INTERNATIONAL STANDARD

ISO
20765-1

First edition
2005-09-15

Natural gas — Calculation of thermodynamic properties —

Part 1:
Gas phase properties for transmission and distribution applications

Gaz naturel — Calcul des propriétés thermodynamiques —

Partie 1: Propriétés de la phase gazeuse utilisée pour des applications de transport et de distribution

Reference number
ISO 20765-1:2005(E)

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Published in Switzerland

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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.

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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 20765-1 was prepared by Technical Committee ISO/TC 193, *Natural gas*, Subcommittee SC 1, *Analysis of natural gas*.

ISO 20765 consists of the following parts, under the general title *Natural gas — Calculation of thermodynamic properties*:

- *Part 1: Gas phase properties for transmission and distribution applications*

The following parts are under preparation:

- *Part 2: Single phase properties (gas, liquid and dense-fluid) for extended ranges of application*

- *Part 3: Two-phase properties (vapour-liquid equilibria)*

Introduction

This part of ISO 20765 specifies methods for the calculation of thermodynamic properties of natural gases, natural gases containing synthetic admixture, and similar mixtures.

This part of ISO 20765 has four normative annexes and three informative annexes.

Natural gas — Calculation of thermodynamic properties —

Part 1:
Gas phase properties for transmission and distribution applications

1 Scope

This part of ISO 20765 specifies a method of calculation for the volumetric and caloric properties of natural gases, natural gases containing synthetic admixture and similar mixtures, at conditions where the mixture can exist only as a gas.

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. For volumetric properties (compression factor and density), the uncertainty of calculation is about ± 0,1 % (95 % confidence interval). For caloric properties (for example enthalpy, heat capacity, Joule-Thomson coefficient, speed of sound), the uncertainty of calculation is usually greater.

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

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

ISO 7504, *Gas analysis — Vocabulary*

ISO 12213-2, *Natural gas — Calculation of compression factor — Part 2: Calculation using molar-composition analysis*

ISO 14532, *Natural gas — Vocabulary*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 31-4, ISO 7504 and ISO 14532 and the following apply.

NOTE See Annex A for the list of symbols and units used in this part of ISO 20765.

3.1
caloric property
characteristic of a gas or homogeneous gas mixture which can be calculated from a fundamental equation of state

NOTE The caloric properties to which this part of ISO 20765 can be applied are internal energy, enthalpy, entropy, isochoric heat capacity, isobaric heat capacity, Joule-Thomson coefficient, isentropic exponent and speed of sound.

3.2

equation of state

mathematical relationship between state variables of a gas or homogeneous gas mixture

NOTE In this part of ISO 20765, it is useful to distinguish between two types of equation of state, namely (1) volumetric equation of state, in which the relationship is between the state variables pressure, temperature and the volume occupied by a given amount of substance, and (2) fundamental equation of state, in which the relationship is between the density, temperature and the Helmholtz free energy.

3.3

residual property

that part of a thermodynamic property which results from the non-ideal (real-gas) behaviour of a gas or homogeneous gas mixture, i.e. the difference between a thermodynamic property of a real gas or gas mixture and the same thermodynamic property for the same gas or gas mixture, in the ideal state, at the same state conditions of temperature and density

3.4

thermodynamic property

volumetric or caloric property

3.5

volumetric property

characteristic of a gas or homogeneous gas mixture that can be calculated from a volumetric equation of state

NOTE The volumetric properties to which this part of ISO 20765 can be applied are compression factor and density.

4 Thermodynamic basis of the method

4.1 Principle

The method recommended is based on the concept that pipeline-quality natural gas is completely characterized for the calculation of its thermodynamic properties by component analysis. Such an analysis, together with the state variables of temperature and density, provides the necessary input data for the method. In practice, the state variables available as input data are more usually temperature and pressure and, in this case, it is necessary first to convert these to temperature and density.

Equations are presented which express the Helmholtz free energy of the gas as a function of density, temperature and composition, from which all of the thermodynamic properties can be obtained in terms of the Helmholtz free energy and its derivatives with respect to temperature and density.

The method uses a detailed molar composition analysis in which all components present in amounts exceeding 0,000 05 mole fraction [50 molar ppm [1]] should be represented. For a typical natural gas, this might include alkane hydrocarbons up to about C_7 or C_8, together with nitrogen, carbon dioxide and helium. Typically, isomers for alkanes above C_5 may be lumped together by molecular weight and treated collectively as the normal isomer.

For some natural gases, it may be necessary to take into consideration additional components such as C_9 and C_{10} hydrocarbons, water vapour and hydrogen sulfide. For manufactured gases, hydrogen and carbon monoxide should be considered.

More precisely, the method uses a 21-component analysis in which all of the major and minor components of natural gas are included (see 6.2). Any trace component present but not identified as one of the 21 specified components may be reassigned appropriately to a specified component.

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[1] ppm is a depredated unit.

4.2 The fundamental equation of Helmholtz free energy

4.2.1 Background

The AGA8 equation [1] was published in 1992 by the Transmission Measurements Committee of the American Gas Association, having been designed specifically as a means for the high accuracy calculation of compression factor. In this respect, it is already the subject of ISO 12213-2. Since then it has become increasingly apparent that the equation has excellent potential for use in the calculation of all thermodynamic properties of natural gas, even though the accuracy of calculation is less well documented.

In order for the AGA8 equation to become useful for the calculation of all thermodynamic properties, there are two major requirements.

a) The equation itself, published initially in a form explicit only for volumetric properties, has to be mathematically recast in a form explicit for the residual Helmholtz free energy. In fact, although not published as such, the original development of the equation was as a fundamental equation in the form of Helmholtz free energy. This formulation [2] is essential in that all residual thermodynamic properties can be calculated from the Helmholtz free energy and its derivatives with respect to the state conditions of temperature and density.

b) For the calculation of caloric properties, a formulation is required for the Helmholtz free energy of the ideal gas as a function of temperature. Most previous formulations for the ideal gas have been explicit in the isobaric heat capacity and so, again, the chosen formulation [3], [4] has to be recast so as to be explicit in the Helmholtz free energy. Again, derivatives of the Helmholtz free energy with respect to the state conditions are needed.

An important aspect of the formulations chosen for both the ideal and residual parts of the Helmholtz free energy is that the derivatives required for calculating the thermodynamic properties can be given in analytical form. Hence, there is no need for numerical differentiation or integration within any computer program that implements the procedures. As a result, numerical problems are avoided and calculation times are shorter.

The method of calculation described is very suitable for use within process simulation programs and, in particular, within programs developed for use in natural gas transmission and distribution applications.

4.2.2 The Helmholtz free energy

The Helmholtz free energy, f, of a homogeneous gas mixture at uniform pressure and temperature can be expressed as the sum of a part f_o describing the ideal gas behaviour and a part f_r describing the residual or real-gas behaviour, as given in Equation (1):

$$f\left(\rho, T, X\right) = f_\mathrm{o}\left(\rho, T, X\right) + f_\mathrm{r}\left(\rho, T, X\right) \tag{1}$$

which, rewritten in the form of dimensionless reduced free energy $\varphi = f/(R \cdot T)$, becomes Equation (2):

$$\varphi\left(\delta, \tau, X\right) = \varphi_\mathrm{o}\left(\delta, \tau, X\right) + \varphi_\mathrm{r}\left(\delta, \tau, X\right) \tag{2}$$

where

X is a vector that defines the composition of the mixture;

τ is the inverse (dimensionless) reduced temperature, related to the temperature, T, as given in Equation (3):

$$\tau = L/T \tag{3}$$

where $L = 1$ K.

Note that Equations (1) and (2) are written in terms of the molar density, ρ, and reduced density, δ, respectively, not in terms of the more commonly available input variable of pressure, p. This is because, from statistical thermodynamics, the Helmholtz free energy appears as a natural consequence of the number and types of molecular interactions in a mixture and, therefore, becomes a natural function of the molar density and mole fractions of the molecules.

The reduced density, δ, is related to the molar density, ρ, as shown in Equation (4):

$$\delta = K^3 \cdot \rho \tag{4}$$

where K is a mixture size parameter.

The ideal part, φ_o, of the reduced Helmholtz free energy is obtained from equations for the isobaric heat capacity in the ideal gas state (see 4.2.3), and the residual part, φ_ris, from the AGA8 equation of state (see 4.2.4).

4.2.3 The Helmholtz free energy of the ideal gas

The Helmholtz free energy of an ideal gas can be expressed in terms of the enthalpy, h_o, and entropy, s_o, as given in Equation (5):

$$f_\mathrm{o}\left(\rho, T, X\right) \; = \; h_\mathrm{o}\left(T, X\right) \; - \; R \cdot T - T \cdot s_\mathrm{o}\left(\rho, T, X\right) \tag{5}$$

The enthalpy, h_o, and entropy, s_o, can in turn be expressed in terms of the isobaric heat capacity, $c_\mathrm{o,p}$, of the ideal gas as given in Equations (6) and (7), where the implied limits of integration are T_θ and T:

$$h_\mathrm{o}\left(T, X\right) = \int c_\mathrm{o,p} \; \mathrm{d}T + h_{\mathrm{o},\theta} \tag{6}$$

$$s_\mathrm{o}(\rho, T, X) = \int \frac{c_\mathrm{o,p}}{T} \mathrm{d}T - R \cdot \ln\left(\frac{\rho}{\rho_\theta}\right) - R \cdot \ln\left(\frac{T}{T_\theta}\right) + s_{\mathrm{o},\theta} - R \cdot \sum_{i=1}^{N} x_i \cdot \ln x_i \tag{7}$$

The reference state of zero enthalpy and zero entropy is here adopted as $T_\theta = 298{,}15$ K and $p_\theta = 0{,}101\,325$ MPa for the ideal unmixed gas. The integration constants, $h_{\mathrm{o},\theta}$ and $s_{\mathrm{o},\theta}$, are then determined so as to conform to this definition. The reference (ideal) density, ρ_θ, is given by $\rho_\theta = p_\theta/(R \cdot T_\theta)$.

The reduced Helmholtz free energy $\varphi_\mathrm{o} = f_\mathrm{o}/(R \cdot T)$ can then be written, using Equations (6) and (7), as a function of δ, τ and X, as given in Equation (8):

$$\varphi_\mathrm{o}\left(\delta, \tau, X\right) = -\tau \int \frac{c_\mathrm{o,p}}{R \cdot \tau^2} \mathrm{d}\tau + \frac{h_{\mathrm{o},\theta} \cdot \tau}{R \cdot L} - 1 + \int \frac{c_\mathrm{o,p}}{R \cdot \tau} \mathrm{d}\tau + \ln\left(\frac{\delta}{\delta_\theta}\right) + \ln\left(\frac{\tau_\theta}{\tau}\right) - \frac{s_{\mathrm{o},\theta}}{R} + \sum_{i=1}^{N} x_i \cdot \ln x_i \tag{8}$$

See Annex B for details of this formulation.

4.2.4 The residual part of the Helmholtz free energy

The residual part of the reduced Helmholtz free energy is obtained, for the purposes of this part of ISO 20765, by use of the AGA8 equation. Written for the compression factor as a function of reduced density, inverse reduced temperature and composition, the AGA8 equation has the form of Equation (9):

$$Z = 1 + \frac{B \cdot \delta}{K^3} - \delta \sum_{n=13}^{18} C_n \cdot \tau^{u_n} + \sum_{n=13}^{58} C_n \cdot \tau^{u_n} \cdot \delta^{b_n} \left(b_n - c_n \cdot k_n \cdot \delta^{k_n}\right) \exp\left(-c_n \cdot \delta^{k_n}\right) \tag{9}$$

where

B	is the second virial coefficient;
b_n, c_n, k_n, u_n	are coefficients of the equation and functions of composition;
C_n	is a function of composition.

The compression factor, Z, is related to the residual part of reduced free energy, φ_r, as given in Equation (10):

$$Z = 1 + \delta \cdot \varphi_{\mathrm{r},\delta} \tag{10}$$

where $\varphi_{\mathrm{r},\delta}$ is the partial derivative of φ_r with respect to reduced density at constant τ and X.

Elimination of Z between Equations (9) and (10), and integration with respect to reduced density leads to the Equation (11) for the residual part of the reduced Helmholtz free energy:

$$\varphi_\mathrm{r}(\delta,\tau,X) = \frac{B\cdot\delta}{K^3} - \delta\sum_{n=13}^{18} C_n\cdot\tau^{u_n} + \sum_{n=13}^{58} C_n\cdot\tau^{u_n}\cdot\delta^{b_n}\exp(-c_n\cdot\delta^{k_n}) \tag{11}$$

See Annexes C and D for details of this formulation.

4.2.5 The reduced Helmholtz free energy

The fundamental equation [Equation (2)] for the reduced Helmholtz free energy, φ, makes it possible, through use of Equation (8) for the ideal part, φ_o, and Equation (11) for the residual part, φ_r, to calculate all thermodynamic properties analytically. The reduced Helmholtz free energy, φ, therefore can be written as given in Equation (12):

$$\begin{aligned}\varphi\left(\delta,\tau,X\right) = {}& -\tau\int\frac{c_{\mathrm{o,p}}}{R\cdot\tau^2}\mathrm{d}\tau + \frac{h_{\mathrm{o},\theta}\cdot\tau}{R} - 1 + \int\frac{c_{\mathrm{o,p}}}{R\cdot\tau}\mathrm{d}\tau + \ln\left(\frac{\delta}{\delta_\theta}\right) + \ln\left(\frac{\tau_\theta}{\tau}\right) - \frac{s_{\mathrm{o},\theta}}{R} + \sum_{i=1}^{N} x_i\cdot\ln x_i + \ldots\\ & \ldots + \frac{B\cdot\delta}{K^3} - \delta\sum_{n=13}^{18} C_n\cdot\tau^{u_n} + \sum_{n=13}^{58} C_n\cdot\tau^{u_n}\cdot\delta^{b_n}\exp(-c_n\cdot\delta^{k_n})\end{aligned} \tag{12}$$

4.3 Thermodynamic properties derived from the Helmholtz free energy

4.3.1 Background

All of the thermodynamic properties can be written explicitly in terms of the reduced Helmholtz free energy, φ, and various derivatives thereof. The required derivatives, φ_τ, $\varphi_{\tau\tau}$, φ_δ, $\varphi_{\delta\delta}$ and $\varphi_{\tau\delta}$, are defined as given in Equations (13):

$$\varphi_\tau = \left(\frac{\partial\varphi}{\partial\tau}\right)_{\delta,\mathrm{X}} \qquad \varphi_{\tau\tau} = \left(\frac{\partial^2\varphi}{\partial\tau^2}\right)_{\delta,\mathrm{X}} \qquad \varphi_\delta = \left(\frac{\partial\varphi}{\partial\delta}\right)_{\tau,\mathrm{X}} \qquad \varphi_{\delta\delta} = \left(\frac{\partial^2\varphi}{\partial\delta^2}\right)_{\tau,\mathrm{X}} \qquad \varphi_{\tau\delta} = \left[\frac{\partial}{\partial\tau}\left(\frac{\partial\varphi}{\partial\delta}\right)_{\tau,\mathrm{X}}\right]_{\delta,\mathrm{X}} \tag{13}$$

Each derivative is the sum of an ideal part (see Annex B) and a residual part (see Annex C). The substitutions given in Equations (14) and (15) help to simplify the appearance of the relevant relationships:

$$\varphi_1 = \left[\frac{\partial\left(\delta^2\cdot\varphi_\delta\right)}{\partial\delta}\right]_{\tau,\mathrm{X}} = 2\cdot\delta\cdot\varphi_\delta + \delta^2\cdot\varphi_{\delta\delta} \tag{14}$$

$$\varphi_2 = -\tau^2 \left[\frac{\partial}{\partial \tau} \left(\frac{\delta \cdot \varphi_\delta}{\tau} \right) \right]_{\delta, X} = \delta \cdot \varphi_\delta - \tau \cdot \delta \cdot \varphi_{\tau\delta} \tag{15}$$

Detailed expressions for φ_τ, $\varphi_{\tau\tau}$, φ_δ, φ_1 and φ_2 can be found in Annex C.

The relevant general relationships for the various thermodynamic properties are given in 4.3.2.1 to 4.3.2.9 [Equations (17) to (26)]. In Equations (19) to (24), lowercase symbols represent molar quantities (i.e. quantity per mole) and the corresponding upper case symbols represent specific quantities (i.e. quantity per kilogram). Conversion of molar variables to mass-basis variables is achieved by division by the molar mass M.

NOTE In these equations, R is the molar gas constant; consequently R/M is the specific gas constant.

The molar mass, M, of the mixture is derived from the composition, X, and molar masses, M_i, of the pure substances as given in Equation (16):

$$M = \sum_{i=1}^{N} x_i \cdot M_i \tag{16}$$

Values for molar masses, M_i, of pure substances are given in References [1] and [2]; these values are identical with those given in ISO 6976:1995 [5].

NOTE The values given in ISO 6976 for the molar masses are in most cases not identical with the most recent values adopted by the international community of metrologists. They are, however, the values that were in general use during the development of the AGA8 equation, and are therefore retained here; the differences are in all cases less than 0,001 kg/kmol.

In Equations (20), (21) and (23) to (26), the basic expressions for the properties h, s, c_p, μ, κ and w have been transformed in several ways, such that values of properties already derived can be used to simplify the subsequent calculations. This approach is useful for applications where several or all of the thermodynamic properties are to be determined. For clarity, the basic thermodynamic relationships are given first in each subclause, and the subsidiary transformations are given below.

4.3.2 Equations for thermodynamic properties

4.3.2.1 Compression factor and density

The expression for the compression factor, Z, is given by Equation (17):

$$Z = \delta \cdot \varphi_\delta \tag{17}$$

where φ_δ is the derivative with respect to the reduced molar density of the Helmholtz free energy [see also Equation (10)]. The molar density, ρ, and specific (mass) density, D, are related to pressure as given in Equation (18):

$$\rho = D / M = p / (Z \cdot R \cdot T) \tag{18}$$

Values of compression factor, Z, calculated in accordance with this part of ISO 20765 should normally be identical with values calculated in accordance with ISO 12213-2. In any case where a requirement for priority is identified, ISO 12213-2 shall take precedence.

4.3.2.2 Internal energy

The expression for the internal energy, u, is given by Equation (19):

$$\frac{u}{R \cdot T} = \frac{U \cdot M}{R \cdot T} = \tau \cdot \varphi_\tau \tag{19}$$

4.3.2.3 Enthalpy

The expression for the enthalpy, h, is given by Equation (20):

$$\begin{aligned}\frac{h}{R\cdot T} &= \frac{H\cdot M}{R\cdot T}\\ &= \tau\cdot\varphi_{\tau}+\delta\cdot\varphi_{\delta}\\ &= \frac{u}{R\cdot T}+Z=\frac{U\cdot M}{R\cdot T}+Z\end{aligned} \tag{20}$$

4.3.2.4 Entropy

The expression for the entropy, s, is given by Equation (21):

$$\begin{aligned}\frac{s}{R} &= \frac{S\cdot M}{R}\\ &= \tau\cdot\varphi_{\tau}-\varphi\\ &= \frac{u}{R\cdot T}-\varphi=\frac{U\cdot M}{R\cdot T}-\varphi\end{aligned} \tag{21}$$

4.3.2.5 Isochoric heat capacity

The expression for the isochoric heat capacity, c_{v}, is given by Equation (22):

$$\frac{c_{\mathrm{v}}}{R}=\frac{C_{\mathrm{v}}\cdot M}{R}=-\tau^{2}\cdot\varphi_{\tau\tau} \tag{22}$$

4.3.2.6 Isobaric heat capacity

The expression for the isobaric heat capacity, c_{p}, is given by Equation (23):

$$\begin{aligned}\frac{c_{\mathrm{p}}}{R} &= \frac{C_{\mathrm{p}}\cdot M}{R}\\ &= -\tau^{2}\cdot\varphi_{\tau\tau}+\frac{\varphi_2^{2}}{\varphi_1}\\ &= \frac{c_{\mathrm{v}}}{R}+\frac{\varphi_2^{2}}{\varphi_1}\\ &= \frac{C_{\mathrm{v}}\cdot M}{R}+\frac{\varphi_2^{2}}{\varphi_1}\end{aligned} \tag{23}$$

4.3.2.7 Joule-Thomson coefficient

The expression for the Joule-Thomson coefficient, μ, is given by Equation (24):

$$\begin{aligned}\mu\cdot R\cdot\rho &= \frac{\mu\cdot R\cdot D}{M}\\ &= \frac{\varphi_2-\varphi_1}{\varphi_2^{2}-\left(\tau^{2}\cdot\varphi_{\tau\tau}\cdot\varphi_1\right)}\\ &= \frac{R}{c_{\mathrm{p}}}\left(\frac{\varphi_2}{\varphi_1}-1\right)\\ &= \frac{R}{C_{\mathrm{p}}\cdot M}\left(\frac{\varphi_2}{\varphi_1}-1\right)\end{aligned} \tag{24}$$

4.3.2.8 Isentropic exponent

The expression for the isentropic exponent, κ, is given by Equation (25):

$$\begin{aligned}\kappa &= \frac{\varphi_1 - \dfrac{\varphi_2^2}{\tau^2 \cdot \varphi_{\tau\tau}}}{\delta \cdot \varphi_\delta} \\ &= \frac{\varphi_1 + \dfrac{R}{c_\mathrm{v}} \varphi_2^2}{Z} \\ &= \frac{\varphi_1 + \dfrac{R}{C_\mathrm{v} \cdot M} \varphi_2^2}{Z} \\ &= \frac{\varphi_1}{Z} \cdot \frac{c_\mathrm{p}}{c_\mathrm{v}} = \frac{\varphi_1}{Z} \cdot \frac{C_\mathrm{p}}{C_\mathrm{v}}\end{aligned} \qquad (25)$$

4.3.2.9 Speed of sound

The expression for the speed of sound, w, is given by Equation (26):

$$\begin{aligned}\frac{w^2 \cdot M}{R \cdot T} &= \varphi_1 - \frac{\varphi_2^2}{\tau^2 \cdot \varphi_{\tau\tau}} \\ &= Z \cdot \kappa = \varphi_1 \frac{c_\mathrm{p}}{c_\mathrm{v}} \\ &= \varphi_1 \frac{C_\mathrm{p}}{C_\mathrm{v}}\end{aligned} \qquad (26)$$

5 Method of calculation

5.1 Input variables

Although the natural formulation of the method presented in this part of ISO 20765 uses reduced density, inverse reduced temperature and molar composition as the input variables, the input variables most usually available for use are the absolute pressure, absolute temperature and the molar composition. In consequence, it is usually necessary first to evaluate the inverse reduced temperature and the reduced density from the available input. The conversion from temperature to inverse reduced temperature is given by Equation (3). The conversion from pressure to reduced density can be carried out as described in 5.2.

If, instead of the pressure, p, the (mass) density, D, is available as input, then δ is obtained directly, without the need for the procedure described in 5.2, as $\delta = D \cdot K^3/M$, where M is the molar mass given by Equation (16).

The composition is required by mole fractions of the following 21 components: nitrogen, carbon dioxide, methane, ethane, propane, n-butane, iso-butane (2-methylpropane), n-pentane, iso-pentane (2-methylbutane), n-hexane, n-heptane, n-octane, n-nonane, n-decane, hydrogen, oxygen, carbon monoxide, water, hydrogen sulfide, helium and argon. For the allowable ranges of mole fraction to which the method applies, see 6.2. Any trace component present but not identified as one of the 21 specified components may be assigned appropriately to one of these 21 components (see Annex E).

The sum of all mole fractions shall be unity. If the sum of all mole fractions is not unity then the composition is either faulty or incomplete. The user shall not proceed until the source of this problem has been identified and eliminated.

If the mole fractions of heptanes, octanes, nonanes and decanes are unknown, then the 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.

NOTE If the composition is known by volume fractions, these will need to be converted to mole fractions using the method given in ISO 6976 [5].

5.2 Conversion from pressure to reduced density

Combination of Equations (4), (9) and (18) results in Equation (27):

$$\frac{p \cdot \tau \cdot K^3}{\delta \cdot R \cdot L} = Z = 1 + \frac{B \cdot \delta}{K^3} - \delta \sum_{n=13}^{18} C_n \cdot \tau^{u_n} + \sum_{n=13}^{58} C_n \cdot \tau^{u_n} \cdot \delta^{b_n} \left(b_n - c_n \cdot k_n \cdot \delta^{k_n} \right) \exp\left(-c_n \cdot \delta^{k_n} \right) \tag{27}$$

If the input variables are available as pressure, inverse reduced temperature and composition, Equation (27) may be solved for the reduced molar density, δ. The variable quantities $B(\tau,X)$, $C_n(X)$, $K(X)$ and the coefficients b_n, c_n, k_n and u_n in Equation (27) may be obtained from equations and tabulations given in Annex D (Equations (D.1), (D.6) and (D.11), and Table D.1, respectively) for these quantities. Numerical values for all pure-component and binary interaction parameters that are also required for the evaluation of Equations (D.1), (D.6) and (D.11) are given in Tables D.2 and D.3, respectively.

The solution may be obtained by any suitable numerical method but, in practice, a standard form of equation-of-state density-search algorithm may be the most convenient and satisfactory. Such algorithms usually use an initial estimate of the density (often the ideal-gas approximation) and proceed, by iterative calculations of p and δ, in order to find the value of δ that reproduces the known value of p to within a pre-established level of agreement. A suitable criterion in the present case is that the pressure calculated from the calculated reduced molar density, δ, shall reproduce the input value of p to within 1 part in 10^6.

5.3 Implementation

The required set of input variables is now available. With this revised set of input variables, reduced density, δ, inverse reduced temperature, τ, and composition, X, it is now possible to use the fundamental equation to calculate the reduced Helmholtz free energy and the other thermodynamic properties. Equation (12) formulates the reduced Helmholtz free energy as $\varphi = \varphi_0 + \varphi_r$. Equation (11) formulates the residual part of the Helmholtz free energy φ_r as a function of reduced density, δ, inverse reduced temperature, τ, and the molar composition, X. The ideal part, φ_0, formulated in Equation (8), may be developed as given by Equation (B.3) of Annex B so as to express φ as given in Equation (28):

$$\begin{aligned}\varphi = \sum_{i=1}^{N} x_i \cdot \Big\{ & (A_{0,1})_i + (A_{0,2})_i \cdot \tau + B_{0,i} \cdot \ln \tau + C_{0,i} \cdot \ln\left[\sinh(D_{0,i} \cdot \tau)\right] - E_{0,i} \cdot \ln\left[\cosh(F_{0,i} \cdot \tau)\right] + \ldots \\ & \ldots + G_{0,i} \cdot \ln\left[\sinh(H_{0,i} \cdot \tau)\right] - I_{0,i} \cdot \ln\left[\cosh(J_{0,i} \cdot \tau)\right] + \ln x_i \Big\} + \ln\left(\frac{\delta}{\delta_\theta}\right) + \ln\left(\frac{\tau_\theta}{\tau}\right) + \ldots \\ & \ldots + \frac{B \cdot \delta}{K^3} - \delta \sum_{n=13}^{18} C_n \cdot \tau^{u_n} + \sum_{n=13}^{58} C_n \cdot \tau^{u_n} \cdot \delta^{b_n} \exp(-c_n \cdot \delta^{k_n})\end{aligned} \tag{28}$$

Values for all of the coefficients $(A_{0,1})_i$, $(A_{0,2})_i$ and $B_{0,i}$ to $J_{0,i}$ for the ideal gas are given in Annex B for all of the 21 possible component gases.

Derivatives of φ with respect to (reduced) density and (inverse reduced) temperature, which are needed for the evaluation of the various thermodynamic properties, may be obtained from Equations (C.2) to (C.6) given in Annex C. Finally, the various thermodynamic properties may be evaluated by means of Equations (17) to (26). Values for the coefficients b_n, c_n, k_n and u_n and the quantities C_n, which are functions of composition, are given in Annex D.

A more detailed description of the implementation procedure is given in Annex F.

6 Ranges of application

6.1 Pressure and temperature

The method described in this part of ISO 20765 applies only to pipeline quality gases (see 6.2) for those ranges of pressure and temperature within which transmission and distribution operations normally take place. The relevant ranges of pressure and temperature are given in Table 1. The method applies strictly to mixtures in the gaseous state and is subject to the specific restriction that it shall not be taken as valid for any set of conditions for which the calculated value of compression factor is less than 0,5.

Table 1 — Ranges of application for pipeline quality gas

Pressure (absolute), MPa	$0 < p \leqslant 30$
Temperature, K	$250 \leqslant T \leqslant 350$

6.2 Pipeline quality gas

Pipeline quality gas shall be taken as a natural (or similar) gas with mole fractions of the various major and minor components that fall within the ranges given in Table 2.

Possible trace components of natural gases, and details of how to deal with these, are discussed in Annex E. The total combined content of all trace components shall not exceed 0,000 5 mole fraction.

Table 2 — Ranges of mole fractions for major and minor components of natural gas

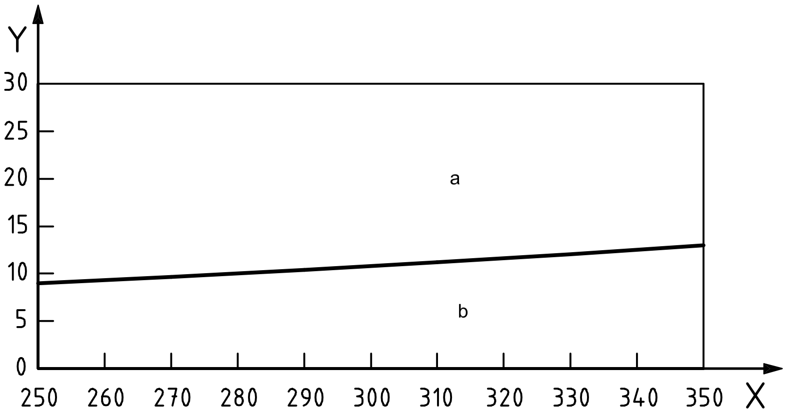
Number i	Component	Range mole fraction
1	nitrogen	$0 \leqslant x_{\mathrm{N2}} \leqslant 0{,}20$
2	carbon dioxide	$0 \leqslant x_{\mathrm{CO2}} \leqslant 0{,}20$
3	methane	$0{,}7 \leqslant x_{\mathrm{CH4}} \leqslant 1{,}00$
4	ethane	$0 \leqslant x_{\mathrm{C2H6}} \leqslant 0{,}10$
5	propane	$0 \leqslant x_{\mathrm{C3H8}} \leqslant 0{,}035$
6 + 7	n-butane + iso-butane	$0 \leqslant x_{\mathrm{C4H10}} \leqslant 0{,}015$
8 + 9	n-pentane + iso-pentane	$0 \leqslant x_{\mathrm{C5H12}} \leqslant 0{,}005$
10	n-hexane	$0 \leqslant x_{\mathrm{C6H14}} \leqslant 0{,}001$
11	n-heptane	$0 \leqslant x_{\mathrm{C7H16}} \leqslant 0{,}000\,5$
12 + 13 + 14	n-octane + n-nonane + n-decane	$0 \leqslant x_{\mathrm{C8+}} \leqslant 0{,}000\,5$
15	hydrogen	$0 \leqslant x_{\mathrm{H2}} \leqslant 0{,}10$
17	carbon monoxide	$0 \leqslant x_{\mathrm{CO}} \leqslant 0{,}03$
18	water	$0 \leqslant x_{\mathrm{H2O}} \leqslant 0{,}000\,15$
20	helium	$0 \leqslant x_{\mathrm{He}} \leqslant 0{,}005$
16	oxygen	$0 \leqslant x_{\mathrm{O2}} \leqslant 0{,}000\,2$
19	hydrogen sulfide	$0 \leqslant x_{\mathrm{H2S}} \leqslant 0{,}000\,2$
21	argon	$0 \leqslant x_{\mathrm{Ar}} \leqslant 0{,}000\,2$

7 Uncertainty

7.1 Uncertainty for pipeline quality gas

7.1.1 Uncertainty diagrams for methane

As a guide to the uncertainty which may be expected for mixtures containing a mole fraction of methane close to unity, Figures 1 to 3 present uncertainty diagrams for pure methane for compression factor, speed of sound and enthalpy, respectively. The uncertainty, expressed as a 95 % confidence limit, given for each region represents the largest value within the region of the sum of (a) the uncertainty in well-documented reference data, and (b) the difference between the reference data and the value of the property calculated using the method presented in this part of ISO 20765. The reference data used are calculated from equations given in Reference [6].



Key

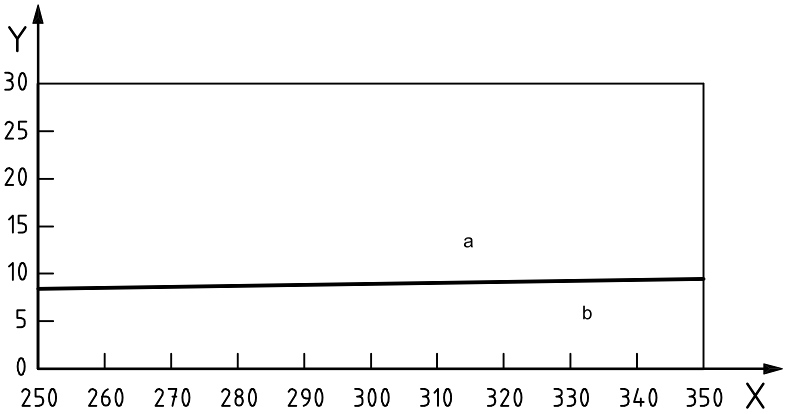
X temperature, expressed in kelvin

Y pressure, expressed in megapascals

[a] Region of uncertainty of ± 0,08 %.

[b] Region of uncertainty of ± 0,04 %.

Figure 1 — Uncertainty diagram for Z, the compression factor of methane



Key

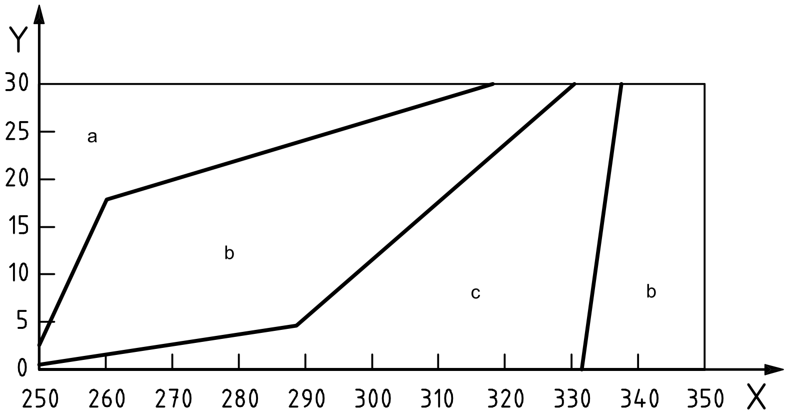
X temperature, expressed in kelvin

Y pressure, expressed in megapascals

[a] Region of uncertainty of ± 0,20 %.

[b] Region of uncertainty of ± 0,05 %.

Figure 2 — Uncertainty diagram for w, the speed of sound of methane



Key

X temperature, expressed in kelvin

Y pressure, expressed in megapascals

[a] Region of uncertainty of ± 3 kJ/kg.

[b] Region of uncertainty of ± 2 kJ/kg.

[c] Region of uncertainty of ± 1 kJ/kg.

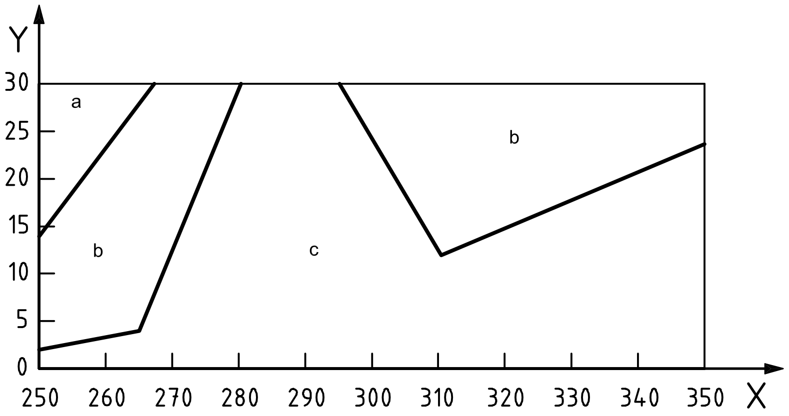
Figure 3 — Uncertainty diagram for H, the enthalpy of methane

7.1.2 Uncertainty diagrams for natural gas

As a guide to the uncertainty that can be expected for natural gases, Figures 4, 5 and 6 present uncertainty diagrams for compression factor, speed of sound and enthalpy, respectively. The uncertainty, expressed as a 95 % confidence limit, given for each region represents the largest difference, for a wide range of natural gases, between the directly measured property and the value calculated using the method presented in this part of ISO 20765. For the compression factor, the directly measured values are taken from Reference [7]; for speed of sound, the values are taken from Reference [8] and for the enthalpy, the values are taken from Reference [9].

NOTE 1 For all gases, the uncertainty diagram for density is identical in form to that for compression factor.

NOTE 2 For all gases, the uncertainty in the isentropic exponent is approximately twice the uncertainty in speed of sound.



Key

X temperature, expressed in kelvin

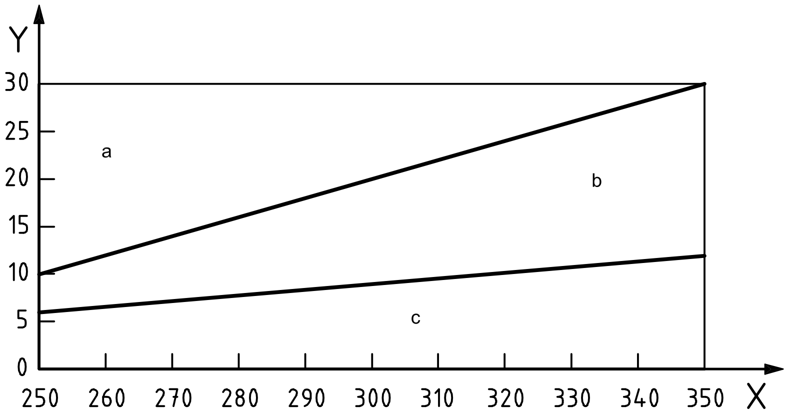
Y pressure, expressed in megapascals

[a] Region of uncertainty of ± 0,4 %.

[b] Region of uncertainty of ± 0,2 %.

[c] Region of uncertainty of ± 0,1 %.

Figure 4 — Uncertainty diagram for Z, the compression factor of natural gas



Key

X temperature, expressed in kelvin

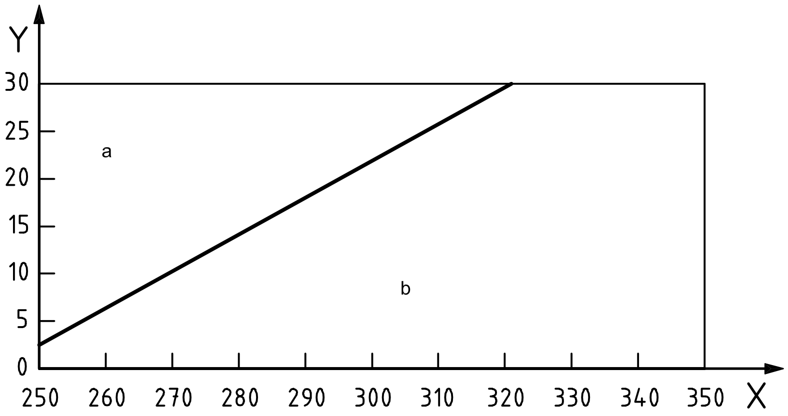
Y pressure, expressed in megapascals

[a] Region of uncertainty of ± 2,0 %.

[b] Region of uncertainty of ± 0,8 %.

[c] Region of uncertainty of ± 0,2 %.

Figure 5 — Uncertainty diagram for w, the speed of sound of natural gas



Key

X temperature, expressed in kelvin

Y pressure, expressed in megapascals

[a] Region of uncertainty of ± 3 kJ/kg.

[b] Region of uncertainty of ± 2 kJ/kg.

Figure 6 — Uncertainty diagram for H, the enthalpy of natural gas

For properties other than compression factor, density (for which the uncertainty diagram is the same as for compression factor), speed of sound and enthalpy, the paucity of experimental data of good (reference) quality makes it impossible to provide definitive numerical estimates of uncertainty. Nevertheless, it is possible to offer some guidelines.

For gases at low pressures (below, say, 1 MPa) having approximately ideal behavior (compression factor greater than, say, 0,95), it is reasonable to expect all of the caloric properties to be predicted with a low uncertainty. This follows from the fact that, in this restricted case, the greater part of each property derives from the ideal part of the Helmholtz free energy that, being derived directly from high-accuracy data for the ideal isobaric heat capacity (see Annex B), is itself known with high accuracy. In this case, the density, compression factor, speed of sound, isochoric and isobaric heat capacities, isentropic exponent and Joule-Thomson coefficient are probably all predicted within 0,1 %.

7.2 Impact of uncertainties of input variables

The user should recognize that uncertainties in the input variables, usually pressure, temperature and composition by mole fractions, will have additional effects upon the uncertainty of any calculated result. In any particular application where the additional uncertainty could be of importance, the user should carry out sensitivity tests to determine its magnitude.

8 Reporting of results

When reported in accordance with the units given in Annex A, results for the thermodynamic properties shall be quoted with the number of digits after the decimal point as given in Table 3. The report shall identify the temperature, pressure (or density) and detailed composition to which the results refer. The method of calculation used shall be identified by reference to this document, e.g. ISO 20765-1.

For validation of computational procedures, it can be useful to carry extra digits (see example calculations in Annex G).

Table 3 — Reporting of results

Symbol	Property	Units	Decimal places
Z	compression factor	—	4
ρ	molar density	kmol/m^3	3
D	density	kg/m^3	2
u	molar internal energy	kJ/kmol	0
U	specific internal energy	kJ/kg	1
h	molar enthalpy	kJ/kmol	0
H	specific enthalpy	kJ/kg	1
s	molar entropy	kJ/(kmol·K)	2
S	specific entropy	kJ/(kg·K)	3
c_v	molar isochoric heat capacity	kJ/(kmol·K)	2
C_v	specific isochoric heat capacity	kJ/(kg·K)	3
c_p	molar isobaric heat capacity	kJ/(kmol·K)	2
C_p	specific isobaric heat capacity	kJ/(kg·K)	3
μ	Joule-Thomson coefficient	K/MPa	2
κ	isentropic exponent	—	2
w	speed of sound	m/s	1

Annex A
(normative)

Symbols and units

Symbol	Meaning	Source of values	Units
a_n	constants in Equations (D.2) and (D.6)	Table D.1	---
$(A_{\mathrm{o},1})_i$	coefficient in the ideal gas equation [Equation (B.3)]	Table B.1	---
$(A_{\mathrm{o},2})_i$	coefficient in the ideal gas equation [(Equation (B.3)]	Table B.1	---
b_n	constants in the real gas equation [(Equation (9)]	Table D.1	---
B	second virial coefficient	Equation (D.1)	$\mathrm{m^3/kmol}$
$B_{\mathrm{o},i}$	coefficient in the ideal gas equation [Equation (B.3)]	Table B.1	---
B_n^*	quantities in Equation (D.1)	Equation (D.2)	---
B_{nij}^*	binary interaction parameter in Equation (D.2)	Equation (D.3)	---
c_n	constants in the real gas equation [Equation (9)]	Table D.1	---
c_p	molar isobaric heat capacity	Equation (23)	kJ/(kmol·K)
c_v	molar isochoric heat capacity	Equation (22)	kJ/(kmol·K)
$C_{\mathrm{o},i}$	coefficient in the ideal gas equation [Equation (B.3)]	Table B.1	---
C_n	coefficients in the real gas equation [Equation (9)]	Equation (D.6)	---
C_p	specific isobaric heat capacity	Equation (23)	kJ/(kg·K)
C_v	specific isochoric heat capacity	Equation (22)	kJ/(kg·K)
D	specific (mass) density	Equation (18)	$\mathrm{kg/m^3}$
$D_{\mathrm{o},i}$	coefficient in the ideal gas equation [Equation (B.3)]	Table B.1	---
E_i	energy parameter in Equations (D.4) and (D.7)	Table D.2	---
$E_{\mathrm{o},i}$	coefficient in the ideal gas equation [Equation (B.3)]	Table B.1	---
E_{ij}	binary interaction energy parameter in Equation (D.2)	Equation (D.4)	---
E_{nij}^*	binary interaction energy parameter in Equation (D.4)	Table D.3	---
f	molar Helmholtz free energy	Equation (1)	kJ/kmol
f_n	constants in Equations (D.3) and (D.6)	Table D.1	---
F	constant in Equation (D.6)	Equation (D.10)	---
F_i	high temperature parameter in Equations (D.3) and (D.10)	Table D.2	---
$F_{\mathrm{o},i}$	coefficient in the ideal gas equation [Equation (B.3)]	Table B.1	---
g_n	constants in Equations (D.3) and (D.6)	Table D.1	---
G	constant in Equation (D.6)	Equation (D.8)	---
G_i	orientation parameter in Equations (D.5) and (D.8)	Table D.2	---
$G_{\mathrm{o},i}$	coefficient in the ideal gas equation [Equation (B.3)]	Table B.1	---
G_{ij}	binary interaction orientation parameter in Equation (D.3)	Equation (D.5)	---
G_{nij}^*	binary interaction orientation parameter in Equations (D.5) and (D.8)	Table D.3	---

h	molar enthalpy	Equation (20)	kJ/kmol
H	specific enthalpy	Equation (20)	kJ/kg
$H_{o,i}$	coefficient in the ideal gas equation [Equation (B.3)]	Table B.1	---
$I_{o,i}$	coefficient in the ideal gas equation [Equation (B.3)]	Table B.1	---
$J_{o,i}$	coefficient in the ideal gas equation [Equation (B.3)]	Table B.1	---
k_n	constants in the AGA8 equation [Equation (9)]	Table D.1	---
K	mixture size parameter in Equation (9)	Equation (D.11)	$(\mathrm{m}^3/\mathrm{kmol})^{1/3}$
K_i	component size parameter in Equations (D.2) and (D.11)	Table D.2	$(\mathrm{m}^3/\mathrm{kmol})^{1/3}$
K_{ij}	binary interaction size parameter in Equation (D.11)	Table D.3	---
L	reference temperature in Equation (3)	$L = 1$	K
M	molar mass of a mixture	Equation (16)	kg/kmol
M_i	molar mass of component i	Table D.2	kg/kmol
N	number of components in gas mixture	input	---
p	pressure	input	MPa
q_n	constants in Equations (D.3) and (D.6)	Table D.1	---
Q	constant in Equation (D.6)	Equation (D.9)	---
Q_i	quadrupole parameter in Equations (D.3) and (D.9)	Table D.2	---
R	molar gas constant	$R = 8{,}314\ 510$	kJ/(kmol·K)

NOTE The value given here for the molar gas constant is not the most recent value adopted by the international community of metrologists. However, it is the value that was in general use during the development of the AGA8 equation, and is therefore retained here. The difference between the value given here and presently accepted value is less than five parts per million.

s	molar entropy	Equation (21)	kJ/(kmol·K)
s_n	constants in Equation (D.3)	Table D.1	---
S	specific entropy	Equation (21)	kJ/(kg·K)
S_i	dipole parameter in Equation (D.3)	Table D.2	---
T	temperature	input	K
u	molar internal energy	Equation (19)	kJ/kmol
u_n	constants in the AGA8 equation [Equation (9)]	Table D.1	---
U	specific internal energy	Equation (19)	kJ/kg
V	constant in Equation (D.6)	Equation (D.7)	---
V_{ij}	binary interaction parameter in Equation (D.7)	Table D.3	---
w	speed of sound	Equation (26)	m/s
w_n	constants in Equation (D.3)	Table D.1	---
W_i	association parameter in Equation (D.3)	Table D.2	---
x	mole fraction	input	---
X	mixture mole fraction vector $(x_1, x_2, x_3 \ldots, x_i \ldots, x_{21})$	input	---
Z	compression factor	Equation (17)	---
δ	reduced density	Equation (4)	---
φ	reduced Helmholtz free energy	Equation (2)	---

κ	isentropic exponent	Equation (25)	---
μ	Joule-Thomson coefficient	Equation (24)	K/MPa
ρ	molar density	Equation (18)	kmol/m^3
τ	inverse reduced temperature	Equation (3)	---

Subscripts

i	for component i ($i = 1$ to N)
j	for the second component j in a binary interaction ($j = 2$ to N)
n	equation of state coefficient counter ($n = 1$ to 58)
o	for the ideal-gas state
r	for the residual part
δ	partial derivative with respect to reduced molar density
θ	for the reference state ($T_\theta = 298{,}15$ K, $p_\theta = 0{,}101\ 325$ MPa)
τ	partial derivative with respect to inverse reduced temperature

Annex B
(normative)

The Helmholtz free energy of the ideal gas

B.1 Calculation of the Helmholtz free energy of the ideal gas

a) The ideal isobaric heat capacity of a single component [3, 4] may be written as in Equation (B.1)

$$\frac{(c_{\text{o,p}})_i}{R} = B_{\text{o},i} + C_{\text{o},i}\left[\frac{D_{\text{o},i}\cdot\tau}{\sinh(D_{\text{o},i}\cdot\tau)}\right]^2 + E_{\text{o},i}\left[\frac{F_{\text{o},i}\cdot\tau}{\cosh(F_{\text{o},i}\cdot\tau)}\right]^2 + G_{\text{o},i}\left[\frac{H_{\text{o},i}\cdot\tau}{\sinh(H_{\text{o},i}\cdot\tau)}\right]^2 + \ldots$$
$$\ldots I_{\text{o},i}\left[\frac{J_{\text{o},i}\cdot\tau}{\cosh(J_{\text{o},i}\cdot\tau)}\right]^2 \tag{B.1}$$

Equation (B.1) may be generalized to the case of an N-component mixture by use of Equation (B.2):

$$\frac{c_{\text{o,p}}}{R} = \sum_{i=1}^{N} x_i \frac{(c_{\text{o,p}})_i}{R} \tag{B.2}$$

b) This formulation for the ideal isobaric heat capacity, $c_{\text{p,o}}$, may be inserted into Equation (8) for the reduced Helmholtz free energy, φ_o. The integrations in Equation (8) may then be performed, yielding Equation (B.3):

$$\varphi_\text{o} = \sum_{i=1}^{N} x_i \cdot \Big\{ (A_{\text{o},1})_i + (A_{\text{o},2})_i \cdot \tau + B_{\text{o},i}\cdot\ln\tau + C_{\text{o},i}\cdot\ln\big[\sinh(D_{\text{o},i}\cdot\tau)\big] - E_{\text{o},i}\cdot\ln\big[\cosh(F_{\text{o},i}\cdot\tau)\big] + \ldots$$
$$\ldots + G_{\text{o},i}\cdot\ln\big[\sinh(H_{\text{o},i}\cdot\tau)\big] - I_{\text{o},i}\cdot\ln\big[\cosh(J_{\text{o},i}\cdot\tau)\big] + \ln x_i \Big\} + \ln\left(\frac{\delta}{\delta_\theta}\right) + \ln\left(\frac{\tau_\theta}{\tau}\right) \tag{B.3}$$

In Equation (B.3), the constants $(A_{\text{o},1})_i$ and $(A_{\text{o},2})_i$ are related to the integration constants $(s_{\text{o},\theta})_i$ and $(h_{\text{o},\theta})_i$ of Equation (8) in accordance with Equations (B.4) and (B.5):

$$(A_{\text{o},1})_i = -(s_{\text{o},\theta})_i / R + B_{\text{o},i} - 1 \tag{B.4}$$

$$(A_{\text{o},2})_i = (h_{\text{o},\theta})_i / R \cdot L \tag{B.5}$$

It is important to observe, in Equation (B.3), that φ_o is a function of the reduced molar density, δ, of the real gas (i.e. not the reduced molar density of the ideal gas) and, therefore, cannot be completely evaluated until a value for δ is available (see Annex D). Equation (B.3) shall be used for the calculation of the reduced Helmholtz free energy of the ideal gas.

c) The best available values in the scientific literature for the ideal isobaric heat capacity, $c_{\text{o,p}}$, have recently been taken as source data and re-correlated[4] so as to provide numerical values of the constants A_o to J_o for the 21 pure component gases considered in this part of ISO 20765.

Values of the constants $(A_{\text{o},1})_i$ and $(A_{\text{o},2})_i$ and constants $B_{\text{o},i}$ to $J_{\text{o},\,i}$ for use in Equation (B.3) are given in Table B.1.

B.2 Derivatives of the Helmholtz free energy of the ideal gas

For some of the thermodynamic properties, the calculation requires first and second partial derivatives of the reduced Helmholtz free energy, φ_o, of the ideal gas equation [Equation (B.3)] with respect to inverse reduced temperature, τ. The relevant mathematical expressions are given in Equations (B.6) and (B.7):

$$\begin{aligned}\varphi_{\mathrm{o},\tau} &= \left(\frac{\partial \varphi_\mathrm{o}}{\partial \tau}\right)_{\delta,x_i} \\ &= \sum_{i=1}^{N} x_i \cdot \left[(A_{\mathrm{o},2})_i + \frac{(B_{\mathrm{o},i}-1)}{\tau} + C_{\mathrm{o},i}\cdot D_{\mathrm{o},i}\frac{\cosh(D_{\mathrm{o},i}\cdot\tau)}{\sinh(D_{\mathrm{o},i}\cdot\tau)} - E_{\mathrm{o},i}\cdot F_{\mathrm{o},i}\frac{\sinh(F_{\mathrm{o},i}\cdot\tau)}{\cosh(F_{\mathrm{o},i}\cdot\tau)} + \ldots \right. \\ &\qquad \left. \ldots + G_{\mathrm{o},i}\cdot H_{\mathrm{o},i}\frac{\cosh(H_{\mathrm{o},i}\cdot\tau)}{\sinh(H_{\mathrm{o},i}\cdot\tau)} - I_{\mathrm{o},i}\cdot J_{\mathrm{o},i}\frac{\sinh(J_{\mathrm{o},i}\cdot\tau)}{\cosh(J_{\mathrm{o},i}\cdot\tau)} \right]\end{aligned} \tag{B.6}$$

and

$$\begin{aligned}\varphi_{\mathrm{o},\tau\tau} &= \left(\frac{\partial^2 \varphi_\mathrm{o}}{\partial \tau^2}\right)_{\delta,x_i} = -\tau^{-2}\left(\frac{c_{\mathrm{o,p}}}{R} - 1\right) \\ &= \sum_{i=1}^{N} x_i \cdot \left\{ -\frac{(B_{\mathrm{o},i}-1)}{\tau^2} - C_{\mathrm{o},i}\left[\frac{D_{\mathrm{o},i}}{\sinh(D_{\mathrm{o},i}\cdot\tau)}\right]^2 - E_{\mathrm{o},i}\left[\frac{F_{\mathrm{o},i}}{\cosh(F_{\mathrm{o},i}\cdot\tau)}\right]^2 - \ldots \right. \\ &\qquad \left. \ldots - G_{\mathrm{o},i}\left[\frac{H_{\mathrm{o},i}}{\sinh(H_{\mathrm{o},i}\cdot\tau)}\right]^2 - I_{\mathrm{o},i}\left[\frac{J_{\mathrm{o},i}}{\cosh(J_{\mathrm{o},i}\cdot\tau)}\right]^2 \right\}\end{aligned} \tag{B.7}$$

Table B.1 — Values for parameters in Equation (B.3) for the Helmholtz free energy of the ideal gas

i	**Component**	$(A_{o,1})_i$	$(A_{o,2})_i$	$B_{o,i}$	$C_{o,i}$	$D_{o,i}$	$E_{o,i}$	$F_{o,i}$	$G_{o,i}$	$H_{o,i}$	$I_{o,i}$	$J_{o,i}$
1	nitrogen	23,265 30	–2 801,729 07	3,500 31	0,137 32	662,738	–0,146 60	680,562	0,900 66	1 740,06	0	0
2	carbon dioxide	26,356 04	–4 902,171 52	3,500 02	2,044 52	919,306	–1,060 44	865,070	2,033 66	483,553	0,013 93	341,109
3	methane	35,536 03	–15 999,691 51	4,000 88	0,763 15	820,659	0,004 60	178,410	8,744 32	1 062,82	–4,469 21	1 090,53
4	ethane	42,427 66	–23 639,653 01	4,002 63	4,339 39	559,314	1,237 22	223,284	13,197 4	1 031,38	–6,019 89	1 071,29
5	propane	50,406 69	–31 236,635 51	4,029 39	6,605 69	479,856	3,197 00	200,893	19,192 1	955,312	–8,372 67	1 027,29
6	n-butane	42,229 97	–38 957,809 33	4,339 44	9,448 93	468,270	6,894 06	183,636	24,461 8	1 914,10	14,782 4	903,185
7	iso-butane	39,999 40	–38 525,502 76	4,067 14	8,975 75	438,270	5,251 56	198,018	25,142 3	1 905,02	16,138 8	893,765
8	n-pentane	48,375 97	–45 215,830 00	4	8,950 43	178,670	21,836 0	840,538	33,403 2	1 774,25	0	0
9	iso-pentane	48,869 78	–51 198,309 46	4	11,761 8	292,503	20,110 1	910,237	33,168 8	1 919,37	0	0
10	n-hexane	52,694 77	–52 746,833 18	4	11,697 7	182,326	26,814 2	859,207	38,616 4	1 826,59	0	0
11	n-heptane	57,773 91	–57 104,810 56	4	13,726 6	169,789	30,470 7	836,195	43,556 1	1 760,46	0	0
12	n-octane	62,955 91	–60 546,763 85	4	15,686 5	158,922	33,802 9	815,064	48,173 1	1 693,07	0	0
13	n-nonane	67,794 07	–66 600,128 37	4	18,024 1	156,854	38,123 5	814,882	53,341 5	1 693,79	0	0
14	n-decane	71,636 69	–74 131,454 83	4	21,006 9	164,947	43,493 1	836,264	58,365 7	1 750,24	0	0
15	hydrogen	18,772 80	–5 836,943 70	2,479 06	0,958 06	228,734	0,454 44	326,843	1,560 39	1 651,71	–1,375 6	1 671,69
16	oxygen	22,499 31	–2 318,322 69	3,501 46	1,075 58	2 235,71	1,013 34	1 116,69	0	0	0	0
17	carbon monoxide	23,155 47	–2 635,244 12	3,500 55	1,028 65	1 550,45	0,004 93	704,525	0	0	0	0
18	water	27,276 42	–7 766,733 08	4,003 92	0,010 59	268,795	0,987 63	1 141,41	3,069 04	2 507,37	0	0
19	hydrogen sulfide	27,280 69	–6 069,035 87	4	3,119 42	1 833,63	1,002 43	847,181	0	0	0	0
20	helium	15,743 99	–745,375 00	2,5	0	0	0	0	0	0	0	0
21	argon	15,743 99	–745,375 00	2,5	0	0	0	0	0	0	0	0

Annex C
(normative)

The equation for the Helmholtz free energy

C.1 Calculation of the Helmholtz free energy

The reduced Helmholtz free energy for the specified gas mixture shall be calculated from Equation (C.1):

$$\varphi = \varphi_0 + \frac{B\cdot\delta}{K^3} - \delta\sum_{n=13}^{18} C_n\cdot\tau^{u_n} + \sum_{n=13}^{58} C_n\cdot\tau^{u_n}\cdot\delta^{b_n}\exp(-c_n\cdot\delta^{k_n}) \tag{C.1}$$

where φ_0 shall be calculated in accordance with the procedure described in Annex B. That part of Equation (C.1) which accounts for the residual part of the Helmholtz free energy (all of the right-hand side except for φ_0) is from Equation (11). Equations for calculation of the variable quantities $B(\tau, X)$, $C_n(X)$ and $K(X)$ in Equation (C.1) are given in D.1. Values of the various constants in Equation (C.1) are given in D.2.

C.2 Derivatives of the Helmholtz free energy

The calculation of various thermodynamic properties requires first and/or second partial derivatives with respect to inverse reduced temperature and/or to reduced density of the reduced Helmholtz free energy. The relevant mathematical expressions are given as Equations (C.2) to (C.6):

$$\begin{aligned}\tau\cdot\varphi_\tau = \tau\left(\frac{\partial\varphi}{\partial\tau}\right)_{\delta,X} &= \tau\cdot\varphi_{0,\tau} + \frac{\delta}{K^3}\cdot\sum_{n=1}^{18} u_n\cdot B_n^*\cdot\tau^{u_n} - \delta\sum_{n=13}^{18} u_n\cdot C_n\cdot\tau^{u_n} + \ldots \\ &\ldots + \sum_{n=13}^{58} u_n\cdot C_n\cdot\tau^{u_n}\cdot\delta^{b_n}\cdot\exp\left(-c_n\cdot\delta^{k_n}\right)\end{aligned} \tag{C.2}$$

$$\begin{aligned}\tau^2\cdot\varphi_{\tau\tau} = \tau^2\left(\frac{\partial^2\varphi}{\partial\tau^2}\right)_{\delta,X} &= \tau^2\cdot\varphi_{0,\tau\tau} + \frac{\delta}{K^3}\sum_{n=1}^{18}(u_n^2 - u_n)\cdot B_n^*\cdot\tau^{u_n} - \delta\sum_{n=13}^{18}(u_n^2 - u_n)\cdot C_n\cdot\tau^{u_n} + \ldots \\ &\ldots + \sum_{n=13}^{58}(u_n^2 - u_n)\cdot C_n\cdot\tau^{u_n}\cdot\delta^{b_n}\cdot\exp\left(-c_n\cdot\delta^{k_n}\right)\end{aligned} \tag{C.3}$$

$$\begin{aligned}\delta\cdot\varphi_\delta = \delta\left(\frac{\partial\varphi}{\partial\delta}\right)_{\tau,X} &= 1 + \frac{B\cdot\delta}{K^3} - \delta\sum_{n=13}^{18} C_n\cdot\tau^{u_n} + \ldots \\ &\ldots + \sum_{n=13}^{58} C_n\cdot\tau^{u_n}\cdot\delta^{b_n}\left(b_n - c_n\cdot k_n\cdot\delta^{k_n}\right)\cdot\exp\left(-c_n\cdot\delta^{k_n}\right)\end{aligned} \tag{C.4}$$

$$\begin{aligned}\varphi_1 = \left(\delta^2\cdot\varphi_\delta\right)_\delta = \left[\frac{\partial(\delta^2\cdot\varphi_\delta)}{\partial\delta}\right]_{\tau,X} &= 1 + 2\cdot\frac{B\cdot\delta}{K^3} - 2\cdot\delta\sum_{n=13}^{18} C_n\cdot\tau^{u_n} + \ldots \\ \ldots + \sum_{n=13}^{58} C_n\cdot\tau^{u_n}\cdot\delta^{b_n}\cdot&\left[b_n - (1+k_n)c_n\cdot k_n\cdot\delta^{k_n} + (b_n - c_n\cdot k_n\cdot\delta^{k_n})^2\right]\exp\left(-c_n\cdot\delta^{k_n}\right)\end{aligned} \tag{C.5}$$

$$\varphi_2 = -\tau^2 \left(\delta \cdot \varphi_\delta / \tau\right)_\tau = -\tau^2 \left[\frac{\partial(\delta \cdot \varphi_\delta / \tau)}{\partial \tau}\right]_{\delta,X} = 1 + \frac{\delta}{K^3} \sum_{n=1}^{18} \left(1 - u_n\right) \cdot B_n^* \cdot \tau^{u_n} - \delta \sum_{n=13}^{18} \left(1 - u_n\right) \cdot C_n \cdot \tau^{u_n} + \ldots$$
$$\ldots + \sum_{n=13}^{58} \left(1 - u_n\right) \cdot C_n \cdot \tau^{u_n} \cdot \delta^{b_n} \cdot \left(b_n - c_n \cdot k_n \cdot \delta^{k_n}\right) \exp\left(-c_n \cdot \delta^{k_n}\right) \qquad \text{(C.6)}$$

Equations and constants required for the evaluation of Equations (C.2) to (C.6) are given in Annex D.

Annex D
(normative)

Detailed documentation for the equation of state

D.1 Subsidiary equations

In order to evaluate Equation (C.1), it is necessary to assign values to the second virial coefficient, $B(\tau, X)$, to the quantities $C_n(X)$ and to the size parameter $K(X)$. In addition, because Equation (C.1) is explicit in the reduced molar density, δ, it is also necessary to have a means to relate this quantity to the usual input variable of pressure. These matters are dealt with in D.1 a) to D.1 d).

a) The second virial coefficient shall be calculated using Equations (D.1) to (D.5), together with the values of the relevant constants from Tables D.1 to D.3:

$$B(\tau, X) = \sum_{n=1}^{18} B_n^* \cdot \tau^{u_n} \tag{D.1}$$

where

$$B_n^* = a_n \sum_{i=1}^{N} \sum_{j=1}^{N} x_i \cdot x_j \cdot B_{nij}^* \cdot E_{ij}^{u_n} \cdot (K_i K_j)^{3/2} \tag{D.2}$$

where

$$B_{nij}^* = (G_{ij} + 1 - g_n)^{g_n} (Q_i Q_j + 1 - q_n)^{q_n} (\sqrt{F_i F_j} + 1 - f_n)^{f_n} (S_i S_j + 1 - s_n)^{s_n} (W_i W_j + 1 - w_n)^{w_n} \tag{D.3}$$

and

$$E_{ij} = E_{ij}^* \cdot \sqrt{E_i E_j} \tag{D.4}$$

$$G_{ij} = G_{ij}^* \cdot (G_i + G_j)/2 \tag{D.5}$$

b) The quantities C_n (for $n = 13$ to 58) shall be calculated using Equations (D.6) to (D.10), together with the values of the relevant constants from Tables D.1 to D.3:

$$C_n(X) = a_n (G + 1 - g_n)^{g_n} (Q^2 + 1 - q_n)^{q_n} (F + 1 - f_n)^{f_n} V^{u_n} \tag{D.6}$$

where

$$V^5 = \left(\sum_{i=1}^{N} x_i \cdot E_i^{5/2} \right)^2 + 2 \cdot \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} x_i \cdot x_j \cdot (V_{ij}^5 - 1)(E_i E_j)^{5/2} \tag{D.7}$$

$$G = \sum_{i=1}^{N} x_i \cdot G_i + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} x_i \cdot x_j \cdot (G_{\text{ast},ij} - 1)(G_i + G_j) \tag{D.8}$$

$$Q = \sum_{i=1}^{N} x_i \cdot Q_i \tag{D.9}$$

$$F = \sum_{i=1}^{N} x_i^2 \cdot F_i \tag{D.10}$$

In Table D.2, F_i is zero for all components except hydrogen, for which $F_{15} = 1{,}0$ and W_i is zero for all components except water, for which $W_{18} = 1{,}0$. Many of the interaction parameters in Table D.3 have a value of unity.

c) The mixture size parameter $K(X)$ shall be calculated using Equation (D.11) together with the values of the relevant constants from Tables D.2 and D.3.

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

Many values of K_{ij} have a value of unity.

d) The reduced molar density, δ (p, τ, X), shall be determined as the solution of Equation (D.12) (Equation (27) of the main text rewritten so as to be explicit in pressure).

$$p = \frac{\delta \cdot R \cdot L}{\tau \cdot K^3} \left[1 + \frac{B \cdot \delta}{K^3} - \delta \cdot \sum_{n=13}^{18} C_n \cdot \tau^{u_n} + \sum_{n=13}^{58} C_n \cdot \tau^{u_n} \cdot \delta^{b_n} (b_n - c_n \cdot k_n \cdot \delta^{k_n}) \exp(-c_n \cdot \delta^{k_n}) \right] \tag{D.12}$$

Equation (D.12) may be solved using a standard equation-of-state density-search algorithm.

D.2 Values of constants for the equation of state

This section lists values for all the constants needed to implement the AGA8 equation of state through Equations (C.1) and (D.1) to (D.12). Table D.1 gives values for those constants generic to the structure of the equation. Table D.2 gives values for those constants that relate to the properties of individual components. Table D.3 gives values for those constants that relate to the properties of pair-wise (binary) unlike molecule interactions between components.

Table D.1 — Constants of the equation of state

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 × 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
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 × 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

Table D.2 — Pure component characterization parameters

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

Table D.3 — Binary interaction parameters

i	*j*	**Component pair**		E_{ij}^*	V_{ij}	K_{ij}	G_{ij}^*
1	2	nitrogen	carbon dioxide	1,022 740	0,835 058	0,982 361	0,982 746
1	3	nitrogen	methane	0,971 640	0,886 106	1,003 630	1,0
1	4	nitrogen	ethane	0,970 120	0,816 431	1,007 960	1,0
1	5	nitrogen	propane	0,945 939	0,915 502	1,0	1,0
1	6	nitrogen	n-butane	0,973 384	0,993 556	1,0	1,0
1	7	nitrogen	iso-butane	0,946 914	1,0	1,0	1,0
1	8	nitrogen	n-pentane	0,945 520	1,0	1,0	1,0
1	9	nitrogen	iso-pentane	0,959 340	1,0	1,0	1,0
1	15	nitrogen	hydrogen	1,086 320	0,408 838	1,032 270	1,0
1	16	nitrogen	oxygen	1,021 000	1,0	1,0	1,0
1	17	nitrogen	carbon monoxide	1,005 710	1,0	1,0	1,0
1	18	nitrogen	water	0,746 954	1,0	1,0	1,0
1	19	nitrogen	hydrogen sulfide	0,902 271	0,993 476	0,942 596	1,0
2	3	carbon dioxide	methane	0,960 644	0,963 827	0,995 933	0,807 653
2	4	carbon dioxide	ethane	0,925 053	0,969 870	1,008 510	0,370 296
2	5	carbon dioxide	propane	0,960 237	1,0	1,0	1,0
2	6	carbon dioxide	n-butane	0,897 362	1,0	1,0	1,0
2	7	carbon dioxide	iso-butane	0,906 849	1,0	1,0	1,0
2	8	carbon dioxide	n-pentane	0,859 764	1,0	1,0	1,0
2	9	carbon dioxide	iso-pentane	0,726 255	1,0	1,0	1,0
2	10	carbon dioxide	n-hexane	0,855 134	1,066 638	0,910 183	1,0
2	11	carbon dioxide	n-heptane	0,831 229	1,077 634	0,895 362	1,0
2	12	carbon dioxide	n-octane	0,808 310	1,088 178	0,881 152	1,0
2	13	carbon dioxide	n-nonane	0,786 323	1,098 291	0,867 520	1,0
2	14	carbon dioxide	n-decane	0,765 171	1,108 021	0,854 406	1,0
2	15	carbon dioxide	hydrogen	1,281 790	1,0	1,0	1,0
2	17	carbon dioxide	carbon monoxide	1,500 000	0,900 000	1,0	1,0
2	18	carbon dioxide	water	0,849 408	1,0	1,0	1,673 090
2	19	carbon dioxide	hydrogen sulfide	0,955 052	1,045290	1,007 790	1,0
3	5	methane	propane	0,994 635	0,990 877	1,007 619	1,0
3	6	methane	n-butane	0,989 844	0,992 291	0,997 596	1,0
3	7	methane	iso-butane	1,019 530	1,0	1,0	1,0
3	8	methane	n-pentane	0,999 268	1,003 670	1,002 529	1,0
3	9	methane	iso-pentane	1,002 350	1,0	1,0	1,0
3	10	methane	n-hexane	1,107 274	1,302 576	0,982 962	1,0
3	11	methane	n-heptane	0,880 880	1,191 904	0,983 565	1,0
3	12	methane	n-octane	0,880 973	1,205 769	0,982 707	1,0

Table D.3 (*continued*)

i	j	**Component pair**		E_{ij}^{*}	V_{ij}	K_{ij}	G_{ij}^{*}
3	13	methane	n-nonane	0,881 067	1,219 634	0,981 849	1,0
3	14	methane	n-decane	0,881 161	1,233 498	0,980 991	1,0
3	15	methane	hydrogen	1,170 520	1,156 390	1,023 260	1,957 310
3	17	methane	carbon monoxide	0,990 126	1,0	1,0	1,0
3	18	methane	water	0,708 218	1,0	1,0	1,0
3	19	methane	hydrogen sulfide	0,931 484	0,736 833	1,000 080	1,0
4	5	ethane	propane	1,022 560	1,065 173	0,986 893	1,0
4	6	ethane	n-butane	1,013 060	1,250 000	1,0	1,0
4	7	ethane	iso-butane	1,0	1,250 000	1,0	1,0
4	8	ethane	n-pentane	1,005 320	1,250 000	1,0	1,0
4	9	ethane	iso-pentane	1,0	1,250 000	1,0	1,0
4	15	ethane	hydrogen	1,164 460	1,616 660	1,020 340	1,0
4	18	ethane	water	0,693 168	1,0	1,0	1,0
4	19	ethane	hydrogen sulfide	0,946 871	0,971 926	0,999 969	1,0
5	6	propane	n-butane	1,004 900	1,0	1,0	1,0
5	15	propane	hydrogen	1,034 787	1,0	1,0	1,0
6	15	n-butane	hydrogen	1,300 000	1,0	1,0	1,0
7	15	iso-butane	hydrogen	1,300 000	1,0	1,0	1,0
10	19	n-hexane	hydrogen sulfide	1,008 692	1,028 973	0,968 130	1,0
11	19	n-heptane	hydrogen sulfide	1,010 126	1,033 754	0,962 870	1,0
12	19	n-octane	hydrogen sulfide	1,011 501	1,038 338	0,957 828	1,0
13	19	n-nonane	hydrogen sulfide	1,012 821	1,042 735	0,952 441	1,0
14	19	n-decane	hydrogen sulfide	1,014 089	1,046 966	0,948 338	1,0
15	17	hydrogen	carbon monoxide	1,100 000	1,0	1,0	1,0

The interaction parameters for any pair of components not listed in Table D.3 shall all have the value 1,0.

Annex E
(informative)

Assignment of trace components

In order to calculate, by use of the method described in this part of ISO 20765, the thermodynamic properties of a natural gas or similar mixture which contains a trace amount of one or more components which do not appear in Table 2, it is necessary to assign each such trace component to one of the 21 major and minor components for which the AGA8 equation was developed. Recommendations for appropriate assignments are given in Table E.1.

Each recommendation is based upon an assessment of which assignment is likely to give the best overall compromise of best accuracy for the complete set of thermodynamic properties. The factors taken into account in this assessment include molar mass, energy parameter (related to critical temperature) and size parameter (related to critical volume). Because, however, no single assignment is likely to be equally satisfactory for all properties, it is not unreasonable that the user may prefer an alternative assignment for a particular application in which, for example, only a single property is needed. For this reason, the recommendations are not normative. Implementations of the method that includes assignments for trace components need to be carefully documented in this respect.

NOTE The set of components completed by the addition of those in Table E.1 to those in Table 2 is the same as the set of components included in ISO 6976:1995 [5].

Table E.1 — Assignment of trace components

Trace component	Formula	Recommended assignment	*i*
2,2-dimethylpropane (neo-pentane)	C_5H_{12}	n-pentane	8
2-methylpentane	C_6H_{14}	n-hexane	10
3-methylpentane	C_6H_{14}	n-hexane	10
2,2-dimethylbutane	C_6H_{14}	n-hexane	10
2,3-dimethylbutane	C_6H_{14}	n-hexane	10
ethylene (ethene)	C_2H_4	ethane	4
propylene (propene)	C_3H_6	propane	5
1-butene	C_4H_8	n-butane	6
cis-2-butene	C_4H_8	n-butane	6
trans-2-butene	C_4H_8	n-butane	6
2-methylpropene	C_4H_8	n-butane	6
1-pentene	C_5H_{10}	n-pentane	8
propadiene	C_3H_4	propane	5
1,2-butadiene	C_4H_6	n-butane	6
1,3-butadiene	C_4H_6	n-butane	6
acetylene (ethyne)	C_2H_2	ethane	4
cyclopentane	C_5H_{10}	n-pentane	8
methylcyclopentane	C_6H_{12}	n-hexane	10
ethylcyclopentane	C_7H_{14}	n-heptane	11
cyclohexane	C_6H_{12}	n-hexane	10
methylcyclohexane	C_7H_{14}	n-heptane	11
ethylcyclohexane	C_8H_{16}	n-octane	12
benzene	C_6H_6	n-pentane	8
toluene (methylbenzene)	C_7H_8	n-hexane	10
ethylbenzene	C_8H_{10}	n-heptane	11
o-xylene	C_8H_{10}	n-heptane	11
all other C_6 hydrocarbons	—	n-hexane	10
all other C_7 hydrocarbons	—	n-heptane	11
all other C_8 hydrocarbons	—	n-octane	12
all other C_9 hydrocarbons	—	n-nonane	13
all other C_{10} hydrocarbons	—	n-decane	14
all higher hydrocarbons	—	n-decane	14
methanol (methyl alcohol)	CH_3OH	ethane	4
methanethiol (methyl mercaptan)	CH_3SH	propane	5
ammonia	NH_3	methane	3
hydrogen cyanide	HCN	ethane	4
carbonyl sulfide (carbon oxysulfide)	COS	n-butane	6
carbon disulfide	CS_2	n-pentane	8
sulfur dioxide	SO_2	n-butane	6
nitrous oxide	N_2O	carbon dioxide	2
neon	Ne	argon	21
krypton	Kr	argon	21
xenon	Xe	argon	21

Annex F
(informative)

Implementation of the method

This annex describes in summary form the sequence of calculations that needs to be carried out in order to implement the evaluation of thermodynamic properties in accordance with this part of ISO 20765. The method is sufficiently complex that it is impractical to perform the calculations without the help of a computer program. Computational aspects of the procedure are also discussed in this annex. Figure F.1 is a flow diagram which follows the step-by-step procedure outlined below for the computer implementation of the calculations.

Step 1

Select the mole fraction, x_i, of each component of the natural gas mixture plus the (absolute) temperature, T, and (absolute) pressure, p, for the calculation.

In one known and validated implementation of the method, the temperature is input in kelvins (K) and the pressure in megapascals (MPa). If either is given in any other unit, the value shall first to be converted to a value in K or MPa, as appropriate. For this purpose, conversion factors given in ISO 31-3 and ISO 31-4 shall be used.

It is sometimes the case that the (mass) density, D, is available as input in place of the pressure, p. In such cases, proceed as follows but take note of the final paragraph of step 4.

Step 2

a) For the selected values of x_i, use Equations (D.2) to (D.5) to calculate values of $B_n^*(X)$.

b) Likewise, for the selected values of x_i, use Equations (D.6) to (D.10) to calculate values of $C_n(X)$.

c) Use Equation (D.11) to calculate a value for the mixture size parameter $K(X)$.

d) Calculate the values of the following:

- the reduced temperature, τ_θ, from Equation (3) with $T = T_\theta$;
- the reduced density, δ_θ, of the ideal gas at reference conditions from Equation (4) with $\rho = \rho_\theta$.

The ideal reference density, ρ_θ, is defined in the text following Equation (7).

Step 3

a) For the selected value of T, use Equation (3) to calculate τ and then use values of $B_n^*(X)$ from step 2 a) in Equation (D.1) to calculate the second virial coefficient, $B(\tau, X)$.

b) Likewise, for the selected value of T, use values of $C_n(X)$ from step 2 b) to calculate values of the quantities $C_n(X) \cdot \tau^{u_n}$ for $n = 13$ to 58.

Step 4

a) Substitute the calculated values of $B(\tau, X)$, $C_n(X)\cdot\tau^{u_n}$ and $K(X)$ from steps 3 a), 3 b) and 2 c), respectively, into Equation (D.12). This equation for p, which is known from step 1, now contains the reduced density, δ, as the only unknown.

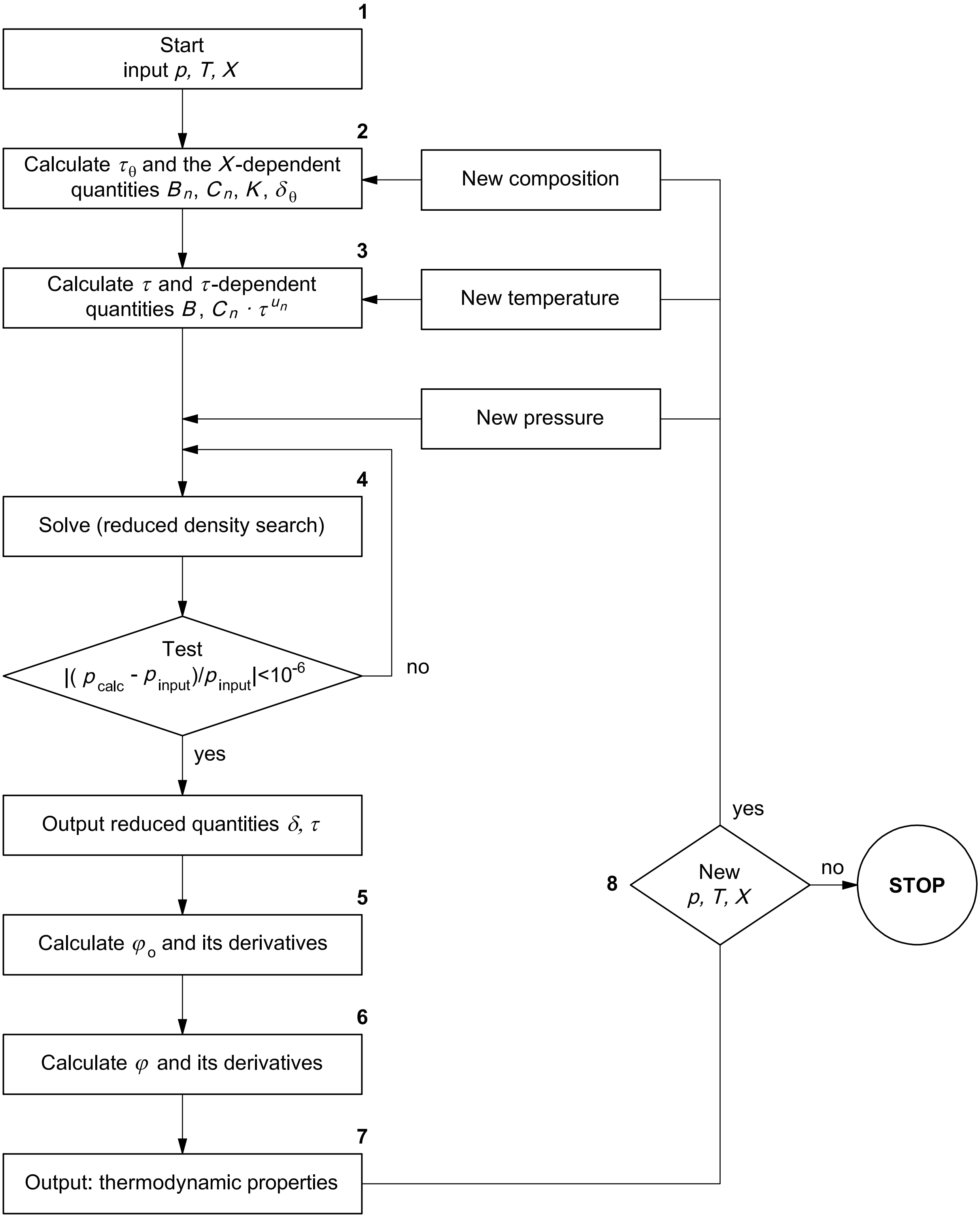


Figure F.1 — Flow diagram for calculation of thermodynamic properties

b) Solve this equation for δ. The required solution may be obtained by any suitable numerical method but, in practice, a standard form of equation-of-state density-search algorithm may be the most convenient and satisfactory. Such algorithms usually use an initial estimate of the density (often the ideal-gas approximation) and proceed, by iterative calculations of p and δ, in order to find the value of δ that reproduces the known value of p to within a pre-established level of agreement. A suitable criterion in the present case is that the pressure calculated from the calculated reduced molar density, δ, reproduces the input value of p to within 1 part in 10^6.

   If, instead of the pressure, p, the (mass) density, D, is available as input, then δ is obtained directly, without the need for any iterative procedure, as $\delta = D \cdot K^3 / M$ where $M(X)$ is the molar mass given by Equation (16) of the main text.

Step 5

Substitute δ and δ_θ into Equation (B.3), together with the various constants and functions of the inverse reduced temperature, τ, in order to calculate the ideal-gas part, φ_o, of the reduced Helmholtz free energy. Also, use Equations (B.6) and (B.7) to calculate the partial first and second derivatives of φ_o with respect to inverse reduced temperature.

Step 6

Use Equation (C.1) to calculate the total reduced Helmholtz free energy $\varphi(\delta, \tau, X)$. Also use Equations (C.2) and (C.4) to calculate the partial first derivatives φ_τ and φ_δ of φ with respect inverse reduced temperature and reduced density, respectively, Equation (C.3) to calculate the partial second derivative, $\varphi_{\tau\tau}$, of φ with respect to inverse reduced temperature, Equation (C.5) to calculate φ_1 and Equation (C.6) to calculate φ_2.

Step 7

a) Use Equations (17) to (26) of the main text to calculate the full set of thermodynamic properties: compression factor, Z; density, ρ; internal energy, u; enthalpy, h; entropy, s; isochoric heat capacity, c_v; isobaric heat capacity, c_p; Joule-Thomson coefficient, μ; isentropic index, κ and speed of sound, w.

b) Note that Equations (18) to (23) give the thermodynamic properties on both the molar basis (using lower-case symbols) and on the specific (i.e. mass) basis (using the corresponding upper-case symbols). The factor which converts between molar-basis and specific quantities is the molar mass, $M(X)$, of the mixture, which is calculated using Equation (16).

Step 8

Return to step 1 (select new input variables) or end.

Annex G
(informative)

Examples

The following example calculations are provided for the purposes of software validation.

Table G.1 — Gas analyses by mole fractions

i	**Component**	**Gas 1**	**Gas 2**	**Gas 3**	**Gas 4**	**Gas 5**	**Gas 6**
1	nitrogen	0,003 000	0,031 000	0,009 617	0,100 000	0,057 000	0,117 266
2	carbon dioxide	0,006 000	0,005 000	0,015 021	0,016 000	0,076 000	0,011 093
3	methane	0,965 000	0,907 000	0,859 284	0,735 000	0,812 000	0,825 198
4	ethane	0,018 000	0,045 000	0,084 563	0,033 000	0,043 000	0,034 611
5	propane	0,004 500	0,008 400	0,023 022	0,007 400	0,009 000	0,007 645
6	n-butane	0,001 000	0,001 500	0,006 985	0,000 800	0,001 500	0,002 539
7	iso-butane	0,001 000	0,001 000	—	0,000 800	0,001 500	—
8	n-pentane	0,000 300	0,000 400	0,001 218	0,000 400	—	0,000 746
9	iso-pentane	0,000 500	0,000 300	—	0,000 400	—	—
10	n-hexane	0,000 700	—	0,000 228	0,000 200	—	0,000 225
11	n-heptane	—	—	0,000 057	0,000 100	—	0,000 110
12	n-octane	—	—	0,000 005	0,000 100	—	0,000 029
13	n-nonane	—	—	—	0,000 100	—	—
14	n-decane	—	—	—	0,000 100	—	—
15	hydrogen	—	—	—	0,095 000	—	—
16	oxygen	—	0,000 100	—	0,000 100	—	—
17	carbon monoxide	—	—	—	0,010 000	—	—
18	water	—	0,000 100	—	0,000 100	—	—
19	hydrogen sulfide	—	0,000 100	—	0,000 100	—	—
20	helium	—	—	—	0,000 200	—	0,000 538
21	argon	—	0,000 100	—	0,000 100	—	—
	SUM	1,000 000	1,000 000	1,000 000	1,000 000	1,000 000	1,000 000

Table G.2 — Results for Gas 1

p MPa	T K	Z	D kg/m^3	U kJ/kg	H kJ/kg	S kJ/(kg·K)	C_v kJ/(kg·K)	C_p kJ/(kg·K)	μ K/MPa	κ	w m/s
5	250	0,819 96	49,295	–280,49	–179,06	–2,422 3	1,690 6	2,834 2	6,153	1,366	372,27
5	260	0,845 44	45,971	–260,09	–151,32	–2,313 4	1,691 0	2,721 9	5,658	1,360	384,59
5	270	0,866 43	43,196	–240,26	–124,51	–2,212 2	1,696 3	2,645 0	5,219	1,354	395,93
5	290	0,898 88	38,764	–201,60	–72,61	–2,026 8	1,718 9	2,555 9	4,473	1,344	416,29
5	310	0,922 62	35,331	–163,45	–21,93	–1,857 8	1,754 1	2,519 1	3,861	1,333	434,32
5	330	0,940 52	32,558	–125,21	+28,36	–1,700 6	1,799 1	2,514 0	3,350	1,322	450,59
5	350	0,954 33	30,253	–86,50	+78,77	–1,552 3	1,851 7	2,529 9	2,918	1,311	465,51
10	250	0,654 44	123,524	–353,94	–272,98	–3,052 2	1,799 6	4,344 8	4,218	1,782	379,77
10	260	0,707 71	109,834	–323,30	–232,25	–2,892 4	1,783 6	3,836 7	4,162	1,663	389,14
10	270	0,750 82	99,693	–295,99	–195,68	–2,754 3	1,774 4	3,499 3	4,010	1,591	399,53
10	290	0,815 67	85,439	–247,10	–130,06	–2,519 7	1,776 2	3,109 8	3,609	1,508	420,07
10	310	0,861 70	75,657	–202,21	–70,03	–2,319 4	1,798 4	2,914 3	3,199	1,458	439,05
10	330	0,895 73	68,371	–159,12	–12,86	–2,140 7	1,834 9	2,814 4	2,821	1,424	456,36
10	350	0,921 62	62,653	–116,71	+42,90	–1,976 6	1,881 6	2,768 5	2,485	1,397	472,24
15	250	0,618 21	196,147	–418,04	–341,57	–3,451 9	1,795 7	4,500 0	1,992	2,912	471,92
15	260	0,661 79	176,182	–382,78	–297,64	–3,279 7	1,803 5	4,271 1	2,250	2,461	457,75
15	270	0,703 50	159,598	–350,25	–256,26	–3,123 4	1,805 8	4,005 6	2,404	2,179	452,49
15	290	0,775 30	134,830	–292,19	–180,93	–2,854 1	1,811 5	3,553 2	2,473	1,865	455,55
15	310	0,830 97	117,682	–240,52	–113,05	–2,627 6	1,829 8	3,259 0	2,363	1,704	466,04
15	330	0,873 68	105,145	–192,45	–49,79	–2,429 8	1,861 8	3,083 5	2,179	1,607	478,79
15	350	0,906 77	95,519	–146,25	+10,79	–2,251 6	1,904 9	2,983 8	1,976	1,541	491,98
20	250	0,676 17	239,112	–455,05	–371,41	–3,662 7	1,777 0	3,998 5	0,950	4,102	585,72
20	260	0,702 15	221,406	–421,87	–331,54	–3,506 3	1,792 7	3,966 6	1,146	3,439	557,37
20	270	0,730 04	205,063	–389,76	–292,23	–3,358 0	1,804 4	3,889 2	1,314	2,965	537,78
20	290	0,785 92	177,345	–329,47	–216,69	–3,088 0	1,823 8	3,655 2	1,529	2,380	518,08
20	310	0,835 93	155,978	–274,20	–145,98	–2,852 1	1,847 2	3,423 8	1,596	2,060	513,90
20	330	0,877 71	139,550	–222,67	–79,35	–2,643 7	1,879 8	3,250 0	1,564	1,867	517,31
20	350	0,911 75	126,664	–173,49	–15,59	–2,456 1	1,921 9	3,134 8	1,478	1,742	524,40
30	250	0,850 42	285,176	–495,51	–390,31	–3,889 8	1,779 4	3,497 4	0,198	5,600	767,57
30	260	0,858 28	271,697	–465,71	–355,30	–3,752 5	1,794 3	3,503 3	0,285	4,865	732,95
30	270	0,868 15	258,660	–436,27	–320,29	–3,620 3	1,807 4	3,496 2	0,369	4,276	704,27
30	290	0,892 15	234,343	–378,74	–250,73	–3,371 8	1,833 8	3,454 9	0,522	3,421	661,74
30	310	0,918 99	212,820	–323,23	–182,27	–3,143 5	1,864 2	3,387 4	0,636	2,860	634,97
30	330	0,945 70	194,277	–269,72	–115,30	–2,934 1	1,900 9	3,309 6	0,702	2,488	619,80
30	350	0,970 32	178,527	–217,87	–49,83	–2,741 5	1,944 3	3,239 9	0,725	2,233	612,55

Table G.3 — Results for Gas 2

p MPa	T K	Z	D kg/m^3	U kJ/kg	H kJ/kg	S kJ/(kg·K)	C_v kJ/(kg·K)	C_p kJ/(kg·K)	μ K/MPa	κ	w m/s
5	250	0,812 60	52,014	–271,30	–175,17	–2,222 7	1,640 7	2,773 0	6,314	1,363	362,01
5	260	0,839 29	48,423	–251,33	–148,07	–2,116 4	1,640 6	2,654 9	5,800	1,356	374,23
5	270	0,861 21	45,443	–231,98	–121,95	–2,017 8	1,645 5	2,574 7	5,346	1,350	385,45
5	290	0,894 98	40,712	–194,31	–71,50	–1,837 5	1,667 5	2,482 3	4,575	1,339	405,56
5	310	0,919 61	37,066	–157,20	–22,31	–1,673 4	1,702 0	2,443 7	3,945	1,328	423,33
5	330	0,938 15	34,131	–120,03	+26,46	–1,521 0	1,746 0	2,437 3	3,420	1,318	439,35
5	350	0,952 44	31,698	–82,41	+75,33	–1,377 2	1,797 3	2,452 0	2,977	1,307	454,03
10	250	0,640 76	131,925	–345,46	–269,66	–2,840 2	1,753 4	4,329 9	4,203	1,814	370,85
10	260	0,696 20	116,751	–314,83	–229,18	–2,681 4	1,736 6	3,801 7	4,186	1,680	379,36
10	270	0,741 12	105,612	–287,73	–193,05	–2,545 0	1,726 4	3,448 8	4,052	1,600	389,27
10	290	0,808 58	90,125	–239,57	–128,62	–2,314 6	1,726 3	3,043 1	3,663	1,510	409,27
10	310	0,856 33	79,609	–195,61	–70,00	–2,119 1	1,747 0	2,840 8	3,252	1,458	427,89
10	330	0,891 56	71,829	–153,56	–14,34	–1,945 0	1,782 1	2,737 5	2,869	1,422	444,91
10	350	0,918 33	65,750	–112,23	+39,86	–1,785 6	1,827 2	2,689 3	2,528	1,394	460,53
15	250	0,610 32	207,758	–407,94	–335,74	–3,222 3	1,743 8	4,365 3	1,917	3,030	467,74
15	260	0,653 29	186,629	–373,37	–293,00	–3,054 6	1,752 9	4,167 3	2,194	2,536	451,45
15	270	0,695 07	168,913	–341,36	–252,55	–2,901 9	1,756 0	3,919 2	2,368	2,227	444,66
15	290	0,768 00	142,331	–284,21	–178,82	–2,638 3	1,761 4	3,476 7	2,470	1,887	445,90
15	310	0,825 03	123,945	–233,50	–112,47	–2,417 0	1,778 4	3,181 5	2,376	1,714	455,43
15	330	0,868 91	110,552	–186,46	–50,78	–2,224 0	1,809 0	3,003 8	2,200	1,611	467,59
15	350	0,902 95	100,306	–141,36	+8,18	–2,050 6	1,850 4	2,902 3	1,999	1,543	480,37
20	250	0,673 18	251,145	–442,98	–363,34	–3,419 3	1,725 2	3,858 6	0,905	4,254	582,02
20	260	0,698 28	232,806	–410,74	–324,83	–3,268 3	1,741 2	3,835 5	1,100	3,552	552,40
20	270	0,725 51	215,770	–379,46	–286,77	–3,124 7	1,753 1	3,769 9	1,273	3,048	531,56
20	290	0,780 93	186,633	–320,57	–213,41	–2,862 4	1,772 5	3,555 8	1,504	2,425	509,77
20	310	0,831 25	164,023	–266,51	–144,57	–2,632 8	1,795 2	3,333 7	1,585	2,085	504,20
20	330	0,873 64	146,606	–216,12	–79,70	–2,430 0	1,826 5	3,163 0	1,563	1,882	506,69
20	350	0,908 32	132,950	–168,11	–17,68	–2,247 5	1,867 1	3,048 5	1,484	1,750	513,14
30	250	0,852 23	297,570	–481,33	–380,51	–3,632 8	1,729 0	3,378 5	0,178	5,753	761,58
30	260	0,859 51	283,704	–452,42	–346,68	–3,500 1	1,743 7	3,386 0	0,264	4,991	726,46
30	270	0,868 84	270,261	–423,84	–312,84	–3,372 4	1,756 3	3,380 4	0,348	4,380	697,27
30	290	0,891 95	245,102	–367,95	–245,55	–3,132 0	1,781 8	3,343 5	0,501	3,492	653,73
30	310	0,918 22	222,731	–313,95	–179,26	–2,910 9	1,811 3	3,282 0	0,618	2,909	625,94
30	330	0,944 65	203,377	–261,85	–114,34	–2,707 9	1,846 7	3,209 6	0,689	2,521	609,85
30	350	0,969 24	186,890	–211,36	–50,84	–2,521 1	1,888 7	3,143 4	0,716	2,256	601,84

Table G.4 — Results for Gas 3

p MPa	T K	Z	D kg/m^3	U kJ/kg	H kJ/kg	S kJ/(kg·K)	C_v kJ/(kg·K)	C_p kJ/(kg·K)	μ K/MPa	κ	w m/s
5	250	0,765 37	59,066	–269,33	–184,68	–2,075 7	1,637 0	2,947 3	7,323	1,346	337,60
5	260	0,800 06	54,331	–248,22	–156,20	–1,964 0	1,639 0	2,763 2	6,681	1,335	350,48
5	270	0,827 89	50,560	–228,09	–129,20	–1,862 1	1,644 8	2,644 4	6,123	1,327	362,19
5	290	0,869 87	44,802	–189,42	–77,82	–1,678 5	1,667 6	2,511 0	5,197	1,314	382,96
5	310	0,899 92	40,512	–151,69	–28,27	–1,513 2	1,703 3	2,453 2	4,454	1,303	401,08
5	330	0,922 30	37,133	–114,07	+20,58	–1,360 5	1,749 0	2,437 1	3,845	1,293	417,27
5	350	0,939 44	34,372	–76,08	+69,39	–1,216 9	1,802 5	2,446 8	3,338	1,283	432,01
10	250	0,547 63	165,102	–364,22	–303,66	–2,753 0	1,756 9	5,094 0	3,980	2,113	357,74
10	260	0,616 07	141,116	–327,13	–256,27	–2,567 0	1,758 1	4,402 3	4,275	1,818	358,90
10	270	0,673 30	124,338	–295,47	–215,05	–2,411 4	1,750 9	3,871 8	4,311	1,665	365,91
10	290	0,758 90	102,706	–241,97	–144,60	–2,159 4	1,745 3	3,249 9	4,028	1,518	384,45
10	310	0,818 33	89,102	–195,19	–82,96	–1,953 8	1,761 0	2,949 3	3,610	1,448	403,07
10	330	0,861 48	79,509	–151,42	–25,65	–1,774 6	1,793 6	2,798 1	3,195	1,405	420,32
10	350	0,893 94	72,244	–108,94	+29,48	–1,612 4	1,838 3	2,724 6	2,818	1,374	436,16
15	250	0,553 63	244,969	–425,70	–364,46	–3,092 5	1,668 3	4,247 9	1,522	4,017	495,98
15	260	0,591 47	220,476	–389,85	–321,81	–2,925 2	1,724 5	4,256 1	1,878	3,129	461,36
15	270	0,632 62	198,500	–355,38	–279,81	–2,766 7	1,754 5	4,124 7	2,169	2,584	441,89
15	290	0,712 30	164,138	–292,85	–201,46	–2,486 5	1,779 5	3,702 9	2,476	2,024	430,12
15	310	0,778 73	140,449	–238,00	–131,20	–2,252 1	1,797 3	3,343 8	2,498	1,768	434,56
15	330	0,830 89	123,654	–188,16	–66,86	–2,050 9	1,825 4	3,109 9	2,370	1,630	444,63
15	350	0,871 54	111,152	–141,13	–6,18	–1,872 3	1,865 2	2,971 3	2,181	1,544	456,50
20	250	0,638 29	283,304	–455,68	–385,08	–3,250 3	1,633 0	3,668 1	0,689	5,499	623,08
20	260	0,658 52	264,036	–423,75	–348,00	–3,104 8	1,693 9	3,737 6	0,883	4,420	578,61
20	270	0,682 13	245,459	–392,00	–310,52	–2,963 4	1,732 9	3,749 9	1,074	3,658	545,96
20	290	0,735 18	212,039	–330,66	–236,34	–2,698 3	1,778 8	3,643 0	1,392	2,727	507,12
20	310	0,788 30	184,992	–273,52	–165,40	–2,461 7	1,809 9	3,446 0	1,565	2,238	491,84
20	330	0,835 57	163,950	–220,40	–98,41	–2,252 2	1,842 6	3,260 2	1,609	1,961	489,08
20	350	0,875 37	147,553	–170,21	–34,66	–2,064 6	1,882 8	3,122 9	1,568	1,790	492,61
30	250	0,836 36	324,314	–489,03	–396,53	–3,426 9	1,627 4	3,191 8	0,083	7,038	806,85
30	260	0,840 62	310,260	–460,88	–364,19	–3,300 1	1,689 1	3,268 4	0,170	5,975	760,08
30	270	0,847 37	296,388	–432,51	–331,29	–3,176 0	1,728 5	3,305 6	0,255	5,148	721,87
30	290	0,866 61	269,821	–376,14	–264,96	–2,939 0	1,779 1	3,318 1	0,416	3,976	664,88
30	310	0,890 85	245,547	–321,02	–198,84	–2,718 5	1,818 5	3,288 8	0,554	3,220	627,21
30	330	0,917 13	224,056	–267,45	–133,55	–2,514 4	1,858 2	3,237 3	0,655	2,721	603,62
30	350	0,942 97	205,462	–215,40	–69,39	–2,325 6	1,902 2	3,179 2	0,711	2,386	590,21

Table G.5 — Results for Gas 4

p MPa	T K	Z	D kg/m^3	U kJ/kg	H kJ/kg	S kJ/(kg·K)	C_v kJ/(kg·K)	C_p kJ/(kg·K)	μ K/MPa	κ	w m/s
5	250	0,869 04	47,932	–258,79	–154,48	–1,927 6	1,566 1	2,485 8	4,934	1,388	380,47
5	260	0,887 70	45,120	–240,75	–129,93	–1,831 3	1,571 1	2,426 8	4,553	1,381	391,19
5	270	0,903 33	42,697	–222,99	–105,89	–1,740 5	1,578 7	2,384 6	4,212	1,375	401,25
5	290	0,927 89	38,700	–187,95	–58,75	–1,572 1	1,601 2	2,335 1	3,624	1,363	419,70
5	310	0,946 08	35,507	–153,09	–12,27	–1,417 1	1,632 2	2,317 0	3,135	1,352	436,38
5	330	0,959 89	32,875	–118,03	+34,06	–1,272 3	1,670 2	2,319 4	2,724	1,341	451,66
5	350	0,970 58	30,655	–82,51	+80,60	–1,135 4	1,713 7	2,336 2	2,373	1,330	465,83
10	250	0,764 51	108,971	–307,61	–215,84	–2,445 5	1,639 7	3,223 4	3,620	1,644	388,42
10	260	0,799 90	100,145	–284,54	–184,68	–2,323 2	1,635 0	3,019 5	3,458	1,591	398,57
10	270	0,829 33	93,013	–262,77	–155,26	–2,212 2	1,634 2	2,872 0	3,279	1,553	408,55
10	290	0,875 07	82,072	–221,73	–99,89	–2,014 3	1,643 9	2,684 6	2,915	1,500	427,47
10	310	0,908 54	73,949	–182,54	–47,32	–1,838 9	1,666 4	2,582 8	2,575	1,463	444,85
10	330	0,933 73	67,593	–144,19	+3,75	–1,679 3	1,698 3	2,530 3	2,268	1,435	460,82
10	350	0,953 09	62,436	–106,06	+54,10	–1,531 1	1,737 4	2,508 7	1,996	1,412	475,61
15	250	0,730 16	171,146	–352,65	–265,01	–2,786 6	1,658 4	3,583 2	2,156	2,200	439,07
15	260	0,766 82	156,696	–325,88	–230,15	–2,649 8	1,662 8	3,390 1	2,210	2,024	440,12
15	270	0,799 39	144,745	–300,76	–197,13	–2,525 2	1,664 5	3,220 3	2,212	1,901	443,82
15	290	0,852 95	126,300	–254,21	–135,44	–2,304 7	1,672 4	2,966 4	2,116	1,744	455,05
15	310	0,893 84	112,748	–210,88	–77,84	–2,112 5	1,691 0	2,807 1	1,955	1,648	468,17
15	330	0,925 27	102,316	–169,34	–22,74	–1,940 2	1,719 5	2,711 8	1,774	1,582	481,59
15	350	0,949 73	93,985	–128,69	+30,91	–1,782 4	1,755 9	2,658 8	1,594	1,534	494,74
20	250	0,761 32	218,856	–385,55	–294,17	–3,005 6	1,643 5	3,498 1	1,204	2,925	517,02
20	260	0,789 17	203,013	–358,14	–259,62	–2,870 0	1,660 6	3,407 1	1,307	2,608	506,85
20	270	0,815 92	189,083	–331,85	–226,07	–2,743 4	1,670 9	3,301 1	1,376	2,379	501,64
20	290	0,863 86	166,274	–282,42	–162,14	–2,514 9	1,686 5	3,098 7	1,425	2,080	500,19
20	310	0,903 41	148,737	–236,27	–101,81	–2,313 7	1,706 5	2,942 8	1,392	1,898	505,16
20	330	0,935 30	134,959	–192,28	–44,09	–2,133 2	1,734 4	2,836 4	1,313	1,777	513,17
20	350	0,960 86	123,862	–149,56	+11,91	–1,968 4	1,769 7	2,769 4	1,213	1,691	522,60
30	250	0,901 69	277,178	–425,72	–317,48	–3,258 9	1,627 7	3,184 3	0,332	4,207	674,76
30	260	0,912 96	263,228	–399,63	–285,66	–3,134 1	1,652 8	3,177 4	0,405	3,733	652,25
30	270	0,925 29	250,102	–373,94	–253,98	–3,014 5	1,670 6	3,155 4	0,469	3,361	634,98
30	290	0,951 24	226,500	–323,99	–191,54	–2,791 4	1,697 5	3,084 4	0,567	2,830	612,24
30	310	0,976 47	206,413	–276,02	–130,68	–2,588 4	1,723 3	3,002 1	0,619	2,482	600,60
30	330	0,999 23	189,486	–229,72	–71,40	–2,403 1	1,753 2	2,929 2	0,633	2,244	595,98
30	350	1,018 93	175,204	–184,62	–13,39	–2,232 4	1,788 5	2,874 4	0,619	2,073	595,76

Table G.6 — Results for Gas 5

p MPa	T K	Z	D kg/m^3	U kJ/kg	H kJ/kg	S kJ/(kg·K)	C_v kJ/(kg·K)	C_p kJ/(kg·K)	μ K/MPa	κ	w m/s
5	250	0,803 18	59,396	–242,65	–158,47	–1,854 4	1,462 8	2,513 7	6,573	1,366	339,12
5	260	0,831 51	55,166	–224,61	–133,98	–1,758 3	1,460 0	2,392 4	6,033	1,358	350,87
5	270	0,854 65	51,685	–207,23	–110,49	–1,669 7	1,462 3	2,310 7	5,557	1,352	361,63
5	290	0,890 10	46,204	–173,55	–65,34	–1,508 3	1,478 6	2,216 2	4,752	1,340	380,87
5	310	0,915 83	42,009	–140,52	–21,49	–1,362 1	1,506 6	2,174 6	4,097	1,330	397,82
5	330	0,935 14	38,648	–107,52	+21,85	–1,226 6	1,543 1	2,163 6	3,552	1,319	413,10
5	350	0,950 00	35,869	–74,21	+65,18	–1,099 1	1,586 0	2,172 1	3,095	1,309	427,09
10	250	0,620 07	153,875	–313,43	–248,44	–2,422 2	1,582 8	4,069 3	4,219	1,854	347,10
10	260	0,679 18	135,079	–284,65	–210,62	–2,273 8	1,561 2	3,529 6	4,259	1,702	354,92
10	270	0,727 01	121,518	–259,55	–177,25	–2,147 8	1,546 5	3,167 8	4,154	1,613	364,35
10	290	0,798 42	103,018	–215,60	–118,53	–1,937 8	1,538 2	2,755 2	3,780	1,516	383,57
10	310	0,848 64	90,670	–175,98	–65,69	–1,761 6	1,551 1	2,550 8	3,365	1,461	401,47
10	330	0,885 52	81,627	–138,36	–15,85	–1,605 7	1,578 1	2,445 2	2,975	1,425	417,81
10	350	0,913 47	74,608	–101,57	+32,47	–1,463 6	1,614 5	2,393 3	2,625	1,397	432,78
15	250	0,591 62	241,909	–371,00	–308,99	–2,765 3	1,564 0	3,990 4	1,867	3,179	443,96
15	260	0,635 26	216,627	–339,09	–269,84	–2,611 7	1,572 4	3,822 1	2,172	2,622	426,12
15	270	0,678 37	195,347	–309,54	–232,75	–2,471 7	1,573 7	3,592 8	2,375	2,279	418,37
15	290	0,754 50	163,524	–257,09	–165,36	–2,230 7	1,572 7	3,165 5	2,519	1,910	418,53
15	310	0,814 32	141,736	–211,02	–105,19	–2,030 0	1,581 9	2,873 8	2,445	1,726	427,40
15	330	0,860 34	126,024	–168,67	–49,64	–1,856 3	1,603 9	2,696 1	2,275	1,619	439,00
15	350	0,895 97	114,097	–128,32	+3,14	–1,700 9	1,636 4	2,592 5	2,074	1,549	451,26
20	250	0,656 80	290,535	–402,27	–333,43	–2,937 7	1,541 1	3,497 4	0,882	4,485	555,64
20	260	0,682 00	269,040	–372,84	–298,50	–2,800 7	1,556 3	3,481 7	1,085	3,706	524,89
20	270	0,709 66	248,978	–344,26	–263,93	–2,670 2	1,566 7	3,425 0	1,268	3,153	503,23
20	290	0,766 73	214,554	–290,51	–197,30	–2,432 1	1,581 1	3,226 3	1,523	2,476	480,39
20	310	0,819 10	187,877	–241,42	–134,96	–2,224 1	1,596 9	3,012 1	1,623	2,112	474,20
20	330	0,863 44	167,428	–195,95	–76,50	–2,041 3	1,620 1	2,844 0	1,613	1,899	476,24
20	350	0,899 79	151,484	–152,88	–20,85	–1,877 6	1,651 8	2,728 8	1,539	1,762	482,29
30	250	0,836 85	342,041	–436,39	–348,68	–3,124 3	1,542 3	3,050 0	0,178	6,046	728,22
30	260	0,844 31	325,979	–410,15	–318,12	–3,004 4	1,555 6	3,058 7	0,267	5,211	692,52
30	270	0,853 96	310,360	–384,21	–287,55	–2,889 1	1,566 3	3,053 5	0,353	4,547	662,93
30	290	0,878 00	281,044	–333,54	–226,80	–2,672 0	1,586 4	3,016 8	0,513	3,590	619,03
30	310	0,905 48	254,934	–284,72	–167,04	–2,472 7	1,609 4	2,955 5	0,638	2,970	591,15
30	330	0,933 26	232,354	–237,77	–108,65	–2,290 2	1,637 2	2,882 6	0,716	2,561	575,03
30	350	0,959 18	213,156	–192,45	–51,70	–2,122 6	1,670 6	2,814 4	0,748	2,284	566,97

Table G.7 — Results for Gas 6

p MPa	T K	Z	D kg/m^3	U kJ/kg	H kJ/kg	S kJ/(kg·K)	C_v kJ/(kg·K)	C_p kJ/(kg·K)	μ K/MPa	κ	w m/s
5	250	0,834 09	53,718	–249,86	–156,78	–1,976 6	1,504 7	2,486 6	5,831	1,377	358,07
5	260	0,857 65	50,234	–231,91	–132,38	–1,880 9	1,506 0	2,399 5	5,369	1,370	369,34
5	270	0,877 16	47,297	–214,42	–108,71	–1,791 6	1,511 1	2,338 7	4,959	1,364	379,78
5	290	0,907 46	42,565	–180,20	–62,74	–1,627 3	1,530 6	2,267 2	4,258	1,353	398,67
5	310	0,929 71	38,866	–146,39	–17,75	–1,477 2	1,560 4	2,237 2	3,680	1,342	415,50
5	330	0,946 51	35,862	–112,50	+26,92	–1,337 6	1,598 1	2,232 8	3,196	1,331	430,77
5	350	0,959 49	33,356	–78,22	+71,68	–1,205 9	1,641 9	2,245 8	2,785	1,320	444,83
10	250	0,690 61	129,758	–309,46	–232,39	–2,515 9	1,594 3	3,583 7	4,052	1,744	366,59
10	260	0,737 64	116,813	–284,01	–198,40	–2,382 5	1,582 8	3,236 0	3,953	1,650	375,82
10	270	0,776 13	106,907	–260,85	–167,31	–2,265 1	1,576 5	2,996 9	3,791	1,589	385,53
10	290	0,834 79	92,540	–218,63	–110,57	–2,062 3	1,579 4	2,709 6	3,405	1,514	404,49
10	310	0,876 93	82,410	–179,37	–58,03	–1,887 0	1,598 5	2,559 9	3,019	1,468	422,02
10	330	0,908 28	74,743	–141,49	–7,70	–1,729 7	1,629 0	2,481 6	2,666	1,434	438,08
10	350	0,932 23	68,662	–104,13	+41,51	–1,584 9	1,667 9	2,445 2	2,350	1,408	452,88
15	250	0,655 98	204,914	–362,28	–289,08	–2,862 8	1,599 0	3,835 0	2,067	2,659	441,19
15	260	0,697 75	185,235	–332,75	–251,77	–2,716 5	1,604 7	3,621 5	2,252	2,318	433,27
15	270	0,736 55	168,978	–305,42	–216,65	–2,583 9	1,605 9	3,405 5	2,351	2,097	431,46
15	290	0,802 22	144,447	–256,08	–152,24	–2,353 6	1,610 2	3,057 9	2,361	1,840	437,07
15	310	0,852 92	127,096	–211,52	–93,50	–2,157 6	1,625 5	2,833 9	2,234	1,699	447,78
15	330	0,891 91	114,173	–169,67	–38,29	–1,985 0	1,652 2	2,698 9	2,054	1,611	460,01
15	350	0,922 20	104,113	–129,24	+14,83	–1,828 7	1,688 0	2,621 4	1,860	1,549	472,47
20	250	0,706 95	253,517	–395,37	–316,48	–3,059 2	1,582 3	3,512 3	1,027	3,705	540,62
20	260	0,733 74	234,868	–366,73	–281,58	–2,922 3	1,597 6	3,461 1	1,198	3,165	519,12
20	270	0,761 43	217,944	–339,14	–247,37	–2,793 2	1,607 6	3,375 1	1,335	2,780	505,07
20	290	0,814 76	189,632	–287,44	–181,97	–2,559 5	1,622 6	3,163 1	1,493	2,298	492,26
20	310	0,861 15	167,841	–239,84	–120,68	–2,355 0	1,641 3	2,973 9	1,526	2,024	491,11
20	330	0,899 49	150,949	–195,16	–62,67	–2,173 6	1,668 0	2,836 0	1,479	1,854	495,66
20	350	0,930 59	137,565	–152,31	–6,92	–2,009 6	1,702 8	2,745 3	1,390	1,740	502,98
30	250	0,874 98	307,248	–432,49	–334,85	–3,274 3	1,580 4	3,103 4	0,229	5,159	709,77
30	260	0,883 65	292,533	–406,36	–303,80	–3,152 5	1,597 3	3,103 9	0,312	4,510	680,11
30	270	0,894 05	278,420	–380,57	–272,82	–3,035 6	1,610 3	3,091 7	0,390	3,994	656,03
30	290	0,918 27	252,383	–330,30	–211,43	–2,816 2	1,633 1	3,042 5	0,527	3,247	621,29
30	310	0,944 24	229,607	–281,91	–151,25	–2,615 5	1,657 7	2,973 1	0,622	2,758	600,30
30	330	0,969 30	210,114	–235,30	–92,52	–2,431 9	1,687 3	2,901 0	0,671	2,430	589,00
30	350	0,991 97	193,580	–190,11	–35,14	–2,263 1	1,722 7	2,840 1	0,681	2,202	584,13

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NOTE Total data points used from References [8](a) to [8](i), 1 194.

[9] OWREN, G., GRINI, P.G., MAEHLUM, H.S. and JORSTAD, O. SINTEF Energy report for GERG WG 1.3 (1 August 1996)

NOTE Total data points used from Reference [9], 206.

ICS 75.060

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