# INTERNATIONAL STANDARD

# ISO
# 12213-3

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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 au moyen des caractéristiques physiques*

ISO 12213-3:1997(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.

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.

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

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*

Annexes A to D form an integral part of this part of ISO 12213. Annexes E to G are for information only.

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# Natural gas — Calculation of compression factor —

## Part 3:
Calculation using physical properties

## 1  Scope

This International Standard 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 $\pm$ 0,1 %. For wider-ranging applications the uncertainty of the results increases (see annex E).

More detail concerning the scope and field of application of the method is given in part 1 of this International Standard.

## 2  Normative references

The following standards contain provisions which, through reference in this text, constitute provisions of this part of ISO 12213. At the time of publication, the editions indicated were valid. All standards are subject to revision, and parties to agreements based on this part of ISO 12213 are encouraged to investigate the possibility of applying the most recent editions of the standards indicated below. Members of IEC and ISO maintain registers of currently valid International Standards.

ISO 31-3:1992, *Quantities and units — Part 3: Mechanics*.

ISO 31-4:1992, *Quantities and units — Part 4: Heat*.

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

ISO 12213-1:1997, *Natural gas — Calculation of compression factor — Part 1: Introduction and guidelines*.

## 3  Definitions

All definitions relevant to the use of this part of ISO 12213 are given in part 1.

## 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

$$Z = 1 + B\rho_m + C\rho_m^2 \qquad \qquad \qquad \text{. .  (1)}$$

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 ($CO_2$ and $H_2$) and the temperature $T$;

  $\rho_m$   is the molar density given by

$$\rho_m = p/(ZRT) \qquad \qquad \qquad \text{. . . (2)}$$

  where

$$Z = f_1\,(p, T, H_S, d, x_{CO_2}, x_{H_2}) \qquad \qquad \qquad \text{. . . (3)}$$

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

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

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 ($x_{H_2} < 0,001$), then set $x_{H_2} = 0$. 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.

**2**

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 $\rho_m$ 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 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 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 MPa | $\leqslant p$ | $\leqslant$ 12 MPa |
| temperature | 263 K | $\leqslant T$ | $\leqslant$ 338 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 MJ·m$^{-3}$ | $\leqslant H_S$ | $\leqslant$ 45 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:

| | | | |
|---|---|---|---|
| methane | $0,7 \leqslant x_{CH_4}$ | $\leqslant$ 1,0 |
| nitrogen | $0 \leqslant x_{N_2}$ | $\leqslant$ 0,20 |
| ethane | $0 \leqslant x_{C_2H_6}$ | $\leqslant$ 0,10 |
| propane | $0 \leqslant x_{C_3H_8}$ | $\leqslant$ 0,035 |
| butanes | $0 \leqslant x_{C_4H_{10}}$ | $\leqslant$ 0,015 |

| pentanes | 0 | $\leqslant x_{C_5H_{12}} \leqslant 0,005$ |
|---|---|---|
| hexanes | 0 | $\leqslant x_{C_6} \leqslant 0,001$ |
| heptanes | 0 | $\leqslant x_{C_7} \leqslant 0,000\ 5$ |
| octanes plus higher hydrocarbons | 0 | $\leqslant x_{C_{8+}} \leqslant 0,000\ 5$ |
| carbon monoxide | 0 | $\leqslant x_{CO} \leqslant 0,03$ |
| helium | 0 | $\leqslant x_{He} \leqslant 0,005$ |
| water | 0 | $\leqslant x_{H_2O} \leqslant 0,000\ 15$ |

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, 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 MPa | $\leqslant p$ | $\leqslant 12$ MPa |
|---|---|---|---|
| temperature | 263 K | $\leqslant T$ | $\leqslant 338$ K |
| mole fraction of carbon dioxide | 0 | $\leqslant x_{CO_2} \leqslant 0,30$ | |
| mole fraction of hydrogen | 0 | $\leqslant x_{H_2} \leqslant 0,10$ | |
| superior calorific value | 20 MJ·m⁻³ | $\leqslant H_S \leqslant 48$ MJ·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 | $\leqslant x_{CH_4} \leqslant 1,0$ |
|---|---|---|
| nitrogen | 0 | $\leqslant x_{N_2} \leqslant 0,50$ |
| ethane | 0 | $\leqslant x_{C_2H_6} \leqslant 0,20$ |
| propane | 0 | $\leqslant x_{C_3H_8} \leqslant 0,05$ |

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.
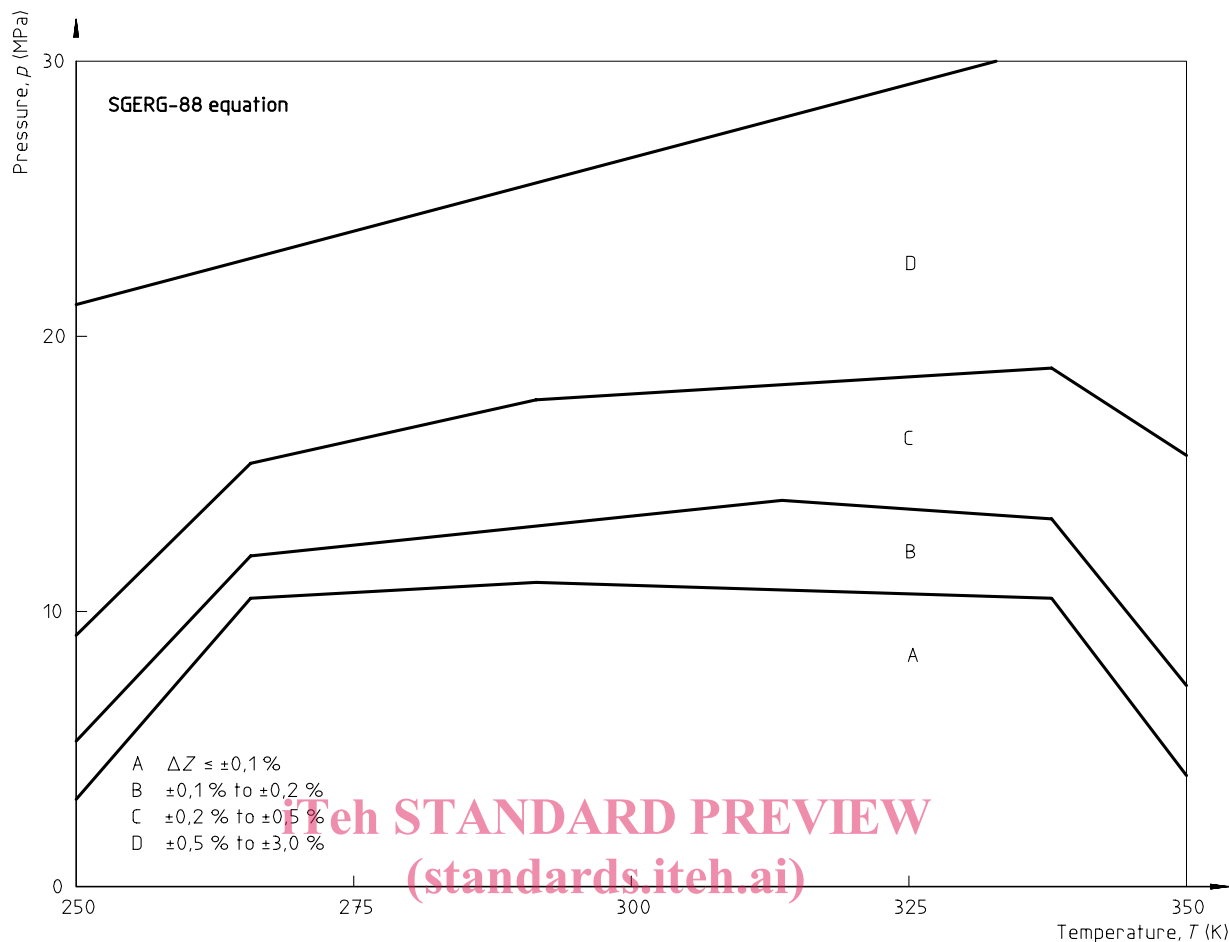
## 4.5 Uncertainty

### 4.5.1 Uncertainty for pipeline quality gas

The uncertainty in the prediction of the compression factor $\Delta Z$ (for the temperature range 263 K to 338 K) is $\pm 0,1$ % at pressures up to 10 MPa and $\pm 0,2$ % between 10 MPa and 12 MPa for natural gases with $x_{N_2} \leqslant 0,20$, $x_{CO_2} \leqslant 0,09$, $x_{C_2H_6} \leqslant 0,10$ and $x_{H_2} \leqslant 0,10$, and for 30 MJ·m⁻³ $\leqslant H_S \leqslant 45$ MJ·m⁻³ and $0,55 \leqslant d \leqslant 0,80$, (see figure 1).

For gases with a $CO_2$ content exceeding 0,09, the uncertainty of $\pm 0,1$ % 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].

SGERG–88 equation

D

C

B

A

A  $\Delta Z \leqslant \pm 0{,}1\,\%$
B  $\pm 0{,}1\,\%$ to $\pm 0{,}2\,\%$
C  $\pm 0{,}2\,\%$ to $\pm 0{,}5\,\%$
D  $\pm 0{,}5\,\%$ to $\pm 3{,}0\,\%$

Pressure, $p$ (MPa)

Temperature, $T$ (K)

**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 $x_2 \leqslant 0{,}20$; $x_{CO_2} \leqslant 0{,}09$; $x_{C_2H_6} \leqslant 0{,}10$ and $x_{H_2} \leqslant 0{,}10$, and for 30 MJ·m$^{-3} \leqslant H_S \leqslant 45$ MJ·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 E.

### 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 $\pm\,0{,}1\,\%$ 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 | $\pm\,0{,}02$ MPa |
| Temperature | $\pm\,0{,}15$ K |
| Mole fraction of carbon dioxide | $\pm\,0{,}002$ |
| Mole fraction of hydrogen | $\pm\,0{,}005$ |
| Relative density | $\pm\,0{,}001\ 3$ |
| Superior calorific value | $\pm\,0{,}06$ MJ·m$^{-3}$ |

## 5 Suppliers of computer programmes

It is planned to make software available which implements this International Standard. Users are invited to contact their ISO member body or ISO Central Secretariat to enquire about the availability of such software.

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

| Symbol | Meaning | Units |
|--------|---------|-------|
| $C_{ijk}$ | 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 (= $1/\rho_m$) | $m^3 \cdot kmol^{-1}$ |
| $x$ | Mole fraction of a component | — |
| $y$ | Combination rule parameters for the binary unlike-interaction virial coefficients $B_{12}$ and $B_{13}$ (table B.1) and the ternary unlike-interaction virial coefficient $C_{ijk}$ [equation (B.32)] | — |
| $Z$ | Compression factor | — |
| $\rho$ | Mass density [equations (B.8) and (B.42)] | $kg \cdot m^{-3}$ |
| $\rho_m$ | 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 $\rho$ 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) |