$$

$$\left|p - p(w)\right| < 10^{-5} \tag{B.40}$$

If this condition is not satisfied, then the current value for the molar density $\rho_\mathrm{m}(w)$ is used as the new value $\rho_\mathrm{m}(w-1)$ in Equation (B.38) and an improved value of the molar density $\rho_\mathrm{m}(w)$ is calculated.

However, if the left-hand side of Equation (B.40) is less than 10^{-5}, the iteration routine is ended, and $\rho_\mathrm{m}(w)$ is the final molar density ρ_m. The compression factor is then given by

$$Z = 1 + B\rho_\mathrm{m} + C\rho_\mathrm{m}^2 \tag{B.41}$$

NOTE The mass density can be calculated as follows:

$$\rho = \left[d\rho_\mathrm{n}(\mathrm{air})pZ_\mathrm{n}T_\mathrm{n}/\left(p_\mathrm{n}ZT\right)\right] \tag{B.42}$$

Z and Z_n being rounded to four places of decimals before being used in the density calculation.

Report the density to three significant figures.

B.5 Consistency checks on the SGERG-88 method

The following tests, which provide partial consistency checks on the input data, shall be applied when carrying out calculations by the SGERG method.

a) The input data shall satisfy the following condition:

$$d > 0{,}55 + 0{,}97x_{\mathrm{CO_2}} - 0{,}45x_{\mathrm{H_2}} \tag{B.43}$$

b) The intermediate calculated value for the mole fraction of nitrogen shall satisfy the following conditions:

$$-0{,}01 \leqslant x_{\mathrm{N_2}} \leqslant 0{,}5 \tag{B.44}$$

$$x_{\mathrm{N_2}} + x_{\mathrm{CO_2}} \leqslant 0{,}5 \tag{B.45}$$

c) Furthermore, the internal consistency of the input data for the third iteration loop shall satisfy the condition:

$$d > 0{,}55 + 0{,}4x_{\mathrm{N_2}} + 0{,}97x_{\mathrm{CO_2}} - 0{,}45x_{\mathrm{H_2}} \tag{B.46}$$

Annex C
(normative)

Example calculations

The following example calculations shall be used for the validation of computer implementations of the SGERG-88 method not cited in Annex B. The calculations have been carried out using the validated executable programme GERG-88.EXE, which incorporates the subroutine SGERG.FOR described in Annex B.

Table C.1 — Input data

	Gas 1	Gas 2	Gas 3	Gas 4	Gas 5	Gas 6
x_{CO_2}	0,006	0,005	0,015	0,016	0,076	0,011
x_{H_2}	0,000	0,000	0,000	0,095	0,000	0,000
d	0,581	0,609	0,650	0,599	0,686	0,644
H_S (MJ·m^{-3})	40,66	40,62	43,53	34,16	36,64	36,58

Table C.2 — Results (Z-values)

Conditions p bar	 t °C	Gas 1	Gas 2	Gas 3	Gas 4	Gas 5	Gas 6
60	− 3,15	0,840 84	0,833 97	0,794 15	0,885 69	0,826 64	0,854 06
60	6,85	0,862 02	0,856 15	0,822 10	0,901 50	0,850 17	0,873 88
60	16,85	0,880 07	0,875 00	0,845 53	0,915 07	0,870 03	0,890 71
60	36,85	0,908 81	0,904 91	0,882 23	0,936 84	0,901 24	0,917 36
60	56,85	0,929 96	0,926 90	0,908 93	0,953 02	0,923 94	0,936 90
120	− 3,15	0,721 46	0,711 40	0,643 22	0,808 43	0,695 57	0,749 39
120	6,85	0,759 69	0,750 79	0,690 62	0,836 13	0,738 28	0,784 73
120	16,85	0,792 57	0,784 72	0,731 96	0,859 99	0,774 63	0,814 90
120	36,85	0,844 92	0,838 77	0,797 78	0,898 27	0,831 66	0,862 66
120	56,85	0,883 22	0,878 32	0,845 54	0,926 62	0,872 69	0,897 49

These gases are the same as the six gases in ISO 12213-2:2006, Annex C, where the complete molar compositions are given.

Annex D
(normative)

Conversion factors

D.1 Reference conditions

The reference conditions for which the standard GERG 88 virial equation was developed and which the SGERG.FOR computer subroutine uses internally are

Calorific value by combustion at $T_1 = 298{,}15$ K ($t_1 = 25$ °C)

$p = 101{,}325$ kPa

gas metered at $T_2 = 273{,}15$ K ($t_2 = 0$ °C)

$p = 101{,}325$ kPa

The latter set of conditions are also the reference conditions for relative density.

Considerable care is needed to ensure that correctly referenced inputs are used for calorific value and relative density. Several countries normally use the above conditions, but others use alternative conditions. This can easily cause confusion, particularly since the unit of calorific-value measurement in each case may still be $\mathrm{MJ{\cdot}m^{-3}}$. Table D.1 is a guide to which of the major international gas-trading countries use which reference conditions.

For those using non-metric units for calorific value (i.e. $\mathrm{Btu{\cdot}ft^{-3}}$), conversion both of units and of reference conditions is required.

The conversion factors used are taken from Reference [3].

Table D.1 — Nationally adopted metric reference conditions for the measurement of calorific value

	t_1 (°C)	t_2 (°C)
Australia	15	15
Austria	25	0
Belgium	25	0
Canada	15	15
Denmark	25	0
France	0	0
Germany	25	0
Ireland	15	15
Italy	25	0
Japan	0	0
Netherlands	25	0
Russia	25	0 or 20
United Kingdom	15	15
United States of America	15	15

NOTE 1 In all countries the reference pressure is 101,325 kPa (= 1,013 25 bar).

NOTE 2 t_1 is the combustion reference temperature.

NOTE 3 t_2 is the gas-metering reference temperature.

D.2 Units and conversion factors for pressure and temperature

If the input variables p and t are not in the necessary units of bar and °C, then conversions must be made in order to use the Fortran implementation. A selection of appropriate conversion factors is given in Table D.2.

Table D.2 — Conversion factors for pressure and temperature

Pressure

$p\ (\mathrm{bar}) = [p(\mathrm{kPa})]/100$

$p\ (\mathrm{bar}) = [p(\mathrm{MPa})] \times 10$

$p\ (\mathrm{bar}) = [p(\mathrm{atm})] \times 1{,}013\,25$

$p\ (\mathrm{bar}) = [p(\mathrm{psia})]/14{,}503\,8$

$p\ (\mathrm{bar}) = [p(\mathrm{psig}) + 14{,}695\,9]/14{,}503\,8$

Temperature

$t\ (^\circ\mathrm{C}) = T(\mathrm{K}) - 273{,}15$

$t\ (^\circ\mathrm{C}) = [t(^\circ\mathrm{F}) - 32]/1{,}8$

$t\ (^\circ\mathrm{C}) = [t(^\circ\mathrm{R})]/1{,}8 - 273{,}15$

D.3 Units and conversion of calorific value and density between reference conditions

Because both superior calorific value and relative density are functions of the composition of a gas mixture, and because the thermophysical properties of the individual components depend upon temperature and pressure in individual ways, it is in principle impossible (without knowledge of the composition) to convert the calorific value and the relative density known at one set of reference conditions to exact corresponding values for any other set of reference conditions.

However, because the relevant reference conditions are always thermodynamically close together, and because natural gases do not vary in their composition to any major extent, it is possible in practice to give conversion factors which may be applied to any typical natural gas with essentially no loss of accuracy in the converted physical properties.

D.3.1 Conversion factors for the units

If the input variable H_S is not in the necessary units $\mathrm{MJ{\cdot}m^{-3}}$, then a conversion must be made.

The appropriate conversion factors for calorific values at a given set of reference conditions (see Clause D.1) are given in Table D.3.

Table D.3 — Conversion factors for calorific value

$H_\mathrm{S}\ (\mathrm{MJ{\cdot}m^{-3}}) = [H_\mathrm{S}(\mathrm{kWh{\cdot}m^{-3}})] \times 3{,}6$

$H_\mathrm{S}\ (\mathrm{MJ{\cdot}m^{-3}}) = [H_\mathrm{S}(\mathrm{Btu{\cdot}ft^{-3}})]/26{,}839\,2$

D.3.2 Conversion between different reference conditions

If the input variables H_S and d are not at the correct reference conditions (see Clause D.1), then a conversion must be made. Table D.4 gives the conversion factors appropriate to the reference conditions in Table D.1.

Table D.4 — Conversion factors for calorific value and relative density

Calorific value H_S at reference conditions $t_1 = 25$ °C, $t_2 = 0$ °C, $p_2 = 1{,}013\ 25$ bar:

$H_S = H_S$ ($t_1 = 0$ °C, $t_2 = 0$ °C, $p_2 = 1{,}013\ 25$ bar) × 0,997 4

$H_S = H_S$ ($t_1 = 15$ °C, $t_2 = 15$ °C, $p_2 = 1{,}013\ 25$ bar) × 1,054 3

$H_S = H_S$ ($t_1 = 60$ °F, $t_2 = 60$ °F, $p_2 = 1{,}015\ 92$ bar) × 1,053 5

$H_S = H_S$ ($t_1 = 60$ °F, $t_2 = 60$ °F, $p_2 = 1{,}015\ 60$ bar) × 1,053 9

Relative density d at reference conditions $t_2 = 0$ °C, $p_2 = 1{,}013\ 25$ bar:

$d = d$ ($t_2 = 15$ °C, $p_2 = 1{,}013\ 25$ bar) × 1,000 2

$d = d$ ($t_2 = 60$ °F, $p_2 = 1{,}015\ 92$ bar or 1,015 60 bar) × 1,000 2

NOTE $p = 1{,}015\ 60$ bar = 14,73 psia (units of pressure customary in US).

Annex E
(informative)

Specification for pipeline quality natural gas

E.1 Maximum limits for mole fractions

The SGERG-88 calculation method [3] is a simplification of the MGERG-88 method [4], for which a full component analysis (CH_4 to C_8H_{18}, N_2 and CO_2 and, if present, H_2 and CO) is required in order to permit the calculation of compression factor or density. This part of ISO 12213 defines various maximum limits for individual mole fractions for the SGERG-88 method (see Table E.1). Column 2 of Table E.1 shows the range of application verified by means of experiment, column 3 lists the maximum mole fractions for pipeline quality natural gas and column 4 defines “wider ranges” of application. The range of natural gas mole fractions with values of compression factor supported by experiment is smaller than the range of pipeline quality natural gas, and also smaller than the wider ranges of application. For pressures up to 10 MPa and the composition limits given in column 2, the experimental values from the GERG databank are reproduced with an uncertainty of 0,1 % (95 % confidence limits).

Table E.1 — Ranges of application of SGERG-88 method (maximum limits of mole fractions)

	Range of application verified by experiment (see Figure 1)	**Range for pipeline quality natural gas** (see 4.4.1)	**Wider ranges of application** (see 4.4.2)
N_2	0,20	0,20	0,50
CO_2	0,09	0,20	0,30
C_2H_6	0,10	0,10	0,20
C_3H_8	0,035	0,035	0,05
C_4H_{10}	0,015	0,015	0,015
H_2	0,10	0,10	0,10

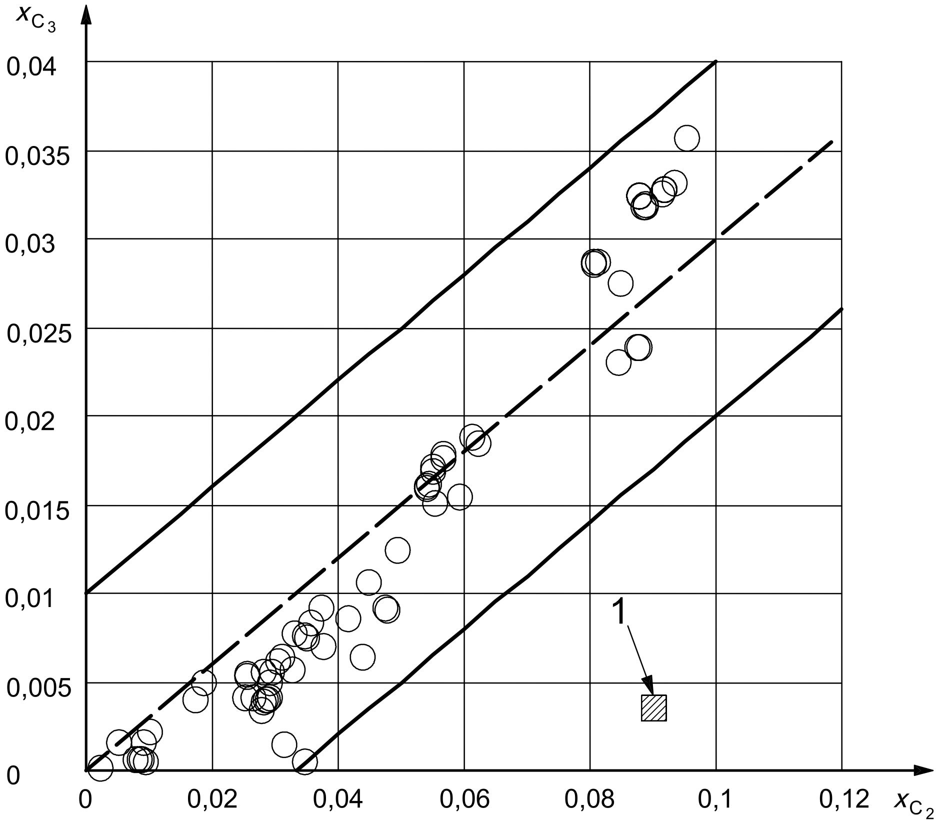
ISO 12213 introduces the term “pipeline quality natural gas” to describe natural gases of the kind usually distributed through natural-gas grids (see Table E.1, column 3). For these natural gases, the maximum limit for the mole fraction of carbon dioxide is given as 0,20. However, for this CO_2 content, the 0,1 % uncertainty limit is only observed up to a pressure of 6 MPa (see 4.5.1).

E.2 Consistency check and specification of input variables

Clause B.5 presents a consistency check of the input variables d, x_{CO_2}, x_{N_2} and x_{H_2} for the SGERG-88 method as a binding (i.e. normative) requirement.

In various publications on the SGERG-88 method [1], [2], [3] and in this part of ISO 12213, it has been emphasized that the method has been derived for natural gases showing the kinds of correlation between higher hydrocarbons which are typical of natural gases. This means, in effect, that the ratio of successive mole fractions in the alkane homologous series is typically 3:1. This rule of thumb has been substantiated and consolidated [10] through a comparison with the GERG databank [5], [6].

In Figures E.1 and E.2, the respective mole fractions $x_{C_3H_8}$ and $x_{C_{4+}}$ have been plotted as functions of the mole fraction of ethane $x_{C_2H_6}$ for the natural gases taken from the GERG databank (TM4, 1990 [5]) as data points (open circles) that meet the pipeline quality natural gas criterion given in Table E.1 (see Table 10 in TM7, 1996 [6]). For both mole fraction ratios, this gives a range of values within which the SGERG-88 method can always be applied safely. The dashed lines in Figures E.1 and E.2 illustrate the one-third rule for the ratios, with 0,3 for $x_{C_3H_8}/x_{C_2H_6}$ and 0,1 for $x_{C_{4+}}/x_{C_2H_6}$. The limiting lines on either side show a range of ± 0,01 for the propane mole fraction and ± 0,003 for the butane+ mole fraction, respectively, within which virtually all the data points from the GERG database can be found. The absolute tolerance limits selected here define the data situation much better than relative tolerance limits [10].



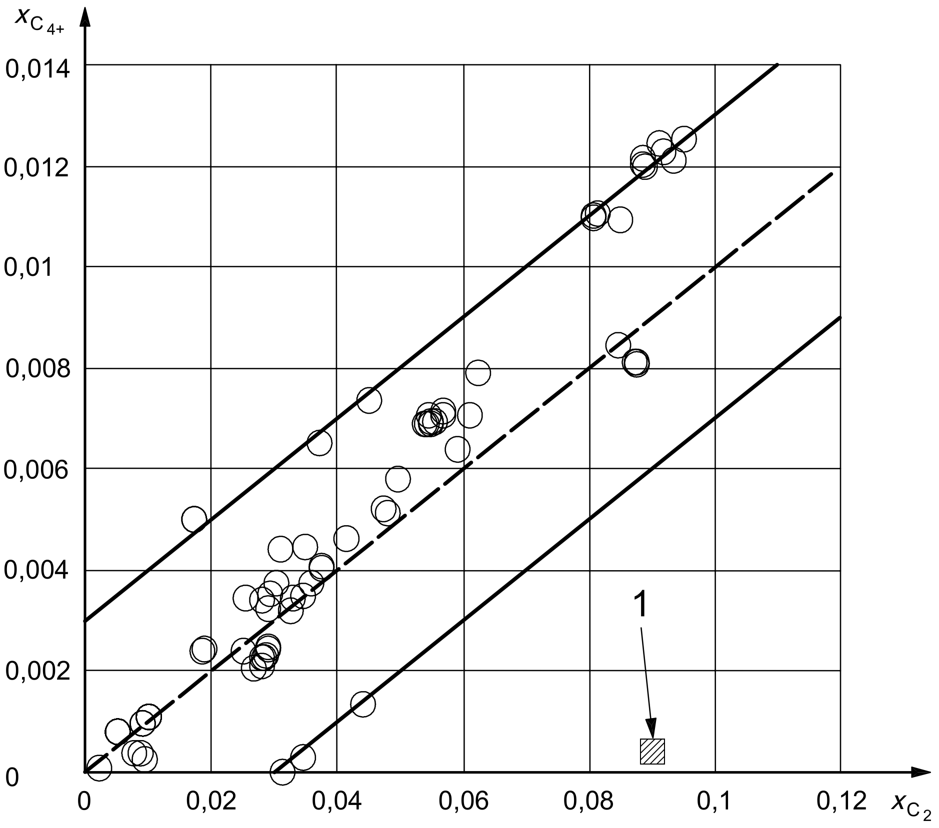
Key

x_{C_3} mole fraction of propane

x_{C_2} mole fraction of ethane

1 03-4605 gas (a North Sea gas) (see text)

Figure E.1 — Mole fraction of propane for natural gases as a function of the mole fraction of ethane



Key

$x_{C_{4+}}$ mole fraction of butane+ components

x_{C_2} mole fraction of ethane

1 03-4605 gas (a North Sea gas) (see text)

Figure E.2 — Mole fraction of butane+ for natural gases as a function of the mole fraction of ethane

Where a natural-gas analysis shows mole fractions that are not covered by the ranges indicated in Figures E.1 and E.2, it is recommended that the applicability of the SGERG-88 method be checked by comparison with other equations of state [4], [7], [11], which will however require a complete component analysis in order to obtain a description of the gas quality.

For one such example (a North Sea gas, designated 03-4605, containing 0,090 2 mole fraction ethane, 0,003 5 mole fraction propane and 0,000 16 mole fraction butanes — see shaded square in Figures E.1 and E.2), a number of comparative calculations have been made [10] with other equations of state [4], [7], [11]. In this case, the SGERG-88 method shows deviations of up to + 0,5 % at a pressure of 10 MPa and temperatures of 275 K to 280 K.

Measurements with a gas density measurement system [10] on the same isotherms show that the experimental density values agree with the density values calculated from a complete analysis [4], [7], [11] within the total measurement uncertainty of 0,04 % and, therefore, that the SGERG-88 method is inappropriate in this particular and unusual instance. The total measurement uncertainty is composed in equal parts of the uncertainty in the density measurement and the measurement uncertainty in the analysis of the natural-gas sample examined.

In cases where the SGERG-88 method should not be employed, it is recommended that the AGA8-DC92 [7] method from Part 2 of this International Standard, or the GERG-2004 equation of state [11], be used, but these options are only open if a complete component analysis is available.

Annex F
(informative)

Performance over wider ranges of application

The standard GERG virial equation has been comprehensively tested, over the temperature range 263 K to 338 K and at pressures up to 12 MPa, with the GERG databank [5] and the Gas Research Institute data [9] for gases within the ranges of composition, superior calorific value and relative density given for pipeline quality gases (see 4.4.1). Within these limits, the uncertainties are as given in 4.5.

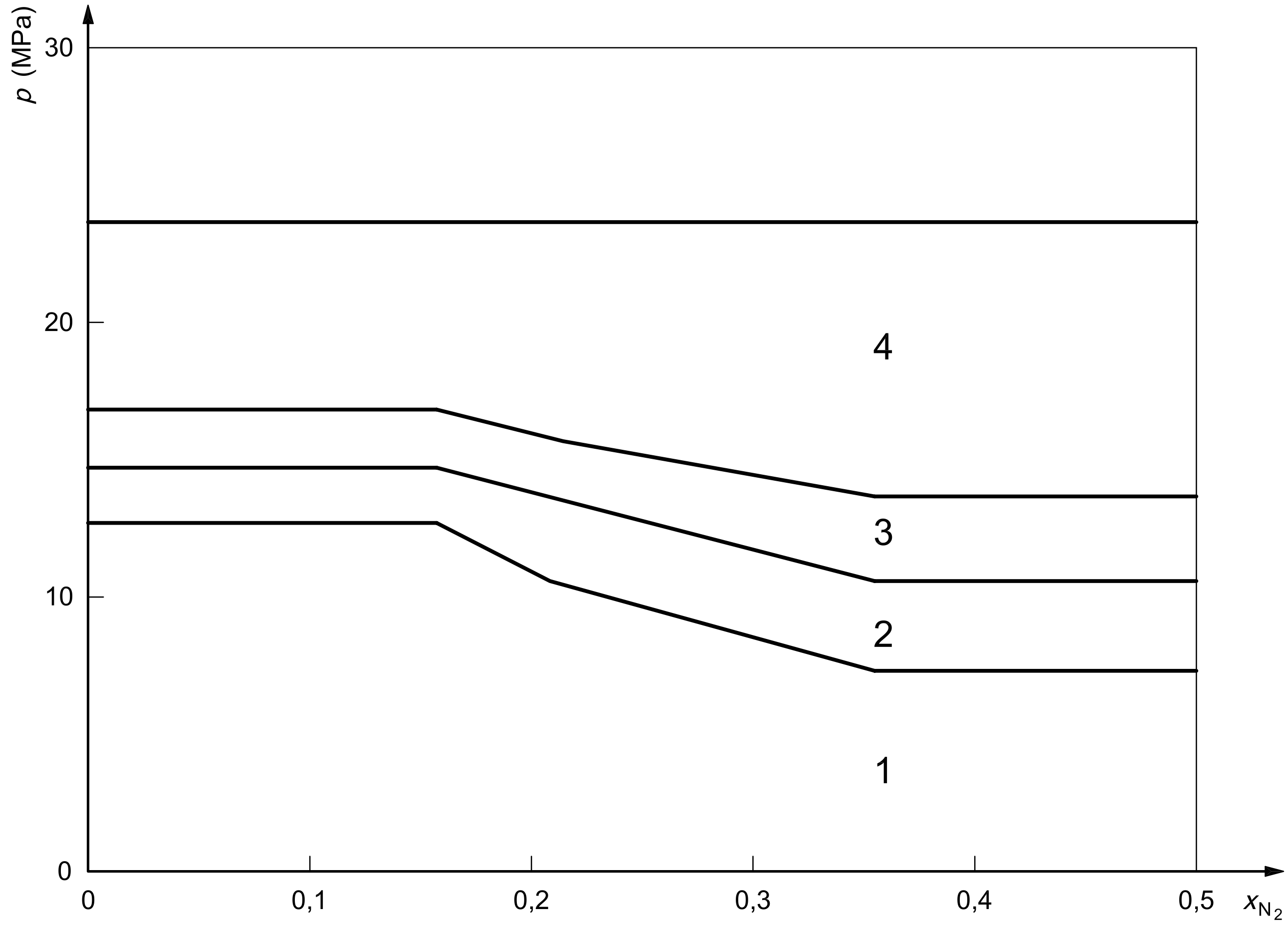
Rough estimates of the uncertainties involved in calculations of compression factors for wider ranges of application are plotted in Figures F.1 to F.4 as pressure-composition plots for nitrogen, carbon dioxide, ethane and propane, respectively.

In Figures F.1 to F.4, the performance of the SGERG equation is illustrated up to a maximum pressure of 30 MPa. This is for informative purposes only and is not intended to imply a recommendation that the equation be used routinely or uncritically above the normal specified limits. The uncertainty limits are dependent upon pressure, temperature and composition, and are also strongly affected by the proximity of the phase boundary. The estimated uncertainty limits presented below are based upon less comprehensive data, published as a supplement to the GERG databank [6], and upon the databanks in References [5] and [9].

The worst-case limits have always been chosen. Dashed lines are used to separate two regions of estimated uncertainty when the experimental evidence is not sufficient to determine the position of the boundary. The detailed composition of the gas will have a strong influence on the position of the phase boundary and the user should, therefore, make his own phase boundary calculation.

The overall results at pressures up to 10 MPa and temperatures within the range 263 K to 338 K can be summarized as follows. Only gases having mole fractions within the limits given below will have uncertainties within ± 0,1 %, ± 0,2 % and ± 0,5 %, respectively, within the given pressure and temperature domain.

Component	**Mole fraction for an uncertainty within**		
	± 0,1 %	± 0,2 %	± 0,5 %
Nitrogen	$< 0{,}20$	$< 0{,}50$	—
Carbon dioxide	$< 0{,}09$	$< 0{,}12$	$< 0{,}23$
Ethane	$< 0{,}10$	$< 0{,}11$	$< 0{,}12$
Propane	$< 0{,}035$	$< 0{,}04$	$< 0{,}045$



SGERG-88 equation (T = 263 K to 338 K)

Key

p pressure

x_{N_2} mole fraction of nitrogen

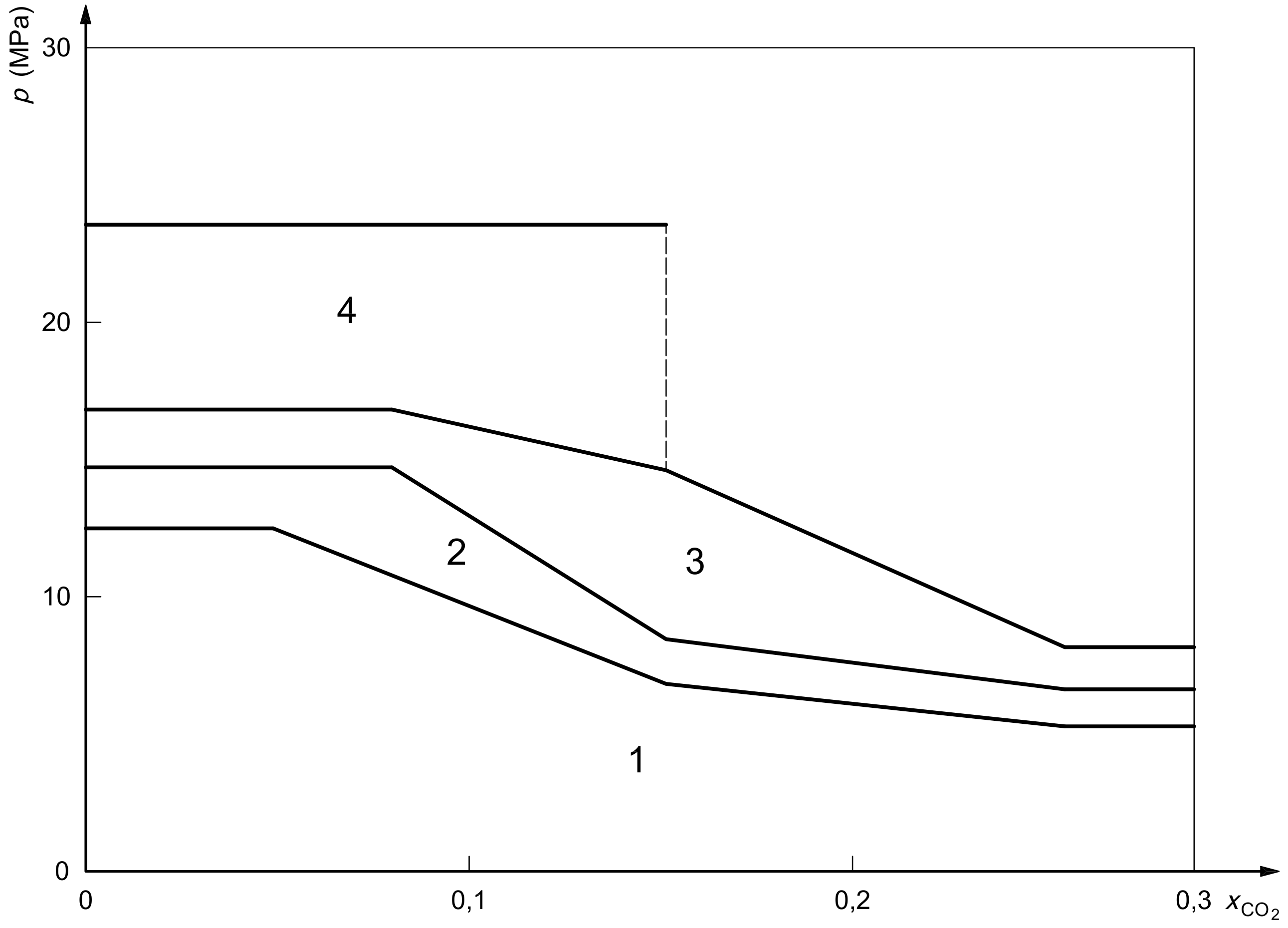
1 ΔZ $\leqslant \pm$ 0,1 %

2 ΔZ ± 0,1 % to ± 0,2 %

3 ΔZ ± 0,2 % to ± 0,5 %

4 ΔZ ± 0,5 % to ± 3,0 %

Figure F.1 — Estimated uncertainty limits for the calculation of compression factors of natural gases with a high nitrogen content



SGERG-88 equation (T = 263 K to 338 K)

Key

p pressure

x_{CO_2} mole fraction of carbon dioxide

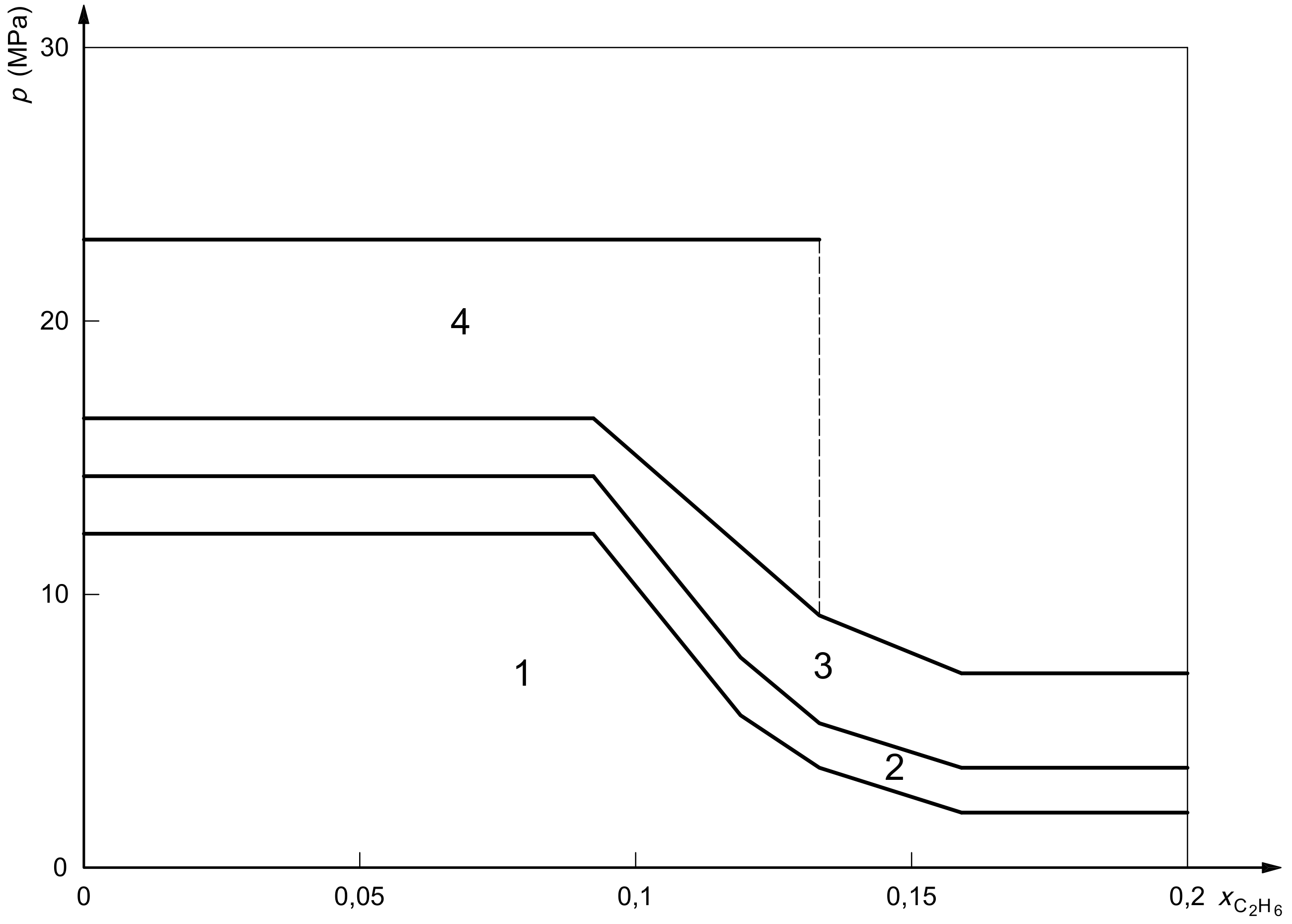
1 ΔZ $\leqslant \pm$ 0,1 %

2 ΔZ $\pm$ 0,1 % to $\pm$ 0,2 %

3 ΔZ $\pm$ 0,2 % to $\pm$ 0,5 %

4 ΔZ $\pm$ 0,5 % to $\pm$ 3,0 %

Figure F.2 — Estimated uncertainty limits for the calculation of compression factors of natural gases with a high carbon dioxide content



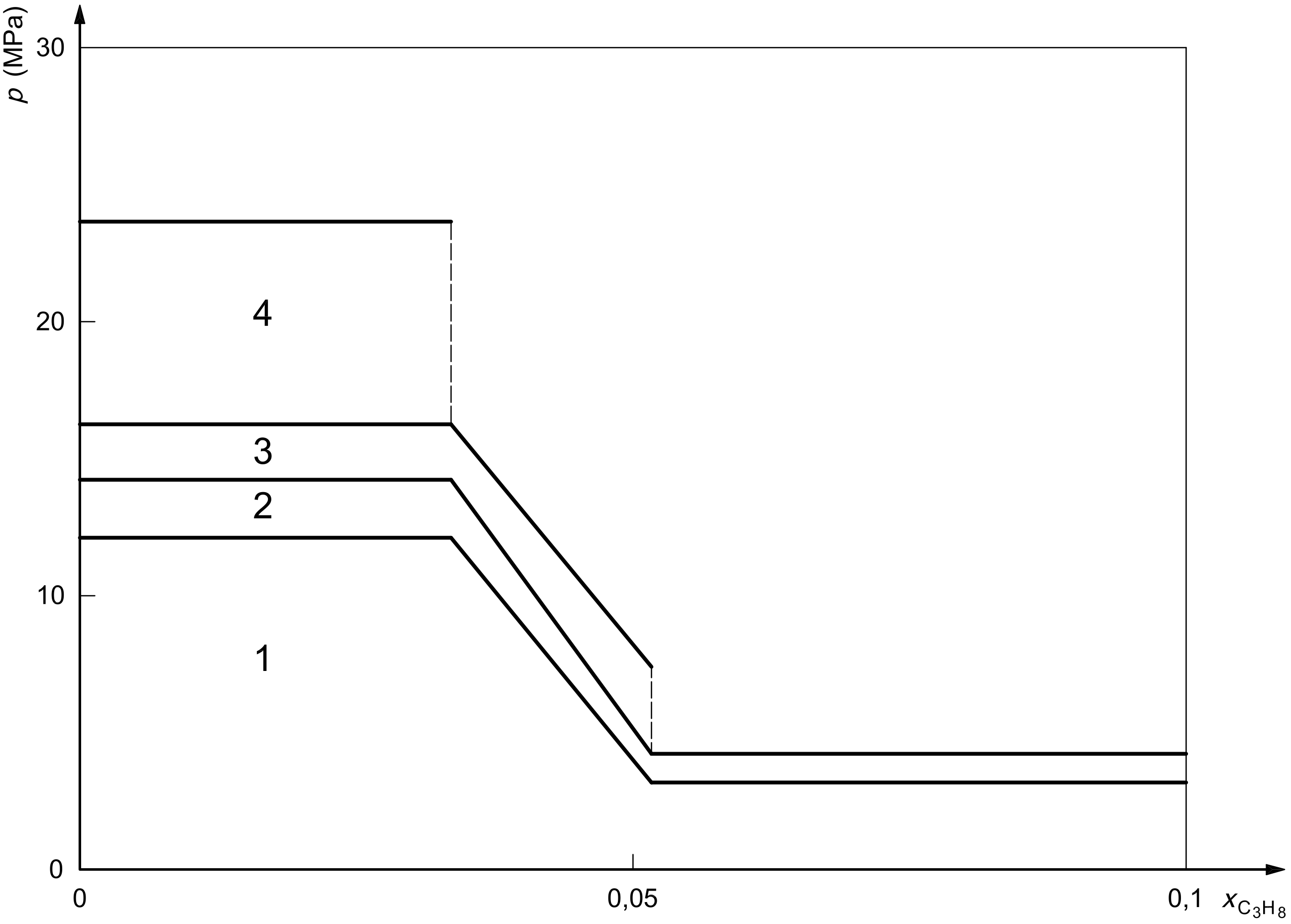
SGERG-88 equation (T = 263 K to 338 K)

Key

p	pressure
$x_{C_2H_6}$	mole fraction of ethane

1	ΔZ	$\leqslant \pm 0{,}1$ %
2	ΔZ	± 0,1 % to ± 0,2 %
3	ΔZ	± 0,2 % to ± 0,5 %
4	ΔZ	± 0,5 % to ± 3,0 %

Figure F.3 — Estimated uncertainty limits for the calculation of compression factors of natural gases with a high ethane content



SGERG-88 equation (T = 263 K to 338 K)

Key

p pressure

$x_{C_3H_8}$ mole fraction of propane

1	ΔZ	$\leqslant \pm 0{,}1$ %
2	ΔZ	± 0,1 % to ± 0,2 %
3	ΔZ	± 0,2 % to ± 0,5 %
4	ΔZ	± 0,5 % to ± 3,0 %

Figure F.4 — Estimated uncertainty limits for the calculation of compression factors of natural gases with a high propane content

Annex G
(informative)

Subroutine SGERG.FOR in Fortran

```
C
C**************************************************************************
C   last update: 07.08.96                  M. Jaeschke, J. Sikora
C
C  *******************  GERG-88  VIRIAL  EQUATION  ************************
C                           SUBROUTINE  SGERG
C
C   'SGERG'     CALCULATES THE COMPRESSION FACTORS OF NATURAL GASES USING
C               A SIMPLIFIED GAS ANALYSIS
C
C               LEGAL COPIES OF THIS PROGRAM MAY ONLY BE OBTAINED FROM THE
C               MEMBERS  OF  THE  GERG  WORKING  GROUP  ON COMPRESSION
C               FACTORS  OF  NATURAL  GAS  AS  GIVEN IN THE GERG TECHNICAL
C               MONOGRAPH TM 5 (1991).
C
C               The calculations are based on the following four
C               input parameters for the gas analysis:
C                                                          (Valid ranges:)
C               -1-  X3: mole fraction CO2                 ( 0.0  -> 0.3 )
C               -2-  HS: calorific value in MJ/m^3  *)     (  20  ->  48 )
C               -3-  RM: relative density           *)     ( 0.55 -> 0.9 )
C               -4-  X5: mole fraction H2                  ( 0.0  -> 0.1 )
C
C              *) note : metering   at T  =  0.0 C  ,  P = 1.01325 bar
C                      : combustion at T  = 25.0 C
C
C               Further input parameters used are:
C
C                    P : pressure in bar                   (  0   -> 120 )
C                    TC: temperature in degrees Celsius    (-23   ->  65 )
C
C               A CALCULATED value for X2, the molar fraction of nitrogen
C               is returned.
C
C               The calculated values are:
C
C                    Z : compression factor
C                    D : molar density in mol/m**3
C
C   ****  For some compilers the SAVE option has to be set explicitly  ****
C
C   SYNTAX :    CALL SGERG(X2,X3,HS,RM,X5,P,TC,Z,D)
C
C               The coefficients used in this program  are conform with the
C               values given in subroutine GAS682, from July 20,1988, appended
C               to report 8807, Van der Waals Laboratory, Amsterdam.
C
C                       J.P.J. Michels   &   J.A. Schouten
C                                August 16, 1991
C
C               Values for the gas constant, molar masses, calorific values
C               and the density of air conform with ISO 6976 (1995).
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
      SUBROUTINE SGERG(X2,X3,HS,RM,X5,P,TC,Z,D)
```

```
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      IF( P.LT.  0.0 .OR. P .GT.120.0)  STOP ' PRESSURE OUT OF RANGE'
      IF(TC.LT.-23.0 .OR. TC.GT .65.0)  STOP ' TEMPERATURE OUT OF RANGE'
      CALL SGERG1(P,TC,X2,X3,X5,HS,RM,Z,D)
      RETURN
      END
C     *******************************************************************
      SUBROUTINE  SGERG1(P,TC,Q2,Q3,Q5,QM,RM,Z,D)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON /RBLOK/ AMOL,HS
      COMMON /XBLOK/ X1,X2,X3,X11,X12,X13,X22,X23,X33
     >              ,X5,X7,X15,X17,X25,X55,X77
      COMMON /MBLOK/ GM1R0,GM1R1,GM2,GM3,GM5,GM7,FA,FB,RL,T0,H5,H7,R
      HS = QM
      X3 = Q3
      X5 = Q5
C      IF(RM.LT. 0.55.OR. RM.GT. 0.90) STOP  'REL. MASS OUT OF RANGE'
C      IF(X3.LT. 0.0 .OR. X3.GT. 0.30) STOP  'CO2 OUT OF RANGE'
C      IF(HS.LT.20.0 .OR. HS.GT.48.0 ) STOP  'CALOR. VALUE OUT OF RANGE'
      IF((0.55+0.97*X3-0.45*X5).GT.RM)STOP  'CONFLICTING INPUT'
      SM = RM*RL
      X7  = X5*0.0964D0
      X33 = X3*X3
      X55 = X5*X5
      X77 = X7*X7
      BEFF= -0.065D0
      H   = 1000.0D0
      AMOL= 1.0D0/(FA+BEFF)
      K  = 0
      KK = 0
 1    CALL SMBER(H,SMT1)
      IF(ABS(SM-SMT1) .GT. 1.D-6) THEN
        CALL SMBER(H+1.0D0,SMT2)
        DH= (SM-SMT1)/(SMT2-SMT1)
        H = H+DH
        KK = KK+1
           IF(KK.GT.20)STOP  ' NO CONVERGENCY  #1'
        GO TO 1
      END IF
      X11 = X1*X1
      X12 = X1*X2
      X13 = X1*X3
      X22 = X2*X2
      X23 = X2*X3
      X25 = X2*X5
      X15 = X1*X5
      X17 = X1*X7
      CALL B11BER(T0,H,B11)
      CALL BBER(T0,B11,BEFF)
      AMOL= 1.0D0/(FA+BEFF)
      HSBER = X1*H*AMOL+(X5*H5+X7*H7)*AMOL
      IF(ABS(HS-HSBER).GT.1.0D-4) THEN
        K = K+1
        IF(K.GT.20)STOP   'NO CONVERGENCY  #2'
        GO TO 1
      END IF
      IF(X2.LT.-0.01 .OR. X2.GT.0.5) STOP    'CALC. N2 OUT OF RANGE'
      IF(X2+X3.GT.0.5) STOP    'N2 + CO2 OUT OF RANGE'
      IF(0.55+.4*X2+0.97*X3-0.45*X5).GT.RM)
     +                STOP    'CONFLICTING RESULT FOR N2'
      Q2 = X2
      T = TC+T0
      CALL B11BER(T,H,B11)
      CALL BBER(T,B11,B)
      CALL CBER(T,H,C)
```

```
      CALL ITER(P,T,B,C,V,Z)
      D = 1.0D0/V
      END
      SUBROUTINE SMBER(H,SM)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON /RBLOK/ AMOL,HS
      COMMON /XBLOK/ X1,X2,X3,X11,X12,X13,X22,X23,X33
     >              ,X5,X7,X15,X17,X25,X55,X77
      COMMON /MBLOK/ GM1R0,GM1R1,GM2,GM3,GM5,GM7,FA,FB,RL,T0,H5,H7,R
      GM1= GM1R0+GM1R1*H
      X1 = (HS-(X5*H5+X7*H7)*AMOL)/H/AMOL
      X2 = 1.0D0-X1-X3-X5-X7
      SM = (X1*GM1+X2*GM2+X3*GM3+X5*GM5+X7*GM7)*AMOL
      END
C
C     ******************************************************************
      SUBROUTINE B11BER(T,H,B11)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON /BBLOK/ BR11H0(3), BR11H1(3), BR11H2(3), BR22(3), BR23(3),
     +               BR33(3), BR15(3), BR17(3), BR55(3), BR77(3), B25
      T2=T*T
      B11=BR11H0(1) + BR11H0(2)*T + BR11H0(3)*T2
     +  +(BR11H1(1) + BR11H1(2)*T + BR11H1(3)*T2)*H
     +  +(BR11H2(1) + BR11H2(2)*T + BR11H2(3)*T2)*H*H
      END
C     ******************************************************************
      SUBROUTINE BBER(T,B11,BEFF)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON /BBLOK/ BR11H0(3), BR11H1(3), BR11H2(3), BR22(3), BR23(3),
     +               BR33(3), BR15(3), BR17(3), BR55(3), BR77(3), B25
      COMMON/ZETA/   Z12,Z13,Y12,Y13,Y123,Y115
      COMMON /XBLOK/ X1,X2,X3,X11,X12,X13,X22,X23,X33
     >              ,X5,X7,X15,X17,X25,X55,X77
      T2=T*T
      B22=BR22(1) + BR22(2)*T + BR22(3)*T2
      B23=BR23(1) + BR23(2)*T + BR23(3)*T2
      B33=BR33(1) + BR33(2)*T + BR33(3)*T2
      B15=BR15(1) + BR15(2)*T + BR15(3)*T2
      B55=BR55(1) + BR55(2)*T + BR55(3)*T2
      B17=BR17(1) + BR17(2)*T + BR17(3)*T2
      B77=BR77(1) + BR77(2)*T + BR77(3)*T2
      BA13= B11*B33
      IF (BA13 .LT. 0.0) STOP  ' NO SOLUTION'
      ZZZ=Z12+(320.0D0-T)**2*1.875D-5
      BEFF =  X11*B11 + X12*ZZZ*(B11+B22) + 2.0D0*X13*Z13*DSQRT(BA13)
     >       +X22*B22 +    2.0D0*X23*B23  + X33*B33       + X55*B55
     > +2.0D0*X15*B15 +    2.0D0*X25*B25  + 2.0D0*X17*B17 + X77*B77
      END
C     ******************************************************************
      SUBROUTINE CBER(T,H,CEFF)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON /CBLOK/ CR111H0(3), CR111H1(3), CR111H2(3), CR222(3),
     +               CR223(3), CR233(3),  CR333(3), CR555(3), CR117(3)
      COMMON /ZETA/  Z12,Z13,Y12,Y13,Y123,Y115
      COMMON /XBLOK/ X1,X2,X3,X11,X12,X13,X22,X23,X33
     >              ,X5,X7,X15,X17,X25,X55,X77
      T2=T*T
      C111=CR111H0(1) + CR111H0(2)*T + CR111H0(3)*T2
     +   +(CR111H1(1) + CR111H1(2)*T + CR111H1(3)*T2)*H
     +   +(CR111H2(1) + CR111H2(2)*T + CR111H2(3)*T2)*H*H
      C222 = CR222(1) +   CR222(2)*T +   CR222(3)*T2
      C223 = CR223(1) +   CR223(2)*T +   CR223(3)*T2
      C233 = CR233(1) +   CR233(2)*T +   CR233(3)*T2
      C333 = CR333(1) +   CR333(2)*T +   CR333(3)*T2
      C555 = CR555(1) +   CR555(2)*T +   CR555(3)*T2
```

```
      C117 = CR117(1) +   CR117(2)*T +   CR117(3)*T2
      CA112=C111*C111*C222
      CA113=C111*C111*C333
      CA122=C111*C222*C222
      CA123=C111*C222*C333
      CA133=C111*C333*C333
      CA115=C111*C111*C555
      IF (CA112.LT.0.0  .OR.  CA113.LT.0.0  .OR.  CA122.LT.0.0
     +    .OR.  CA123.LT.0.0  .OR.  CA133.LT.0.0 .OR. CA115. LT. 0.0)
     +    STOP  ' NO SOLUTION'
      D3REP=1.0D0/3.0D0
      CEFF=X1*X11*C111 +3.0D0*X11*X2*(CA112)**D3REP*(Y12+(T-270.0D0)
     +   *0.0013D0)
     +   + 3.0D0*X11*X3  *(CA113)**D3REP  *Y13
     +   + 3.0D0*X1*X15  *(CA115)**D3REP  *Y115
     +   + 3.0D0*X1*X22  *(CA122)**D3REP  *(Y12+(T-270.0D0)*0.0013D0)
     +    +6.0D0*X1*X2*X3*(CA123)**D3REP  *Y123
     +    +3.0D0*X1*X33  *(CA133)**D3REP  *Y13
     +    +X22*X2*C222 + 3.0D0*X22*X3*C223 + 3.0D0*X2*X33*C233
     +    +X3*X33*C333 +       X5*X55*C555 + 3.0D0*X11*X7*C117
      RETURN
      END
C     ********************************************************************
      SUBROUTINE ITER(P,T,B,C,V,Z)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON /MBLOK/ GM1R0,GM1R1,GM2,GM3,GM5,GM7,FA,FB,RL,T0,H5,H7,R
      RT = R*T
      RTP= RT/P
      V  = RTP+B
      KK = 0
  5   V  = RTP*(1.0D0+B/V+C/V**2)
      KK = KK+1
      IF (KK .GT. 20) STOP  ' NO CONVERGENCY #3'
      Z  = 1.0D0+B/V+C/V**2
      PA = RT/V*Z
      IF(ABS(PA-P) .GE. 1.D-5)GO TO 5
      RETURN
      END
C     ********************************************************************
      BLOCK DATA
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON /BBLOK/ BR11H0(3), BR11H1(3), BR11H2(3), BR22(3), BR23(3),
     +               BR33(3), BR15(3), BR17(3), BR55(3), BR77(3), B25
      COMMON /CBLOK/ CR111H0(3), CR111H1(3), CR111H2(3), CR222(3),
     +               CR223(3), CR233(3),  CR333(3), CR555(3), CR117(3)
      COMMON /ZETA/  Z12,Z13,Y12,Y13,Y123,Y115
      COMMON /MBLOK/ GM1R0,GM1R1,GM2,GM3,GM5,GM7,FA,FB,RL,T0,H5,H7,R
      DATA BR11H0/-0.425468D0, 0.286500D-2, -.462073D-5 /,
     +     BR11H1/0.877118D-3, -.556281D-5, 0.881510D-8 /,
     +     BR11H2/-.824747D-6, 0.431436D-8, -.608319D-11/,
     +     BR22 / -.144600D0 , 0.740910D-3, -.911950D-6 /,
     +     BR23 / -.339693D0 , 0.161176D-2, -.204429D-5 /,
     +     BR33 / -.868340D0 , 0.403760D-2, -.516570D-5 /,
     +     BR15 / -.521280D-1, 0.271570D-3, -.25   D-6 /,
     +     BR17 / -.687290D-1, -.239381D-5, 0.518195D-6 /,
     +     BR55 / -.110596D-2, 0.813385D-4, -.987220D-7 /,
     +     BR77 / -.130820D0 , 0.602540D-3, -.644300D-6 /,
     +     B25  / 0.012D0 /
      DATA CR111H0/ -.302488D0 , 0.195861D-2, -.316302D-5 /,
     +     CR111H1/ 0.646422D-3, -.422876D-5, 0.688157D-8 /,
     +     CR111H2/ -.332805D-6, 0.223160D-8, -.367713D-11/,
     +     CR222 /  0.784980D-2, -.398950D-4, 0.611870D-7 /,
     +     CR223 /  0.552066D-2, -.168609D-4, 0.157169D-7 /,
     +     CR233 /  0.358783D-2, 0.806674D-5, -.325798D-7 /,
     +     CR333 /  0.205130D-2, 0.348880D-4, -.837030D-7 /,
```

```
     +     CR555 /  0.104711D-2, -.364887D-5,  .467095D-8 /,
     +     CR117 /  0.736748D-2, -.276578D-4,  .343051D-7 /
      DATA  Z12 /   0.72D0 /, Z13 / -.865D0/,
     +      Y12 /   0.92D0 /, Y13 /  0.92D0/, Y123 /1.10D0/,
     +      Y115/   1.2D0/
      DATA GM1R0/-2.709328D0/, GM1R1/.021062199D0/,
     +     GM2  /  28.0135D0/, GM3  /    44.010D0/,
     +     GM5  /   2.0159D0/, GM7  /    28.010D0/,
     +     FA   /22.414097D0/, FB   / 22.710811D0/,
     +     RL   / 1.292923D0/, T0   /    273.15D0/,
     +     H5   /   285.83D0/, H7   /    282.98D0/
     +     R    /0.0831451D0/
      END
C
C
```

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