INTERNATIONAL STANDARD

ISO 12213-2

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Natural gas — Calculation of compression factor —

Part 2:
Calculation using molar-composition analysis

Gaz naturel — Calcul du facteur de compression —
Partie 2: Calcul par analyse de la composition molaire

Contents

Page

Annexes

International Organization for Standardization
Case postale 56 • CH-1211 Genève 20 • Switzerland
Internet central@iso.ch
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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 12213-2 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.

Natural gas — Calculation of compression factor —

Part 2:
Calculation using molar-composition analysis

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 detailed composition of the gas by mole fractions is known, together with the relevant pressures and temperatures.

The method is 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 %. It can be applied, with greater uncertainty, to wider ranges of gas composition, pressure and temperature (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 an equation based on the concept that pipeline quality natural gas may be uniquely characterized for calculation of its volumetric properties by component analysis. This analysis, together with the pressure and temperature, are used as input data for the method.

The method uses a detailed molar-composition analysis in which all constituents present in amounts exceeding a mole fraction of 0,000 05 should be represented. Typically, this includes all alkane hydrocarbons up to about C_7 or C_8 together with nitrogen, carbon dioxide and helium.

For other gases, additional components such as water vapour, hydrogen sulfide and ethylene need to be taken into consideration (see reference [1] in annex G).

For manufactured gases, hydrogen and carbon monoxide are also likely to be significant components.

4.2 The AGA8-92DC equation

The compression factor is determined using the AGA8 detailed characterization equation (denoted hereafter as the AGA8-92DC equation). This is an extended virial-type equation. The equation is described in AGA Report No. 8[1]. It may be written as

$$Z = 1 + B\rho_m - \rho_r \sum_{n=13}^{18} C_n^* + \sum_{n=13}^{58} C_n^* \left(b_n - c_n k_n \rho_r^{k_n}\right) \rho_r^{b_n} \exp\left(-c_n \rho_r^{k_n}\right) \quad \ldots (1)$$

where

Z is the compression factor;

B is the second virial coefficient;

ρ_m is the molar density (moles per unit volume);

ρ_r is the reduced density;

b_n, c_n, k_n are constants (see table B.1);

C_n^* are coefficients which are functions of temperature and composition.

The reduced density ρ_r is related to the molar density ρ_m by the equation

$$\rho_r = K^3 \rho_m \quad \ldots (2)$$

where K is a mixture size parameter.

The molar density can be written as

$$\rho_m = p/(ZRT) \quad \ldots (3)$$

where

p is the absolute pressure;

R is the universal gas constant;

T is the absolute temperature.

Z is calculated as follows: first the values of B and C_n^* (n = 13 to 58) are calculated, using relationships given in annex B. Equations (1) and (3) are then solved simultaneously for ρ_m and Z by a suitable numerical method (see figure B.1).

4.3 Input variables

The input variables required for use with the AGA8-92DC equation are the absolute pressure, absolute temperature and molar composition.

The composition is required, by mole fraction, of the following components: nitrogen, carbon dioxide, argon, methane, ethane, propane, *n*-butane, methyl-2-propane (iso-butane), *n*-pentane, methyl-2-butane (iso-pentane), hexanes, heptanes, octanes, nonanes, decanes, hydrogen, carbon monoxide, hydrogen sulfide, helium, oxygen and water.

NOTE — If the mole fractions of the heptanes, octanes, nonanes and decanes are unknown, then use of a composite C_{6+} fraction may be acceptable. The user should carry out a sensitivity analysis in order to test whether a particular approximation of this type degrades the result.

All components with mole fractions greater than 0,000 05 shall be accounted for. Trace components (such as ethylene) shall be treated as given in table 1.

If the composition is known by volume fractions, these shall be converted to mole fractions using the method given in ISO 6976. The sum of all mole fractions shall be unity to within 0,000 1.

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	$263 \text{ K} \leqslant T \leqslant 338 \text{ K}$
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 the natural-gas components shall be within the following ranges:

methane	$0{,}7 \leqslant x_{CH_4} \leqslant 1{,}00$
nitrogen	$0 \leqslant x_{N_2} \leqslant 0{,}20$
carbon dioxide	$0 \leqslant x_{CO_2} \leqslant 0{,}20$
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	$0 \leqslant x_{C_{8+}} \leqslant 0{,}000\,5$
hydrogen	$0 \leqslant x_{H_2} \leqslant 0{,}10$
carbon monoxide	$0 \leqslant x_{CO} \leqslant 0{,}03$
helium	$0 \leqslant x_{He} \leqslant 0{,}005$
water	$0 \leqslant x_{H_2O} \leqslant 0{,}000\,15$

Any component for which x_i is less than 0,000 05 can be neglected.

Minor and trace components are listed in table 1.

Table 1 — Minor and trace components

Minor or trace component	Assigned component
Oxygen	oxygen
Argon	argon
Hydrogen sulfide	hydrogen sulfide
Ethylene, acetylene	carbon dioxide
Propylene, propadiene	propane
Butenes, butadienes	*n*-butane
Neo-pentane, pentenes, benzene, cyclopentane	*n*-pentane
All C_6-isomers, cyclohexane, ethylbenzene, xylenes	*n*-hexane
All C_7-isomers, cycloheptane, toluene	*n*-heptane
All C_8-isomers	*n*-octane
All C_9-isomers	*n*-nonane
All C_{10}-isomers and all higher hydrocarbons	*n*-decane

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.

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	$\leqslant p \leqslant$	65 MPa
temperature	225 K	$\leqslant T \leqslant$	350 K
relative density	0,55	$\leqslant d \leqslant$	0,90
superior calorific value	20 MJ·m^{-3}	$\leqslant H_S \leqslant$	48 MJ·m^{-3}

The allowable mole fractions of the major natural gas components are:

methane	0,50	$\leqslant x_{CH_4} \leqslant$	1,00
nitrogen	0	$\leqslant x_{N_2} \leqslant$	0,50
carbon dioxide	0	$\leqslant x_{CO_2} \leqslant$	0,30
ethane	0	$\leqslant x_{C_2H_6} \leqslant$	0,20
propane	0	$\leqslant x_{C_3H_8} \leqslant$	0,05
hydrogen	0	$\leqslant x_{H_2} \leqslant$	0,10

The limits for minor and trace gas components are as given in 4.4.1 for pipeline quality gas. For use of the method outside these ranges, see annex E.

4.5 Uncertainty

4.5.1 Uncertainty for pipeline quality gas

The uncertainty of results for use on all pipeline quality gas within the limits described in 4.4.1 is ± 0,1 % (for the temperature range 263 K to 350 K and pressures up to 12 MPa) (see figure 1). For temperatures above 290 K and at pressures up to 30 MPa the uncertainty of the result is also ± 0,1 %.

For lower temperatures, the uncertainty of ± 0,1 % is at least maintained for pressures up to about 10 MPa.

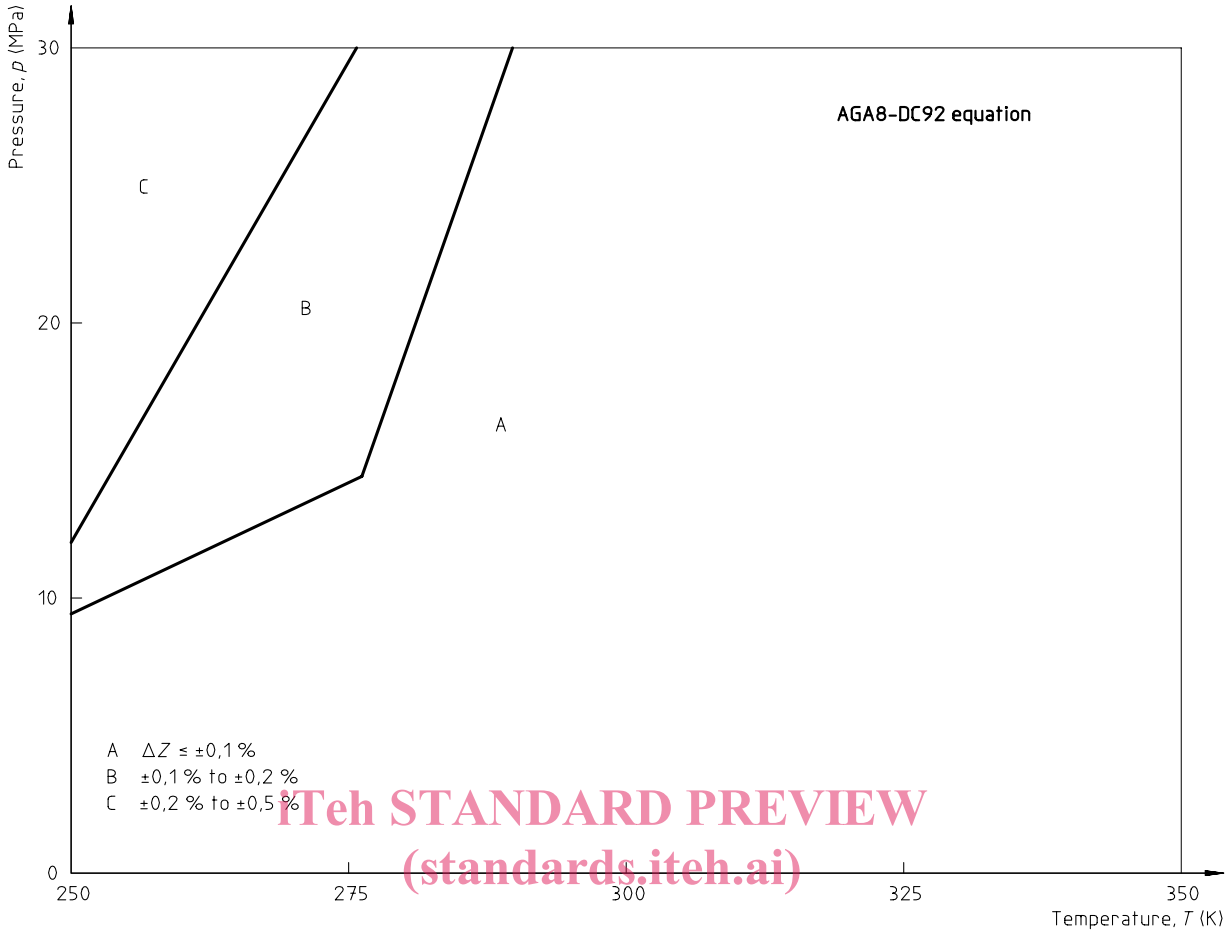

Figure 1 — Uncertainty limits for the calculation of compression factors (The uncertainty limits given are expected to be valid for natural gases and similar gases with $x_N \leqslant 0{,}20$, $x_{CO_2} \leqslant 0{,}20$, $x_{C_2H_6} \leqslant 0{,}10$ and $x_{H_2} \leqslant 0{,}10$, and for 30 MJ·m$^{-3} \leqslant H_S \leqslant$ 45 MJ·m^{-3} and $0{,}55 \leqslant d \leqslant 0{,}80$)

This uncertainty level has been determined by comparison with the GERG databank of measurements of the compression factor for natural gases [2], [3]. A detailed comparison was also made with the GRI PVT data on gravimetrically prepared simulated natural-gas mixtures [4], [5].

The uncertainty of the measurements in both databanks used to test the method is of the order of ± 0,1 %.

4.5.2 Uncertainty for wider ranges of application

The estimated uncertainties for calculations of compression factors beyond the limits of quality given in 4.4.1 are discussed in annex E.

4.5.3 Impact of uncertainties of input variables

Listed in table 2 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 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.

Table 2 — Uncertainties of input variables

Input variable	Absolute uncertainty
Absolute pressure	± 0,02 MPa
Temperature	± 0,15 K
Mole fraction of	
inerts	± 0,001
nitrogen	± 0,001
carbon dioxide	± 0,001
methane	± 0,001
ethane	± 0,001
propane	± 0,000 5
butanes	± 0,000 3
pentanes plus higher hydrocarbons	± 0,000 1
hydrogen and carbon monoxide	± 0,001

4.5.4 Reporting of results

Results for compression factor and molar density shall be reported to four and to five places of decimals, respectively, together with the pressure and temperature values and the calculation method used (ISO 12213-2, AGA8-92DC equation). For verification of calculation procedures, it is useful to carry extra digits.

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.

Annex A
(normative)

Symbols and units

Symbol	Meaning	Units
a_n	Constant in table B.1	—
B	Second virial coefficient	$m^3 \cdot kmol^{-1}$
B^*_{nij}	Mixture interaction coefficient [equations (B.1) and (B.2)]	—
B_n	Constant in table B.1	—
c_n	Constant in table B.1	—
C^*_n	Coefficients which are functions of temperature and composition	—
E_i	Characteristic energy parameter for ith component (table B.2)	K
E_j	Characteristic energy parameter for jth component (table B.2)	K
E_{ij}	Binary energy parameter for second virial coefficient	K
E^*_{ij}	Binary energy interaction parameter for second virial coefficient (table B.3)	—
F	Mixture high-temperature parameter	—
F_i	High-temperature parameter for ith component (table B.2)	—
F_j	High-temperature parameter for jth component (table B.2)	—
f_n	Constant in table B.1	—
G	Mixture orientation parameter	—
G_i	Orientation parameter for ith component (table B.2)	—
G_j	Orientation parameter for jth component (table B.2)	—
G_{ij}	Binary orientation parameter	—
G^*_{ij}	Binary interaction parameter for orientation (table B.2)	—
g_n	Constant in table B.1	—
H_S	Superior calorific value	$MJ \cdot m^3$
K	Size parameter	$(m^3/kmol)^{1/3}$
K_i	Size parameter for ith component (table B.2)	$(m^3/kmol)^{1/3}$
K_j	Size parameter for jth component (table B.2)	$(m^3/kmol)^{1/3}$
K_{ij}	Binary interaction parameter for size (table B.3)	—
k_n	Constant in table B.1	—
M	Molar mass	$kg \cdot kmol^{-1}$
M_i	Molar mass of ith component	$kg \cdot kmol^{-1}$
N	Number of components in gas mixture	
n	An integer (from 1 to 58)	—
p	Absolute pressure	MPa
Q	Quadrupole parameter	—
Q_i	Quadrupole parameter for ith component	—
Q_j	Quadrupole parameter for jth component	—
q_n	Constant (table B.1)	—
R	Gas constant (= 0,008 314 510)	$MJ \cdot (kmol \cdot K)^{-1}$
S_i	Dipole parameter for ith component (table B.2)	—
S_j	Dipole parameter for jth component (table B.2)	—
s_n	Constant (table B.1)	—

Symbol	Meaning	Units
T	Absolute temperature	K
U	Mixture energy parameter	K
U_{ij}	Binary interaction parameter for mixture energy (table B.3)	—
u_n	Constant in table B.1	—
W_i	Association parameter for ith component (table B.2)	—
W_j	Association parameter for jth component (table B.2)	—
w_n	Constant (table B.1)	—
x_i	Mole fraction of ith component in gas mixture	—
x_j	Mole fraction of jth component in gas mixture	—
Z	Compression factor	—
ρ	Mass density	$kg \cdot m^{-3}$
ρ_r	Reduced density of gas	—
ρ_m	Molar density	$kmol \cdot m^{-3}$