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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 à partir de l'analyse de la composition molaire

Reference number
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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 12213-2 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 12213-2:1997), Table 1 of which has been technically revised.

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*

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Natural gas — Calculation of compression factor —

Part 2:
Calculation using molar-composition analysis

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 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 $\pm$ 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 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, *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.

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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 the Bibliography).

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

$$Z = 1 + B\rho_{\mathrm{m}} - \rho_{\mathrm{r}} \sum_{n=13}^{18} C_n^* + \sum_{n=13}^{58} C_n^* \left(b_n - c_n k_n \rho_{\mathrm{r}}^{k_n} \right) \rho_{\mathrm{r}}^{b_n} \exp\left(-c_n \rho_{\mathrm{r}}^{k_n} \right) \tag{1}$$

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

$$\rho_{\mathrm{r}} = K^3 \rho_{\mathrm{m}} \tag{2}$$

where K is a mixture size parameter.

The molar density can be written as

$$\rho_{\mathrm{m}} = p / (ZRT) \tag{3}$$

where

p is the absolute pressure;

R is the universal gas constant;

T is the absolute temperature.

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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 MPa	$\leqslant p \leqslant$		12 MPa
temperature	263 K	$\leqslant T \leqslant$		338 K
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 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

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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 and trace component	Assigned component
Oxygen	Oxygen
Argon, neon, krypton, xenon	Argon
Hydrogen sulfide	Hydrogen sufide
Nitrous oxide	Carbon dioxide
Ammonia	Methane
Ethylene, acetylene, methanol (methyl alcohol), hydrogen cyanide	Ethane
Propylene, propadiene, methanethiol (methyl mercaptan)	Propane
Butenes, butadienes, carbonyl sulfide (carbon oxysulfide), sulfur dioxide	*n*-Butane
Neo-pentane, pentenes, benzene, cyclopentane, carbon disulfide	*n*-Pentane
All C_6–isomers, cyclohexane, toluene, methylcyclopentane	*n*-Hexane
All C_7–isomers, ethylcyclopentane, methylcyclohexane, cycloheptane, ethylbenzene, xylenes	*n*-Heptane
All C_8–isomers, ethylcyclohexane	*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}

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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 $\pm$ 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 $\pm$ 0,1 %.

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

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 $\pm$ 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.

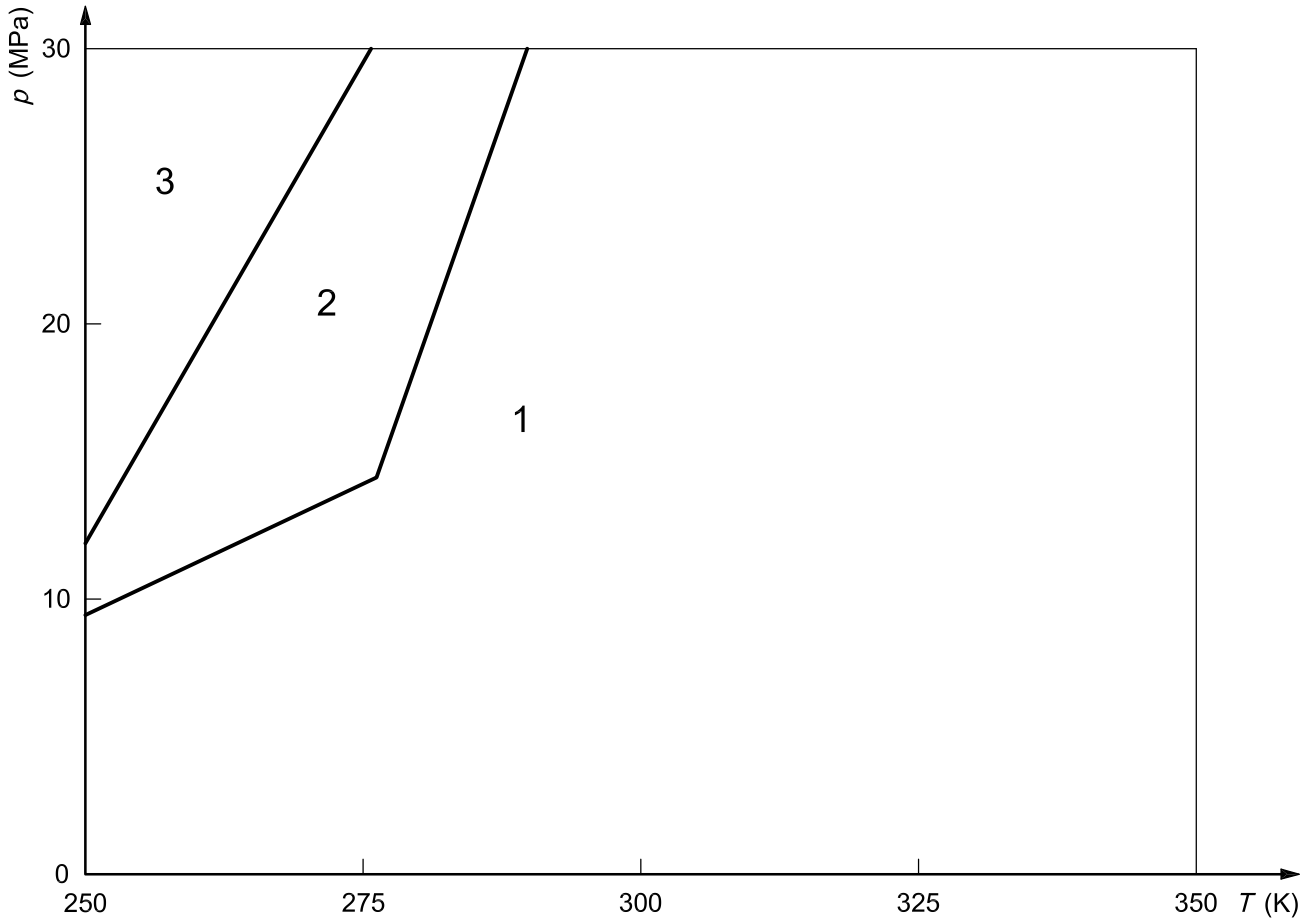
4.5.3 Impact of uncertainties of input variables

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 $\pm$ 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.

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AGA8-DC92 equation

Key

p pressure

T temperature

1 ΔZ $\leqslant \pm 0{,}1$ %

2 ΔZ $\pm 0{,}1$ % to $\pm 0{,}2$ %

3 ΔZ $\pm 0{,}2$ % to $\pm 0{,}5$ %

NOTE The uncertainty limits given are expected to be valid for natural gases and similar gases with $x_{N_2} \leqslant 0{,}20$, $x_{CO_2} \leqslant 0{,}20$, $x_{C_2H_6} \leqslant 0{,}10$ and $x_{H_2} \leqslant 0{,}10$, and for 30 MJ·m^{-3} $\leqslant H_S \leqslant$ 45 MJ·m^{-3} and $0{,}55 \leqslant d \leqslant 0{,}80$.

Figure 1 — Uncertainty limits for the calculation of compression factors

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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 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.

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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	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	—
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	—
G_{ij}	Binary orientation parameter	—
G^*_{ij}	Binary interaction parameter for orientation (Table B.3)	—
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	$(m^3/kmol)^{1/3}$
K_{ij}	Binary interaction parameter for size (Table B.3)	—
k_n	Constant in Table B.1	—

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Symbol	Meaning	Units
M	Molar mass	kg·kmol^{-1}
M_i	Molar mass of ith component	kg·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·(kmol·K)$^{-1}$
S_i	Dipole parameter for ith component (Table B.2)	—
S_j	Dipole parameter for jth component	—
s_n	Constant (Table B.1)	—
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	—
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·m^{-3}
ρ_r	Reduced density of gas	—
ρ_m	Molar density	kmol·m^{-3}

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Annex B
(normative)

Description of the AGA8-92DC method

B.1 General

For gas mixtures, the compression factor Z is calculated using the equations given in 4.2. This annex gives a detailed description of the computations and the necessary numerical values. The description is based upon that given in AGA Report No. 8 [1]. A program implementing this description is given in Annex F, and as such provides the correct solution. Other computational procedures are acceptable provided that they can be demonstrated to yield identical numerical results (see Annex C for examples).

B.2 Computer implementation of the AGA8-92DC method

B.2.1 Overview of the calculation procedure

I Input the absolute temperature T, absolute pressure p and mole fraction of each component x_i of the mixture.

NOTE For pressure and temperature, values known in any other units will first have to be converted precisely to values in megapascals and kelvins, respectively (see ISO 80000-4 and ISO 80000-5 and Annex D for relevant conversion factors).

II Compute the equation of state coefficients B and C_n^* (n = 13 to 58) that depend on T and x_i.

III Solve iteratively for the molar density ρ_m, using the equation of state rearranged to give the pressure p.

IV Output the compression factor after the computed pressure from step III and the input pressure from step I agree within a specified range of convergence (e.g. 1E-06).

Figure B.1 shows a flow diagram of these steps.

B.2.2 Details of the calculation procedure

Step I

Input the absolute temperature T, absolute pressure p and mole fraction x_i of each constituent in the natural-gas mixture.

Step II

At the absolute temperature T and the mole fractions x_i of the natural gas (as input from step I), compute the composition- and temperature-dependent coefficients B and C_n^* (n = 13 to 58).

The second virial coefficient B is given by the following equations:

$$B = \sum_{n=1}^{18} a_n T^{-u_n} \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j B_{nij}^{*} E_{ij}^{u_n} \left(K_i K_j\right)^{3/2} \tag{B.1}$$

$$B_{nij}^{*} = \left(G_{ij} + 1 - g_n\right)^{g_n} \left(Q_i Q_j + 1 - q_n\right)^{q_n} \left(F_i^{1/2} F_j^{1/2} + 1 - f_n\right)^{f_n} \left(S_i S_j + 1 - s_n\right)^{s_n} \left(W_i W_j + 1 - w_n\right)^{w_n} \tag{B.2}$$

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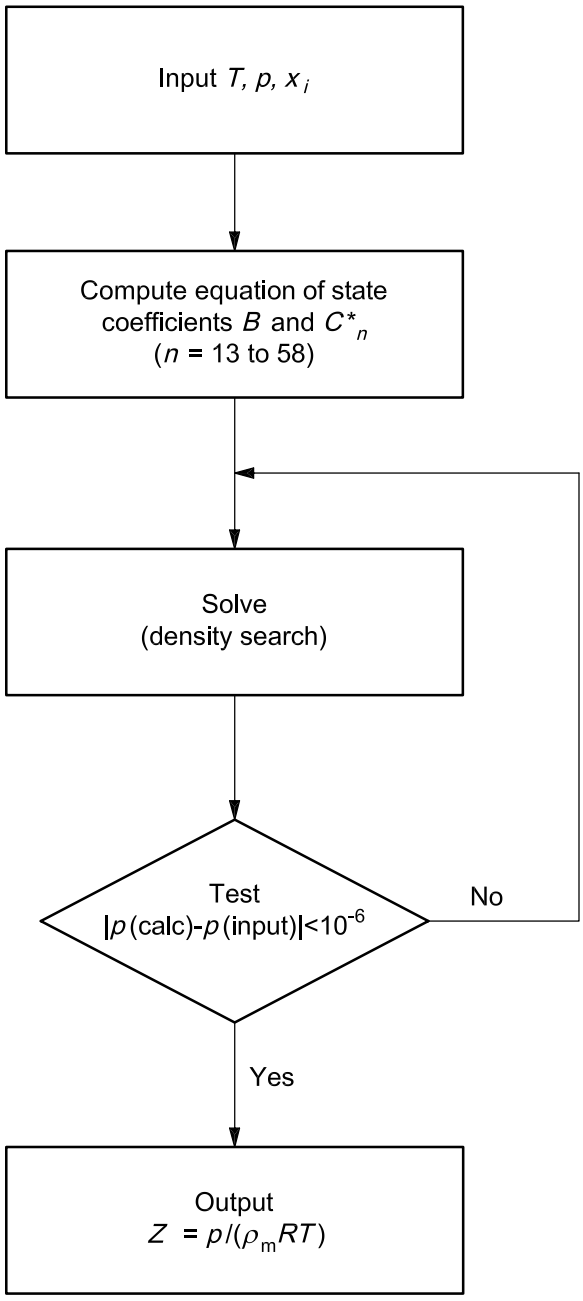


Figure B.1 — AGA8-92DC equation — Calculation flow diagram

The binary parameters E_{ij} and G_{ij} are calculated using the following equations:

$$E_{ij} = E^*_{ij}\left(E_i E_j\right)^{1/2} \tag{B.3}$$

$$G_{ij} = G^*_{ij}\left(G_i + G_j\right)/2 \tag{B.4}$$

Note that all values of the binary interaction parameters E^*_{ij} and G^*_{ij} are 1,0 except for the values given in Table B.3.

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The coefficients C_n^* (n = 13 to 58) are given by the equation:

$$C_n^* = a_n \left(G + 1 - g_n\right)^{g_n} \left(Q^2 + 1 - q_n\right)^{q_n} \left(F + 1 - f_n\right)^{f_n} U^{u_n} T^{-u_n} \tag{B.5}$$

The mixture parameters U, G, Q and F are calculated using the following conformal solution mixing equations, where in the double sums i ranges from 1 to $N - 1$ and, for each value of i, j ranges from i + 1 to N:

$$U^5 = \left(\sum_{i=1}^{N} x_i E_i^{5/2} \right)^2 + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} x_i x_j \left(U_{ij}^5 - 1\right)\left(E_i E_j\right)^{5/2} \tag{B.6}$$

$$G = \sum_{i=1}^{N} x_i G_i + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} x_i x_j \left(G_{ij}^* - 1\right)\left(G_i + G_j\right) \tag{B.7}$$

$$Q = \sum_{i=1}^{N} x_i Q_i \tag{B.8}$$

$$F = \sum_{i=1}^{N} x_i^2 F_i \tag{B.9}$$

It should be noted that all values of the binary interaction parameters K_{ij}, E_{ij}^*, G_{ij}^* and U_{ij} are 1,0 except for the values given in Table B.3. Also note that F_i is zero for all components except hydrogen, for which $F(H_2) = 1{,}0$, and that W_i is zero for all components except water, for which $W(H_2O) = 1{,}0$.

Step III

In the computation of the compression factor Z, the composition of the gas is known, the absolute temperature T of the gas is known and the absolute pressure is known. The problem then is to compute the molar density ρ_m, using the equation of state expression for the pressure p. For this purpose, the definition of the compression factor Z as given in Equation (1) (see 4.2) is substituted into Equation (3) to obtain an equation for the pressure as given in Equation (B.10):

$$p = \rho_m RT \left[1 + B\rho_m - \rho_r \sum_{n=13}^{18} C_n^* + \sum_{n=13}^{58} C_n^* \left(b_n - c_n k_n \rho_r^{k_n}\right) \rho_r^{b_n} \exp\left(- c_n \rho_r^{k_n}\right) \right] \tag{B.10}$$

Equation (B.10) is solved using standard equation of state density search algorithms. Having obtained an equation for the pressure p [Equation (B.10)], the problem is then to search for the value of the molar density ρ_m that will yield the pressure that is within a preset limit (e.g. 1×10^{-6}) equal to the input pressure.

The reduced density ρ_r is related to the molar density ρ_m by the mixture size parameter [see Equation (2) in 4.2].

The mixture size parameter K is calculated using the following equation:

$$K^5 = \left(\sum_{i=1}^{N} x_i K_i^{5/2} \right)^2 + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} x_i x_j \left(K_{ij}^5 - 1\right)\left(K_i K_j\right)^{5/2} \tag{B.11}$$

Note that in the summations the subscript i refers to the ith component in the gas mixture and the subscript j refers to the jth component in the gas mixture. The quantity N is the number of components in the mixture. Thus, in the single summation, i ranges over the integer values from 1 to N. For example, for a mixture of 12 components, $N = 12$ and there would be 12 terms in the single sum. In the double summation, i ranges

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from 1 to $N-1$ and, for each value of i, j ranges from $i+1$ to N. For example, for a mixture of 12 components, there would be 66 terms in the double summation if all values of K_{ij} differed from 1,0. However, because many of the values of K_{ij} are 1,0, the number of non-zero terms in the double summation is small for many natural-gas mixtures. Note that all values of K_{ij} are 1,0 except for the values given in Table B.3.

Step IV

Once the molar density ρ_{m} has been obtained in step III, the compression factor is calculated in step IV using the pressure, temperature, molar density and gas constant:

$$Z = p/\left(\rho_{\mathrm{m}} RT\right) \tag{B.12}$$

NOTE The density ρ (mass per unit volume) can be calculated as follows:

$$\rho = M\rho_{\mathrm{m}} \tag{B.13}$$

where M is calculated from the equation:

$$M = \sum_{i=1}^{N} x_i M_i \tag{B.14}$$

Report the density to three places of decimals.

Table B.1 — Equation of state parameters

n	a_n	b_n	c_n	k_n	u_n	g_n	q_n	f_n	s_n	w_n
1	0,153 832 600	1	0	0	0,0	0	0	0	0	0
2	1,341 953 000	1	0	0	0,5	0	0	0	0	0
3	− 2,998 583 000	1	0	0	1,0	0	0	0	0	0
4	− 0,048 312 280	1	0	0	3,5	0	0	0	0	0
5	0,375 796 500	1	0	0	− 0,5	1	0	0	0	0
6	− 1,589 575 000	1	0	0	4,5	1	0	0	0	0
7	− 0,053 588 470	1	0	0	0,5	0	1	0	0	0
8	0,886 594 630	1	0	0	7,5	0	0	0	1	0
9	− 0,710 237 040	1	0	0	9,5	0	0	0	1	0
10	− 1,471 722 000	1	0	0	6,0	0	0	0	0	1
11	1,321 850 350	1	0	0	12,0	0	0	0	0	1
12	− 0,786 659 250	1	0	0	12,5	0	0	0	0	1
13	$2{,}291\,290 \times 10^{-9}$	1	1	3	− 6,0	0	0	1	0	0
14	0,157 672 400	1	1	2	2,0	0	0	0	0	0
15	− 0,436 386 400	1	1	2	3,0	0	0	0	0	0
16	− 0,044 081 590	1	1	2	2,0	0	1	0	0	0
17	− 0,003 433 888	1	1	4	2,0	0	0	0	0	0
18	0,032 059 050	1	1	4	11,0	0	0	0	0	0
19	0,024 873 550	2	0	0	− 0,5	0	0	0	0	0
20	0,073 322 790	2	0	0	0,5	0	0	0	0	0
21	− 0,001 600 573	2	1	2	0,0	0	0	0	0	0

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Table B.1 (*continued*)

n	a_n	b_n	c_n	k_n	u_n	g_n	q_n	f_n	s_n	w_n
22	0,642 470 600	2	1	2	4,0	0	0	0	0	0
23	− 0,416 260 100	2	1	2	6,0	0	0	0	0	0
24	− 0,066 899 570	2	1	4	21,0	0	0	0	0	0
25	0,279 179 500	2	1	4	23,0	1	0	0	0	0
26	− 0,696 605 100	2	1	4	22,0	0	1	0	0	0
27	− 0,002 860 589	2	1	4	− 1,0	0	0	1	0	0
28	− 0,008 098 836	3	0	0	− 0,5	0	1	0	0	0
29	3,150 547 000	3	1	1	7,0	1	0	0	0	0
30	0,007 224 479	3	1	1	− 1,0	0	0	1	0	0
31	− 0,705 752 900	3	1	2	6,0	0	0	0	0	0
32	0,534 979 200	3	1	2	4,0	1	0	0	0	0
33	− 0,079 314 910	3	1	3	1,0	1	0	0	0	0
34	− 1,418 465 000	3	1	3	9,0	1	0	0	0	0
35	$-5{,}999\,05 \times 10^{-17}$	3	1	4	− 13,0	0	0	1	0	0
36	0,105 840 200	3	1	4	21,0	0	0	0	0	0
37	0,034 317 290	3	1	4	8,0	0	1	0	0	0
38	− 0,007 022 847	4	0	0	− 0,5	0	0	0	0	0
39	0,024 955 870	4	0	0	0,0	0	0	0	0	0
40	0,042 968 180	4	1	2	2,0	0	0	0	0	0
41	0,746 545 300	4	1	2	7,0	0	0	0	0	0
42	− 0,291 961 300	4	1	2	9,0	0	1	0	0	0
43	7,294 616 000	4	1	4	22,0	0	0	0	0	0
44	− 9,936 757 000	4	1	4	23,0	0	0	0	0	0
45	− 0,005 399 808	5	0	0	1,0	0	0	0	0	0
46	− 0,243 256 700	5	1	2	9,0	0	0	0	0	0
47	0,049 870 160	5	1	2	3,0	0	1	0	0	0
48	0,003 733 797	5	1	4	8,0	0	0	0	0	0
49	1,874 951 000	5	1	4	23,0	0	1	0	0	0
50	0,002 168 144	6	0	0	1,5	0	0	0	0	0
51	− 0,658 716 400	6	1	2	5,0	1	0	0	0	0
52	0,000 205 518	7	0	0	− 0,5	0	1	0	0	0
53	0,009 776 195	7	1	2	4,0	0	0	0	0	0
54	− 0,020 487 080	8	1	1	7,0	1	0	0	0	0
55	0,015 573 220	8	1	2	3,0	0	0	0	0	0
56	0,006 862 415	8	1	2	0,0	1	0	0	0	0
57	− 0,001 226 752	9	1	2	1,0	0	0	0	0	0
58	0,002 850 908	9	1	2	0,0	0	1	0	0	0

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Table B.2 — Characterization parameters

Identification number	Compound	Molar mass M_i kg·kmol^{-1}	Energy parameter E_i K	Size parameter K_i (m^3/kmol)$^{1/3}$	Orientation parameter G_i	Quadrupole parameter Q_i	High-temp. parameter F_i	Dipole parameter S_i	Association parameter W_i
1	Methane	16,043 0	151,318 300	0,461 925 5	0,0	0,0	0,0	0,0	0,0
2	Nitrogen	28,013 5	99,737 780	0,447 915 3	0,027 815	0,0	0,0	0,0	0,0
3	Carbon dioxide	44,010 0	241,960 600	0,455 748 9	0,189 065	0,690 000	0,0	0,0	0,0
4	Ethane	30,070 0	244,166 700	0,527 920 9	0,079 300	0,0	0,0	0,0	0,0
5	Propane	44,097 0	298,118 300	0,583 749 0	0,141 239	0,0	0,0	0,0	0,0
6	Water	18,015 3	514,015 600	0,382 586 8	0,332 500	1,067 750	0,0	1,582 200	1,0
7	Hydrogen sulfide	34,082 0	296,355 000	0,461 826 3	0,088 500	0,633 276	0,0	0,390 000	0,0
8	Hydrogen	2,015 9	26,957 940	0,351 491 6	0,034 369	0,0	1,0	0,0	0,0
9	Carbon monoxide	28,010 0	105,534 800	0,453 389 4	0,038 953	0,0	0,0	0,0	0,0
10	Oxygen	31,998 8	122,766 700	0,418 695 4	0,021 000	0,0	0,0	0,0	0,0
11	iso-Butane	58,123 0	324,068 900	0,640 693 7	0,256 692	0,0	0,0	0,0	0,0
12	*n*-Butane	58,123 0	337,638 900	0,634 142 3	0,281 835	0,0	0,0	0,0	0,0
13	iso-Pentane	72,150 0	365,599 900	0,673 857 7	0,332 267	0,0	0,0	0,0	0,0
14	*n*-Pentane	72,150 0	370,682 300	0,679 830 7	0,366 911	0,0	0,0	0,0	0,0
15	*n*-Hexane	86,177 0	402,636 293	0,717 511 8	0,289 731	0,0	0,0	0,0	0,0
16	*n*-Heptane	100,204 0	427,722 630	0,752 518 9	0,337 542	0,0	0,0	0,0	0,0
17	*n*-Octane	114,231 0	450,325 022	0,784 955 0	0,383 381	0,0	0,0	0,0	0,0
18	*n*-Nonane	128,258 0	470,840 891	0,815 273 1	0,427 354	0,0	0,0	0,0	0,0
19	*n*-Decane	142,285 0	489,558 373	0,843 782 6	0,469 659	0,0	0,0	0,0	0,0
20	Helium	4,002 6	2,610 111	0,358 988 8	0,0	0,0	0,0	0,0	0,0
21	Argon	39,948 0	119,629 900	0,421 655 1	0,0	0,0	0,0	0,0	0,0

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Table B.3 — Binary interaction parameter values

Identification number		Component pair	E_{ij}^{*}	U_{ij}	K_{ij}	G_{ij}^{*}
i	j					
1	2	Methane + nitrogen	0,971 640	0,886 106	1,003 630	
	3	carbon dioxide	0,960 644	0,963 827	0,995 933	0,807 653
	4	ethane				
	5	propane	0,994 635	0,990 877	1,007 619	
	6	water	0,708 218			
	7	hydrogen sulfide	0,931 484	0,736 833	1,000 080	
	8	hydrogen	1,170 520	1,156 390	1,023 260	1,957 310
	9	carbon monoxide	0,990 126			
	10	oxygen				
	11	iso-butane	1,019 530			
	12	*n*-butane	0,989 844	0,992 291	0,997 596	
	13	iso-pentane	1,002 350			
	14	*n*-pentane	0,999 268	1,003 670	1,002 529	
	15	*n*-hexane	1,107 274	1,302 576	0,982 962	
	16	*n*-heptane	0,880 880	1,191 904	0,983 565	
	17	*n*-octane	0,880 973	1,205 769	0,982 707	
	18	*n*-nonane	0,881 067	1,219 634	0,981 849	
	19	*n*-decane	0,881 161	1,233 498	0,980 991	
2	3	Nitrogen + carbon dioxide	1,022 740	0,835 058	0,982 361	0,982 746
	4	ethane	0,970 120	0,816 431	1,007 960	
	5	propane	0,945 939	0,915 502		
	6	water	0,746 954			
	7	hydrogen sulfide	0,902 271	0,993 476	0,942 596	
	8	hydrogen	1,086 320	0,408 838	1,032 270	
	9	carbon monoxide	1,005 710			
	10	oxygen	1,021 000			
	11	iso-butane	0,946 914			
	12	*n*-butane	0,973 384	0,993 556		
	13	iso-pentane	0,959 340			
	14	*n*-pentane	0,945 520			
3	4	Carbon dioxide + ethane	0,925 053	0,969 870	1,008 510	0,370 296
	5	propane	0,960 237			
	6	water	0,849 408			1,673 090
	7	hydrogen sulfide	0,955 052	1,045 290	1,007 790	
	8	hydrogen	1,281 790			
	9	carbon monoxide	1,500 000	0,900 000		

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Table B.3 (*continued*)

Identification number		Component pair	E_{ij}^{*}	U_{ij}	K_{ij}	G_{ij}^{*}
i	*j*					
	10	oxygen				
	11	iso-butane	0,906 849			
	12	*n*-butane	0,897 362			
	13	iso-pentane	0,726 255			
	14	*n*-pentane	0,859 764			
	15	*n*-hexane	0,855 134	1,066 638	0,910 183	
	16	*n*-heptane	0,831 229	1,077 634	0,895 362	
	17	*n*-octane	0,808 310	1,088 178	0,881 152	
	18	*n*-nonane	0,786 323	1,098 291	0,867 520	
	19	*n*-decane	0,765 171	1,108 021	0,854 406	
4	5	Ethane + propane	1,022 560	1,065 173	0,986 893	
	6	water	0,693 168			
	7	hydrogen sulfide	0,946 871	0,971 926	0,999 969	
	8	hydrogen	1,164 460	1,616 660	1,020 340	
	9	carbon monoxide				
	10	oxygen				
	11	iso-butane		1,250 000		
	12	*n*-butane	1,013 060	1,250 000		
	13	iso-pentane		1,250 000		
	14	*n*-pentane	1,005 320	1,250 000		
5	8	Propane + hydrogen	1,034 787			
	12	*n*-butane	1,004 900			
7	15	Hydrogen sulfide + *n*-hexane	1,008 692	1,028 973	0,968130	
	16	*n*-heptane	1,010 126	1,033 754	0,962870	
	17	*n*-octane	1,011 501	1,038 338	0,957828	
	18	*n*-nonane	1,012 821	1,042 735	0,952 441	
	19	*n*-decane	1,014 089	1,046 966	0,948 338	
8	9	Hydrogen + carbon monoxide	1,100 000			
	10	oxygen				
	11	iso-butane	1,300 000			
	12	*n*-butane	1,300 000			

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Annex C
(normative)

Example calculations

The following example calculations have been carried out using the validated computer program described in Reference [1], which incorporates the subroutine described in Annex B.

Table C.1 — Gas analysis in mole fractions

	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_{N_2}	0,003	0,031	0,010	0,100	0,057	0,117
x_{H_2}	0,00	0,00	0,00	0,095	0,00	0,00
x_{CO}	0,00	0,00	0,00	0,010	0,00	0,00
x_{CH_4}	0,965	0,907	0,859	0,735	0,812	0,826
$x_{C_2H_6}$	0,018	0,045 0	0,085	0,033	0,043	0,035
$x_{C_3H_8}$	0,004 5	0,008 4	0,023	0,007 4	0,009	0,007 5
$x_{\text{iso-}C_4H_{10}}$	0,001 0	0,001 0	0,003 5	0,001 2	0,001 5	0,001 2
$x_{n\text{-}C_4H_{10}}$	0,001 0	0,001 5	0,003 5	0,001 2	0,001 5	0,001 2
$x_{\text{iso-}C_5H_{12}}$	0,000 5	0,000 3	0,000 5	0,000 4	0,00	0,000 4
$x_{n\text{-}C_5H_{12}}$	0,000 3	0,000 4	0,000 5	0,000 4	0,00	0,000 4
$x_{C_6H_{14}}$	0,000 7	0,000 4	0,00	0,000 2	0,00	0,000 2
$x_{C_7H_{16}}$	0,00	0,00	0,00	0,000 1	0,00	0,000 1
$x_{C_8H_{18}}$	0,00	0,00	0,00	0,000 1	0,00	0,00

Table C.2 — Results (Z-values)

Conditions		Gas 1	Gas 2	Gas 3	Gas 4	Gas 5	Gas 6
p	t						
bar	°C						
60	− 3,15	0,840 53	0,833 48	0,793 80	0,885 50	0,826 09	0,853 80
60	6,85	0,861 99	0,855 96	0,822 06	0,901 44	0,849 69	0,873 70
60	16,85	0,880 06	0,874 84	0,845 44	0,915 01	0,869 44	0,890 52
60	36,85	0,908 67	0,904 66	0,881 83	0,936 74	0,900 52	0,917 23
60	56,85	0,930 11	0,926 96	0,908 68	0,953 18	0,923 68	0,937 30
120	− 3,15	0,721 33	0,710 44	0,641 45	0,810 24	0,695 40	0,750 74
120	6,85	0,760 25	0,750 66	0,689 71	0,837 82	0,737 80	0,785 86
120	16,85	0,793 17	0,784 75	0,731 23	0,861 37	0,773 69	0,815 69
120	36,85	0,845 15	0,838 63	0,796 97	0,899 13	0,830 22	0,863 11
120	56,85	0,883 83	0,878 70	0,845 53	0,927 66	0,872 11	0,898 62

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Annex D
(normative)

Pressure and temperature conversion factors

If the input variables pressure and temperature are not in the necessary units of megapascals and kelvins, then conversions will have to be made in order to use the Fortran implementation. A selection of appropriate conversion factors is given below.

Pressure

p (MPa) = [p(bar)] × 10^{-1}

p (MPa) = [p(atm)] × 0,101 325

p (MPa) = [p(psia)]/145,038

p (MPa) = [p(psig) + 14,695 9]/145,038

Temperature

T (K) = t(°C) + 273,15

T (K) = [t(°F) − 32]/1,8 + 273,15

T (K) = [t(°R)]/1,8

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Annex E
(informative)

Performance over wider ranges of application

The AGA8-92DC equation has been comprehensively tested, over the temperature range 263 K to 338 K and at pressures up to 30 MPa, with the GERG data [2], [3] and the Gas Research Institute data [4] for gases within the ranges of composition given for pipeline quality gases (see 4.4.1). Within these limits, the uncertainties are as given in 4.5.

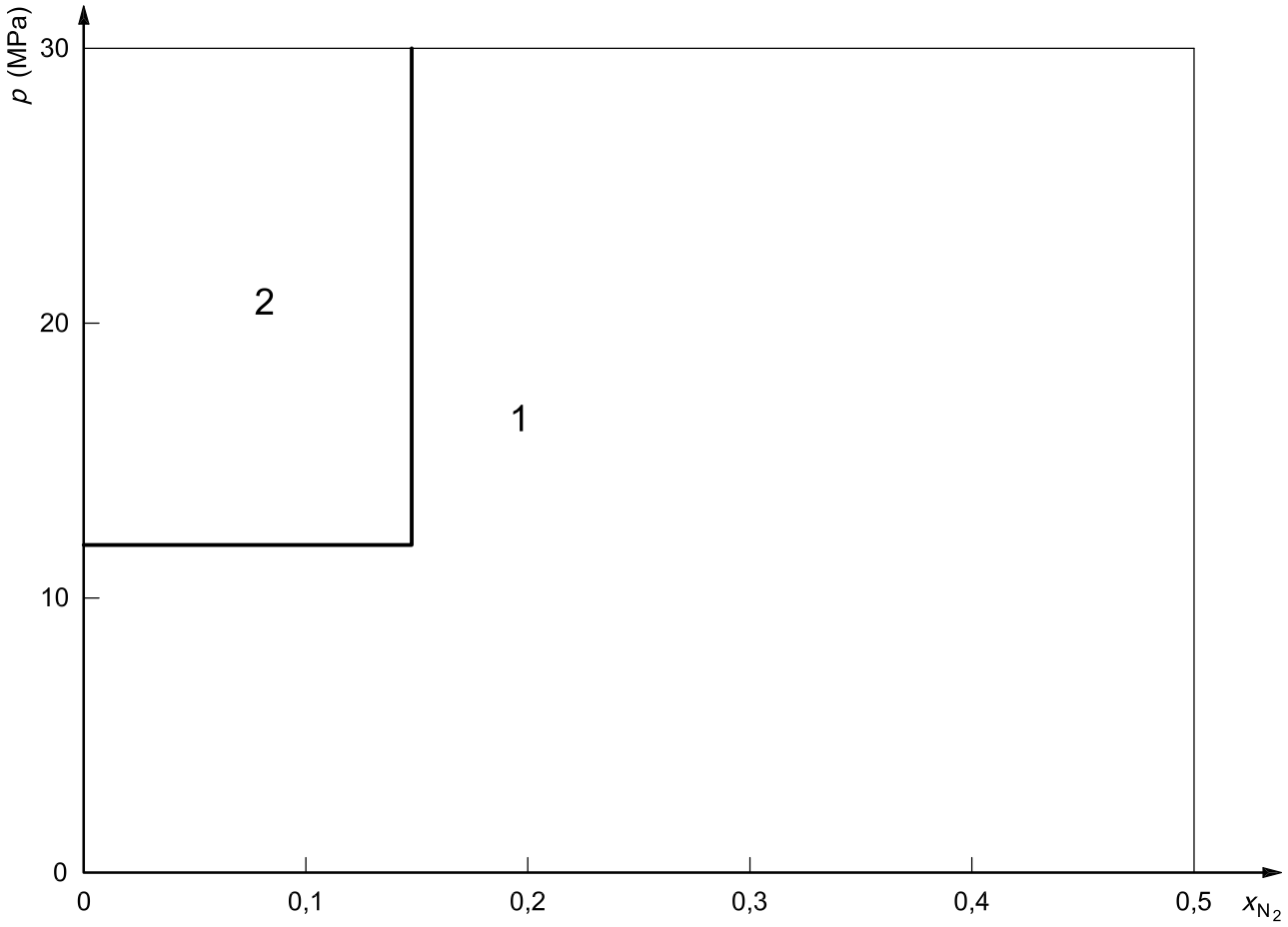
Rough estimates of the uncertainties involved in calculations of compression factors for wider ranges of application (with respect to composition) (see 4.4.2) are plotted in Figures E.1 to E.4 as pressure-composition plots for nitrogen, carbon dioxide, ethane and propane, respectively.

In Figures E.1 to E.4, the performance of the AGA8-92DC method is illustrated up to a maximum pressure of 30 MPa. 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 [3], and upon the databanks in References [2] and [4]. Reference [4] also provides data up to 70 MPa. The uncertainty limits given in Figures E.1 to E.4 are always for the worst-case result, i.e. they are the least optimistic choice.

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.

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AGA8-DC92 equation (T = 263 K to 338 K)

Key

p pressure

x_{N_2} mole fraction of nitrogen

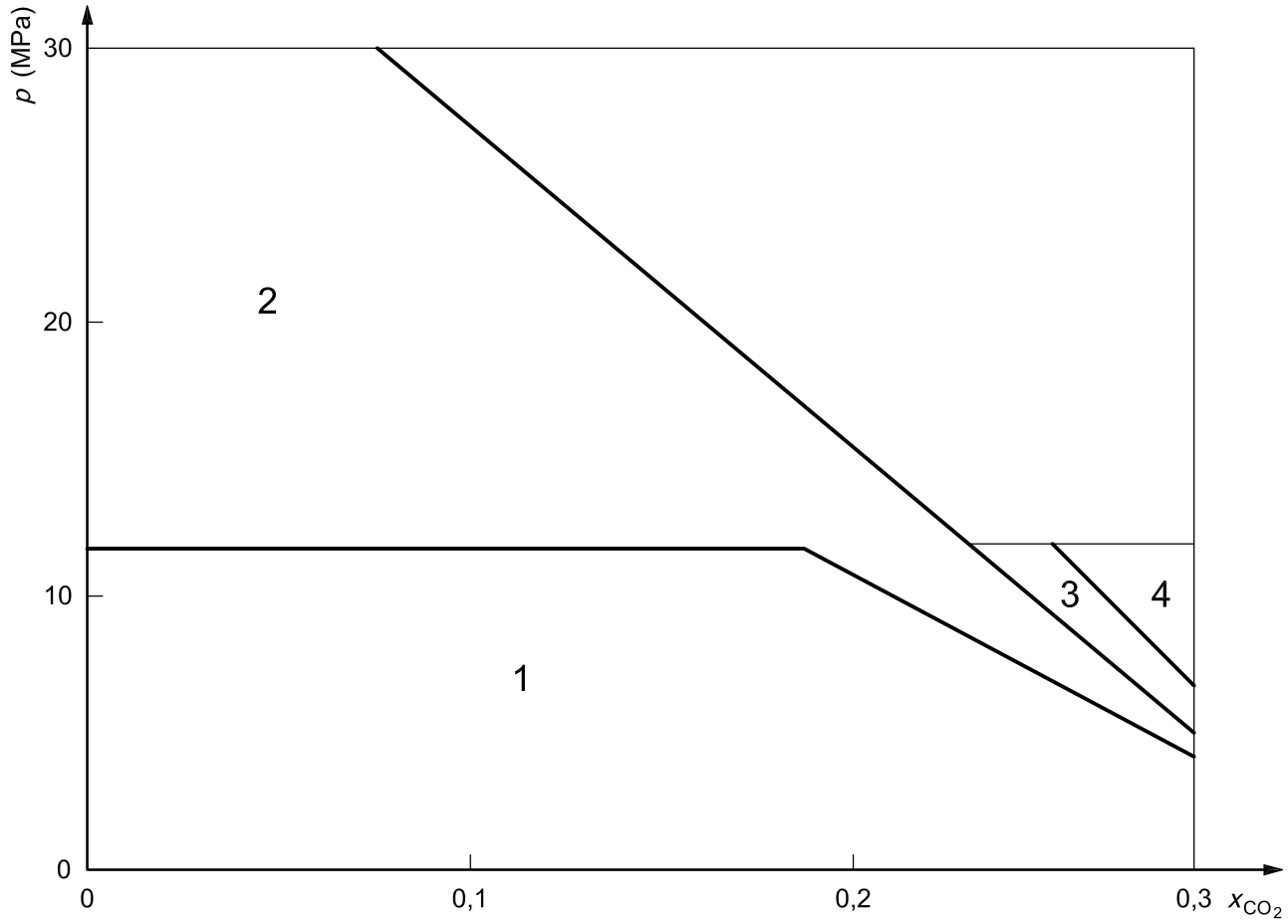
1 $\Delta Z \leqslant \pm 0{,}1$ %

2 ΔZ $\pm 0{,}1$ % to $\pm 0{,}2$ %

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

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AGA8-DC92 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 %

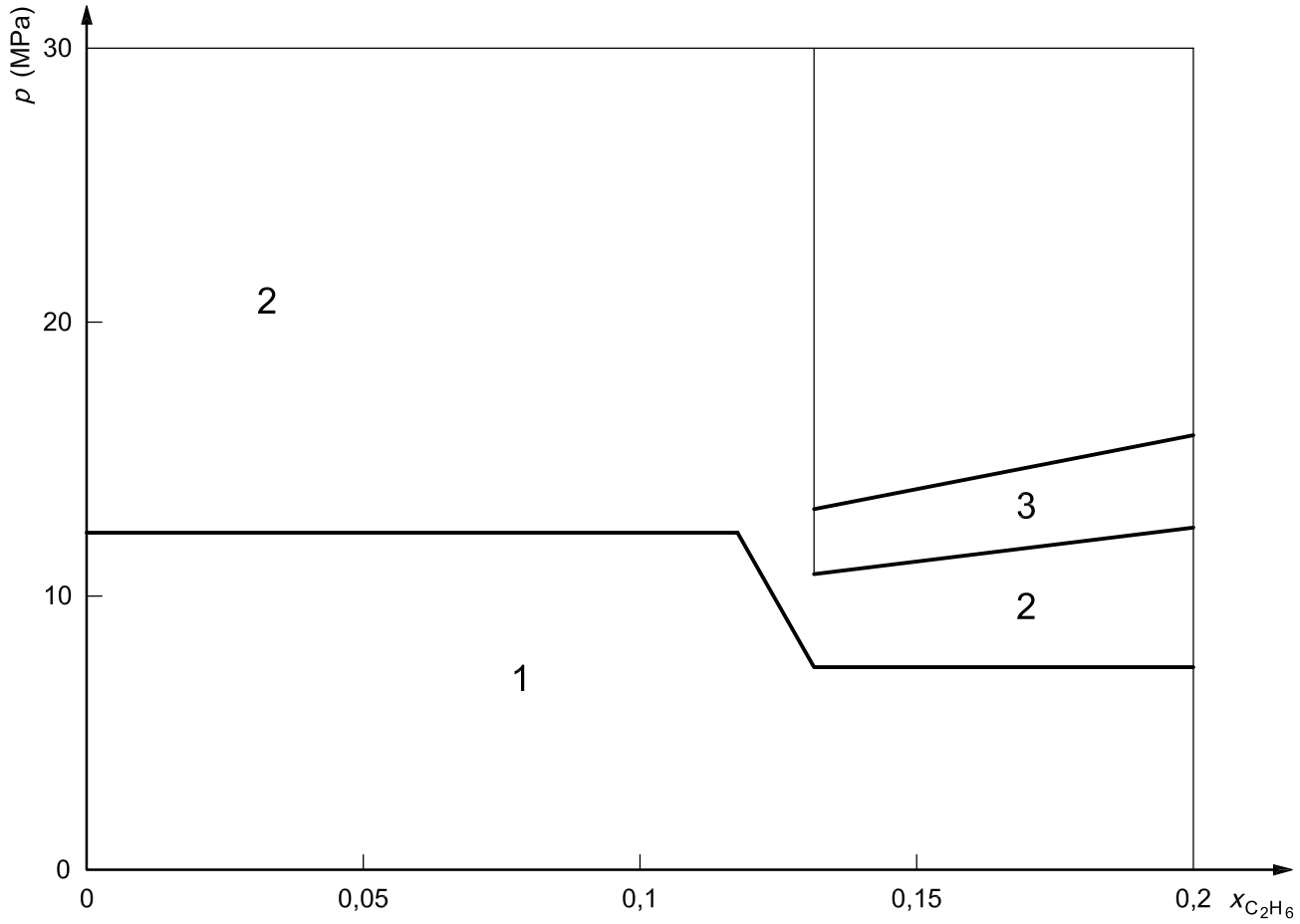
3 ΔZ $\pm$ 0,2 % to $\pm$ 0,5 %

4 ΔZ $\pm$ 0,5 % to $\pm$ 3,0 %

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

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AGA8-DC92 equation (T = 263 K to 338 K)

Key

p pressure

$x_{C_2H_6}$ mole fraction of ethane

1 ΔZ $\leqslant \pm 0{,}1$ %

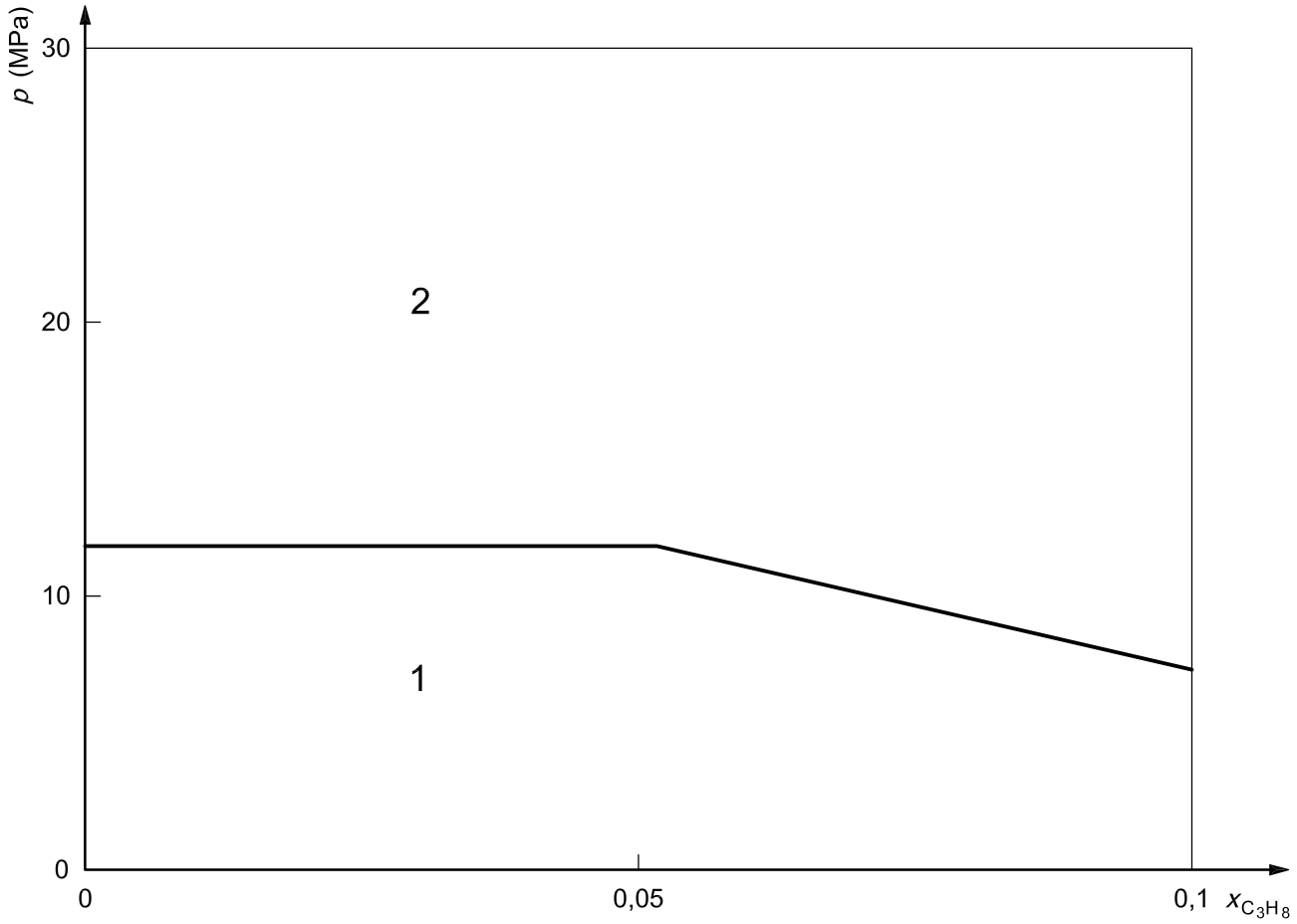
2 ΔZ $\pm 0{,}1$ % to $\pm 0{,}2$ %

3 ΔZ $\pm 0{,}2$ % to $\pm 0{,}5$ %

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

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AGA8-DC92 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 $\pm 0{,}1$ % to $\pm 0{,}2$ %

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

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 $\pm$ 0,1 %, $\pm$ 0,2 % and $\pm$ 0,5 %, respectively, within the given pressure and temperature domain.

Component	Mole fraction for an uncertainty within		
	$\pm$ 0,1 %	$\pm$ 0,2 %	$\pm$ 0,5 %
Nitrogen	$\leqslant$ 0,50	—	—
Carbon dioxide	$\leqslant$ 0,23	$\leqslant$ 0,26	$\leqslant$ 0,28
Ethane	$\leqslant$ 0,13	$\leqslant$ 0,20	—
Propane	$\leqslant$ 0,06	$\leqslant$ 0,10	—

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Annex F
(informative)

Subroutines in Fortran for the AGA8-92DC method

```
C
C     update:  17.05.94              E.W. Lemmon/S.W. Beyerlein/J.L. Savidge
C     update:   4.09.95              M. Jaeschke J. Sikora
================================================================================
C     AGA8-DC92 COMPRESSION FACTOR EQUATION
================================================================================
C                                    SUBROUTINE DCAGA
C
C     This program was written to accompany ISO 12213.
C
C     "DCAGA"   Calculates the compression factor of natural gases using
C                   a detailed gas analysis.
C
C     For information contact: DR. Jeffrey L. Savidge
C                              gas research institute
C                              8600 W. Bryn Mawr Ave.
C                              Chicago, IL 60631
C                              (312) 399-8100, FAX (312) 399-8125
C
C
C     This program calculates compression factors and molar densities for
C     natural gases from the input of gas composition in accordance with the
C     AGA8-DC92 compression equation developed by the Gas
C     Research Institute, Chicago, Illinois.  (K.E. Starling and J.L.
C     Savidge, Compressibility Factors of Natural Gas and Other Related
C     Hydrocarbon Gases, American Gas Association, AGA Transmission
C     Measurement Committee Report No. 8, American Petroleum Institute MPMS
C     Chapter 14.2, Second Edition, November 1992, Catalog No. XQ9212).
C
C
C     The coefficients used in this program are the same as the values found
C     in AGA Report No. 8, November 1992.
C     Values for the gas constant and molar masses conform with ISO 6976
C     (1995) and GPA 2172 (1988).
C
C
C     Ranges of application for compression factor calculation
C     with the AGA8 - DC92 equation:
C
C     p-T-ranges
C                    absolute pressure      0 to  65 MPa
C                    temperature          225 to 350 K
C
C     Ranges for percentage molar composition:
C
C          A: pipeline quality natural gas
C          B: wider ranges of application
C
C                            A             B
C     methane           70 to 100     50 to 100
C     nitrogen           0 to  20      0 to  50
C     carbon dioxide     0 to  20      0 to  30
C     ethane             0 to  10      0 to  20
C     propane            0 to   3.5    0 to   5
C     butanes            0 to   1.5    0 to   1.5
C     pentanes           0 to   0.5    0 to   0.5
```

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```
C     hexanes           0 to   0.1    0 to   0.1
C     heptanes          0 to   0.05   0 to   0.05
C     octanes plus      0 to   0.05   0 to   0.05
C     hydrogen          0 to  10      0 to  10
C     carbon monoxide   0 to   3      0 to   3
C     helium            0 to   0.5    0 to   0.5
C     water             0 to   0.015  0 to   0.015
C
C     The expected uncertainty of the calculated results are for
C     pipeline quality natural gases:
C     +/- 0,1%     within p-T range  0 to 12 MPa, 263 to 350 K
C     +/- 0,6%     within p-T range  0 to 60 MPa, 225 to 350 K
C     The expected uncertainty in the wider range of application
C     (composition) is often even for pressures up to 12 MPa larger.
C     For more details see ISO 12213 part 2.
C
      SUBROUTINE DCAGA (XJ)

      INTEGER B(58),C(58),K(58),G(58)
      INTEGER Q(58),F(58),S(58),W(58)
      REAL*8 A(58),U(58)
      COMMON /CONSTANTS/ A,B,C,K,U,G,Q,F,S,W

      REAL*8 MW(21),EI(21),KI(21),GI(21),QI(21),FI(21),SI(21),WI(21)
      REAL*8 EIJ(21,21),UIJ(21,21),KIJ(21,21),GIJ(21,21)
      COMMON /PARAMETERS/ MW,EI,KI,GI,QI,FI,SI,WI,EIJ,UIJ,KIJ,GIJ

      REAL*8 K1, CNS(58), BI(18)
      COMMON /COEF/ K1, CNS, BI

      REAL*8 MWX, RGAS, TCM, DCM
      COMMON /MW/ MWX, RGAS, TCM, DCM

      INTEGER I, J, N
      REAL*8 SUM, XI(21), XJ(21)
      REAL*8 U1, G1, Q1, F1, E1
      REAL*8 XIJ, EIJ0, GIJ0, BN

      XI( 1) = XJ( 1)
      XI( 4) = XJ( 2)
      XI( 5) = XJ( 3)
      XI(11) = XJ( 4)
      XI(12) = XJ( 5)
      XI(13) = XJ( 6)
      XI(14) = XJ( 7)
      XI(15) = XJ( 8)
      XI(16) = XJ( 9)
      XI(17) = XJ(10)
      XI(18) = XJ(11)
      XI(19) = XJ(12)
      XI( 3) = XJ(13)
      XI( 2) = XJ(14)
      XI( 7) = XJ(15)
      XI(20) = XJ(16)
      XI( 6) = XJ(17)
      XI(10) = XJ(18)
      XI(21) = XJ(19)
      XI( 8) = XJ(20)
      XI( 9) = XJ(21)

C.....Normalize mole fractions
      SUM = 0
      MWX = 0
      DO 10 I=1, 21
 10   SUM = SUM + XI(I)
```

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```
      DO 20 I=1, 21
 20   XI(I) = XI(I)/SUM

C.....Calculate molecular weight
      RGAS = 8.31451D-3
      MWX = 0
      DO 30 I=1, 21
 30   MWX = MWX + XI(I)*MW(I)

      DO 40 N=1, 18
 40   BI(N) = 0

      K1  = 0
      U1  = 0
      G1  = 0
      Q1  = 0
      F1  = 0
      E1  = 0

      DO 50 I=1, 21
        K1 = K1 + XI(I)*KI(I)**2.5D0
        U1 = U1 + XI(I)*EI(I)**2.5D0
        G1 = G1 + XI(I)*GI(I)
        Q1 = Q1 + XI(I)*QI(I)
        F1 = F1 + XI(I)*XI(I)*FI(I)
        E1 = E1 + XI(I)*EI(I)
 50   CONTINUE
      TCM = 1.261*E1
      DCM = K1**(-1.2D0)
      K1 = K1*K1
      U1 = U1*U1

      DO 60 I=1, 8
        DO 60 J=I+1, 19
          XIJ = XI(I)*XI(J)
          IF (XIJ.NE.0) THEN
            K1 = K1+2.D0*XIJ*(KIJ(I,J)**5.D0-1.D0)*(KI(I)*KI(J))**2.5D0
            U1 = U1+2.D0*XIJ*(UIJ(I,J)**5.D0-1.D0)*(EI(I)*EI(J))**2.5D0
            G1 = G1+XIJ*(GIJ(I,J) - 1.D0)*(GI(I) + GI(J))
          ENDIF
 60   CONTINUE

      DO 80 I=1, 21
        DO 80 J=I, 21
          XIJ = XI(I)*XI(J)
          IF (XIJ.NE.0) THEN
            IF (I.NE.J) XIJ = 2.D0*XIJ
            EIJ0 = EIJ(I,J)*DSQRT(EI(I)*EI(J))
            GIJ0 = GIJ(I,J)*(GI(I) + GI(J))/2.D0
            DO 70 N=1, 18
              BN = (GIJ0 + 1.D0 - G(N))**G(N)
     &           * (QI(I)*QI(J) + 1.D0 - Q(N))**Q(N)
     &           * (DSQRT(FI(I)*FI(J)) + 1.D0 - F(N))**F(N)
     &           * (SI(I)*SI(J) + 1.D0 - S(N))**S(N)
     &           * (WI(I)*WI(J) + 1.D0 - W(N))**W(N)
              BI(N) = BI(N)+A(N)*XIJ*EIJ0**U(N)*(KI(I)*KI(J))**1.5D0*BN
 70         CONTINUE
          ENDIF
 80   CONTINUE

      K1 = K1**0.2D0
      U1 = U1**0.2D0
      DO 90 N=13, 58
 90   CNS(N) = (G1 + 1.D0 - G(N))**G(N)
     &       * (Q1**2 + 1.D0 - Q(N))**Q(N)
```

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```
     &       * (F1 + 1.D0 - F(N))**F(N)
     &       * A(N)*U1**U(N)
      END
C=======================================================================
      SUBROUTINE PZOFDT(D, T, P, Z, BMIX)

      INTEGER B(58),C(58),K(58),G(58)
      INTEGER Q(58),F(58),S(58),W(58)
      REAL*8 A(58),U(58)
      COMMON /CONSTANTS/ A,B,C,K,U,G,Q,F,S,W

      REAL*8 K1, CNS(58), BI(18)
      COMMON /COEF/ K1, CNS, BI

      REAL*8 MWX, RGAS, TCM, DCM
      COMMON /MW/ MWX, RGAS, TCM, DCM

      INTEGER N
      REAL*8 D, T, P, Z, BMIX, DR

      DR = D*K1**3
      BMIX = 0
      DO 10 N=1, 18
 10   BMIX = BMIX + BI(N)/T**U(N)

      Z = 1.D0 + BMIX*D
      DO 20 N=13, 18
 20   Z = Z - DR*CNS(N)/T**U(N)

      DO 30 N=13, 58
 30   Z = Z + CNS(N)/T**U(N)*(B(N) - C(N)*K(N)*DR**K(N))*DR**B(N)
     &      *DEXP(-C(N)*DR**K(N))
      P = D*RGAS*T*Z
      END
C=======================================================================
      SUBROUTINE DZOFPT(P, T, D, Z, BMIX)

      REAL*8 P, T, D, Z, BMIX
      REAL*8 X1, X2, X3, F, F1, F2, F3, TOL
      INTEGER I

      TOL = 0.5D-9
      X1 = 0.000001D0
      X2 = 40.D0
      D = 0

      CALL PZOFDT(X1, T, F1, Z, BMIX)
      CALL PZOFDT(X2, T, F2, Z, BMIX)
      F1 = F1 - P
      F2 = F2 - P
      IF (F1*F2.GE.0) RETURN
C-----------------------------------------------------------------------
C  BEGIN ITERATING
C-----------------------------------------------------------------------
      DO 60 I = 1, 50
C     ...Use False Position to get point 3.
        X3 = X1 - F1*(X2 - X1)/(F2 - F1)
        CALL PZOFDT(X3, T, F3, Z, BMIX)
        F3 = F3 - P

C     ...Use points 1, 2, and 3 to estimate the root using Chamber's
C     ...method (quadratic solution).
        D = X1*F2*F3/((F1 - F2)*(F1 - F3))
     &    + X2*F1*F3/((F2 - F1)*(F2 - F3))
     &    + X3*F1*F2/((F3 - F1)*(F3 - F2))
```

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```
         IF ((D - X1)*(D - X2).GE.0) D = (X1 + X2)/2.D0
         CALL PZOFDT(D, T, F, Z, BMIX)
         F = F - P
         IF (DABS(F).LE.TOL) RETURN

C     ...Discard quadratic solution if false position root is closer.
         IF (DABS(F3).LT.DABS(F) .AND. F*F3.GT.0) THEN
           IF (F3*F1.GT.0) THEN
             X1 = X3
             F1 = F3
           ELSE
             X2 = X3
             F2 = F3
           ENDIF
         ELSE

C       ...Swap in new value from quadratic solution
           IF (F*F3.LT.0) THEN
             X1 = D
             F1 = F
             X2 = X3
             F2 = F3
           ELSEIF (F3*F1.GT.0) THEN
             X1 = D
             F1 = F
            ELSE
             X2 = D
             F2 = F
           ENDIF
         ENDIF
 60    CONTINUE
       D = 0
       END
C=======================================================================
       BLOCK DATA
       INTEGER B(58),C(58),K(58),G(58)
       INTEGER Q(58),F(58),S(58),W(58)
       REAL*8 A(58),U(58)
       COMMON /CONSTANTS/ A,B,C,K,U,G,Q,F,S,W

       REAL*8 MW(21),EI(21),KI(21),GI(21),QI(21),FI(21),SI(21),WI(21)
       REAL*8 EIJ(21,21),UIJ(21,21),KIJ(21,21),GIJ(21,21)
       COMMON /PARAMETERS/ MW,EI,KI,GI,QI,FI,SI,WI,EIJ,UIJ,KIJ,GIJ

       REAL*8 XN(21), XH(21)
       COMMON /GRENZDATA/ XN,XH

C.....Equation of state parameters
       DATA A/
      &  0.153832600D0,  1.341953000D0, -2.998583000D0, -0.048312280D0,
      &  0.375796500D0, -1.589575000D0, -0.053588470D0,  0.886594630D0,
      & -0.710237040D0, -1.471722000D0,  1.321850350D0, -0.786659250D0,
      &  0.2291290D-08,  0.157672400D0, -0.436386400D0, -0.044081590D0,
      & -0.003433888D0,  0.032059050D0,  0.024873550D0,  0.073322790D0,
      & -0.001600573D0,  0.642470600D0, -0.416260100D0, -0.066899570D0,
      &  0.279179500D0, -0.696605100D0, -0.002860589D0, -0.008098836D0,
      &  3.150547000D0,  0.007224479D0, -0.705752900D0,  0.534979200D0,
      & -0.079314910D0, -1.418465000D0, -0.5999050D-16,  0.105840200D0,
      &  0.034317290D0, -0.007022847D0,  0.024955870D0,  0.042968180D0,
      &  0.746545300D0, -0.291961300D0,  7.294616000D0, -9.936757000D0,
      & -0.005399808D0, -0.243256700D0,  0.049870160D0,  0.003733797D0,
      &  1.874951000D0,  0.002168144D0, -0.658716400D0,  0.000205518D0,
      &  0.009776195D0, -0.020487080D0,  0.015573220D0,  0.006862415D0,
      & -0.001226752D0,  0.002850908D0/
       DATA B/1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,2,2,2,2,2,2,2,2,3,3,
```

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```
     &       3,3,3,3,3,3,3,3,4,4,4,4,4,4,5,5,5,5,6,6,7,7,8,8,8,9,9/
      DATA C/0,0,0,0,0,0,0,0,0,0,0,1,1,1,1,1,1,0,0,1,1,1,1,1,1,1,0,1,
     &       1,1,1,1,1,1,1,1,0,0,1,1,1,1,1,1,0,1,1,1,1,0,1,0,1,1,1,1,1,1/
      DATA K/0,0,0,0,0,0,0,0,0,0,0,0,3,2,2,2,4,4,0,0,2,2,2,4,4,4,4,0,1,
     &       1,2,2,3,3,4,4,4,0,0,2,2,2,4,4,0,2,2,4,4,0,2,0,2,1,2,2,2,2,2/
      DATA G/0,0,0,0,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,1,
     &       0,0,1,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,1,0,1,0,0/
      DATA Q/0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,0,1,0,
     &       0,0,0,0,0,0,0,1,0,0,0,0,1,0,0,0,0,1,0,1,0,0,1,0,0,0,0,0,1/
      DATA F/0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,1,0,0,
     &       1,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
      DATA S/0,0,0,0,0,0,0,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,
     &       0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
      DATA W/0,0,0,0,0,0,0,0,0,0,1,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,
     &       0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0/
      DATA U/0,0.5D0,1,3.5D0,-0.5D0,4.5D0,0.5D0,7.5D0,9.5D0,6,12,12.5D0,
     &      -6,2,3,2,2,11,-0.5D0,0.5D0,0,4,6,21,23,22,-1,-0.5D0,7,-1,6,
     &       4,1,9,-13,21,8,-0.5D0,0,2,7,9,22,23,1,9,3,8,23,1.5D0,5,
     &      -0.5D0,4,7,3,0,1,0/

C.....Characterization Parameters
      DATA MW/16.0430D0, 28.0135D0, 44.0100D0, 30.0700D0, 44.0970D0,
     &        18.0153D0, 34.0820D0,  2.0159D0, 28.0100D0, 31.9988D0,
     &        58.1230D0, 58.1230D0, 72.1500D0, 72.1500D0, 86.1770D0,
     &       100.2040D0,114.2310D0,128.2580D0,142.2850D0,  4.0026D0,
     &        39.9480D0/
      DATA EI/151.318300D0,  99.737780D0, 241.960600D0, 244.166700D0,
     &        298.118300D0, 514.015600D0, 296.355000D0,  26.957940D0,
     &        105.534800D0, 122.766700D0, 324.068900D0, 337.638900D0,
     &        365.599900D0, 370.682300D0, 402.636293D0, 427.722630D0,
     &        450.325022D0, 470.840891D0, 489.558373D0,   2.610111D0,
     &        119.629900D0/
      DATA KI/0.4619255D0, 0.4479153D0, 0.4557489D0, 0.5279209D0,
     &        0.5837490D0, 0.3825868D0, 0.4618263D0, 0.3514916D0,
     &        0.4533894D0, 0.4186954D0, 0.6406937D0, 0.6341423D0,
     &        0.6738577D0, 0.6798307D0, 0.7175118D0, 0.7525189D0,
     &        0.7849550D0, 0.8152731D0, 0.8437826D0, 0.3589888D0,
     &        0.4216551D0/
      DATA GI/0,         0.027815D0, 0.189065D0, 0.079300D0, 0.141239D0,
     &       0.332500D0, 0.088500D0, 0.034369D0, 0.038953D0, 0.021000D0,
     &       0.256692D0, 0.281835D0, 0.332267D0, 0.366911D0, 0.289731D0,
     &       0.337542D0, 0.383381D0, 0.427354D0, 0.469659D0, 0, 0/
      DATA QI/2*0, 0.69D0, 2*0, 1.06775D0, 0.633276D0, 14*0/
      DATA FI/7*0, 1, 13*0/
      DATA SI/5*0, 1.5822D0, 0.390D0, 14*0/
      DATA WI/5*0, 1, 15*0/

C.....Binary interaction parameters
      DATA EIJ/441*1/
      DATA UIJ/441*1/
      DATA KIJ/441*1/
      DATA GIJ/441*1/

      DATA (EIJ(1,J),J=2,19)/
     &     0.971640D0, 0.960644D0, 1,          0.994635D0, 0.708218D0,
     &     0.931484D0, 1.170520D0, 0.990126D0, 1,          1.019530D0,
     &     0.989844D0, 1.002350D0, 0.999268D0, 1.107274D0, 0.880880D0,
     &     0.880973D0, 0.881067D0, 0.881161D0/
      DATA (EIJ(2,J),J=3,14)/
     &     1.022740D0, 0.970120D0, 0.945939D0, 0.746954D0, 0.902271D0,
     &     1.086320D0, 1.005710D0, 1.021000D0, 0.946914D0, 0.973384D0,
     &     0.959340D0, 0.945520D0/
      DATA (EIJ(3,J),J=4,19)/
     &     0.925053D0, 0.960237D0, 0.849408D0, 0.955052D0, 1.281790D0,
     &     1.5D0,      1,          0.906849D0, 0.897362D0, 0.726255D0,
```

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     &     0.859764D0, 0.855134D0, 0.831229D0, 0.808310D0, 0.786323D0,
     &     0.765171D0/
      DATA (EIJ(4,J),J=5,14)/1.022560D0, 0.693168D0, 0.946871D0,
     &     1.164460D0, 3*1, 1.013060D0, 1, 1.00532D0/
      DATA (EIJ(5,J),J=8,12)/1.034787D0, 3*1, 1.0049D0/
      DATA (EIJ(7,J),J=15,19)/1.008692D0, 1.010126D0, 1.011501D0,
     &     1.012821D0, 1.014089D0/
      DATA (EIJ(8,J),J=9,12)/1.1D0, 1, 1.3D0, 1.3D0/

      DATA (UIJ(1,J),J=2,19)/
     &     0.886106D0, 0.963827D0, 1, 0.990877D0, 1, 0.736833D0,
     &     1.156390D0, 3*1, 0.992291D0, 1, 1.003670D0, 1.302576D0,
     &     1.191904D0, 1.205769D0, 1.219634D0, 1.233498D0/
      DATA (UIJ(2,J),J=3,12)/0.835058D0, 0.816431D0, 0.915502D0, 1,
     &     0.993476D0, 0.408838D0, 3*1, 0.993556D0/
      DATA (UIJ(3,J),J=4,19)/0.969870D0, 2*1, 1.045290D0, 1, 0.9D0,
     &     5*1, 1.066638D0, 1.077634D0, 1.088178D0, 1.098291D0,
     &     1.108021D0/
      DATA (UIJ(4,J),J=5,14)/
     &     1.065173D0, 1, 0.971926D0, 1.616660D0, 2*1, 4*1.25D0/
      DATA (UIJ(7,J),J=7,19)/8*1, 1.028973D0, 1.033754D0,
     &     1.038338D0, 1.042735D0, 1.046966D0/

      DATA (KIJ(1,J),J=2,19)/
     &     1.003630D0, 0.995933D0, 1, 1.007619D0, 1, 1.000080D0,
     &     1.023260D0, 3*1, 0.997596D0, 1, 1.002529D0, 0.982962D0,
     &     0.983565D0, 0.982707D0, 0.981849D0, 0.980991D0/
      DATA (KIJ(2,J),J=3,8)/
     &     0.982361D0, 1.007960D0, 1, 1, 0.9425960D0,1.032270D0/
      DATA (KIJ(3,J),J=4,19)/1.008510D0, 2*1, 1.00779D0,7*1.0D0,
     &     0.910183D0, 0.895362D0, 0.881152D0, 0.867520D0, 0.854406D0/
      DATA (KIJ(4,J),J=5,8)/0.986893D0, 1, 0.999969D0, 1.020340D0/
      DATA (KIJ(7,J),J=7,21)/8*1, 0.968130D0, 0.962870D0,
     &     0.957828D0, 0.952441D0, 0.948338D0, 2*1/

      DATA GIJ(1,3) /0.807653D0/
      DATA GIJ(1,8) /1.957310D0/
      DATA GIJ(2,3) /0.982746D0/
      DATA GIJ(3,4) /0.370296D0/
      DATA GIJ(3,6) /1.673090D0/

C
      DATA XN/
     &  50.0  ,  0.0  ,  0.0  ,  0.0  ,  0.0  ,  0.0  ,  0.0  ,  0.0  ,
     &   0.0  ,  0.0  ,  0.0  ,  0.0  ,  0.0  ,  0.0  ,  0.0  ,  0.0  ,
     &   0.0  ,  0.0  ,  0.0  ,  0.0  ,  0.0/
C
      DATA XH/
     & 100.0  , 20.0  ,  5.0  ,  1.5  ,  1.5  ,  0.5  ,  0.5  ,  0.1  ,
     &   0.05 ,  0.05 ,  0.05 ,  0.05 , 30.0  , 50.0  ,  0.02 ,  0.5  ,
     &   0.015,  0.02 ,  0.02 , 10.0  ,  3.0/
      END
```

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