SLOVENSKI STANDARD
SIST EN ISO 6976:2005

01-julij-2005

Zemeljski plin ï Izraį un kaloriį nih vrednosti, gostote, relativne gostote in Wobbejevega indeksa iz kompozicije (ISO 6976:1995 vključ ujoį Popravek 2:1997 in Popravek 3:1999)

Natural gas - Calculation of calorific values, density, relative density and Wobbe index from composition (ISO 6976:1995 including Corrigendum 1:1997, Corrigendum 2:1997 and Corrigendum 3:1999)

Erdgas - Berechnung von Brenn- und Heizwert, Dichte, relativer Dichte und Wobbeindex aus der Zusammensetzung (ISO 6976:1995 + Corrigendum 1:1997 + Corrigendum 2:1997 + Corrigendum 3:1999)

Gaz naturel - Calcul du pouvoir calorifique, de la masse volumique, de la densité relative et de l'indice de Wobbe a partir de la composition (ISO 6976:1995, Corrigendum 1:1997, Corrigendum 2:1997 et Corrigendum 3:1999 inclus)

Ta slovenski standard je istoveten z: **EN ISO 6976:2005**

ICS:

75.060	Zemeljski plin	Natural gas

SIST EN ISO 6976:2005 **en**

EUROPEAN STANDARD

NORME EUROPÉENNE

EUROPÄISCHE NORM

EN ISO 6976

May 2005

ICS 75.060

English version

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This European Standard was approved by CEN on 17 April 2005.

CEN members are bound to comply with the CEN/CENELEC Internal Regulations which stipulate the conditions for giving this European Standard the status of a national standard without any alteration. Up-to-date lists and bibliographical references concerning such national standards may be obtained on application to the Central Secretariat or to any CEN member.

This European Standard exists in three official versions (English, French, German). A version in any other language made by translation under the responsibility of a CEN member into its own language and notified to the Central Secretariat has the same status as the official versions.

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Ref. No. EN ISO 6976:2005: E

Foreword

The text of ISO 6976:1995 has been prepared by Technical Committee ISO/TC 193 "Natural gas” of the International Organization for Standardization (ISO) and has been taken over as EN ISO 6976:2005 by CMC.

This European Standard shall be given the status of a national standard, either by publication of an identical text or by endorsement, at the latest by November 2005, and conflicting national standards shall be withdrawn at the latest by November 2005.

According to the CEN/CENELEC Internal Regulations, the national standards organizations of the following countries are bound to implement this European Standard: Austria, Belgium, Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Netherlands, Norway, Poland, Portugal, Slovakia, Slovenia, Spain, Sweden, Switzerland and United Kingdom.

Endorsement notice

The text of ISO 6976:1995 has been approved by CEN as EN ISO 6976:2005 without any modifications.

INTERNATIONAL
STANDARD

ISO
6976

Second edition
1995-12-01

Corrected and reprinted
1996-02-01

Natural gas — Calculation of calorific values, density, relative density and Wobbe index from composition

Gaz naturel — Calcul du pouvoir calorifique, de la masse volumique, de la densité relative et de l'indice de Wobbe à partir de la composition

Reference number
ISO 6976:1995(E)

Contents

International Organization for Standardization
Case Postale 56 • CH-1211 Genève 20 • Switzerland
Printed in Switzerland

Annexes

Foreword

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

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

International Standard ISO 6976 was prepared by Technical Committee ISO/TC 193, *Natural gas*, Subcommittee SC 1, *Analysis of natural gas*.

This second edition cancels and replaces the first edition (ISO 6976:1983), of which it constitutes a technical revision.

Annexes A and B form an integral part of this International Standard. Annexes C, D, E, F, G, H, J, K, L and M are for information only.

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INTERNATIONAL STANDARD © ISO **ISO 6976:1995(E)**

Natural gas — Calculation of calorific values, density, relative density and Wobbe index from composition

1 Scope

This International Standard specifies methods for the calculation of the superior calorific value, inferior calorific value, density, relative density and Wobbe index of dry natural gases, natural gas substitutes and other combustible gaseous fuels, when the composition of the gas by mole fraction is known. The methods provide a means of calculating the properties of the gas mixture at commonly used metric reference conditions.

The methods of calculation require values for various physical properties of the pure components; these values are provided in tables and their sources are identified.

Methods are given for estimating the precision of calculated properties.

The methods of calculation of the values of properties on either a molar or mass basis are applicable to any dry natural gas, natural gas substitute or other combustible fuel which is normally gaseous. For the calculation of the values of properties on a volumetric basis, the methods are restricted to gases consisting preponderantly of methane (not less than 0,5 mole fraction).

Examples of calculations are given in annex D for the recommended methods of calculation.

NOTES

1 The symbols used in this International Standard, together with their meanings, are given in annex A.

2 The qualifiers "higher", "upper", "total" and "gross" are, for the purposes of this International Standard, synonymous with "superior"; likewise, "lower" and "net" are synonymous with "inferior". The term "heating value" is synonymous with "calorific value"; "specific gravity" is synonymous with "relative density"; "Wobbe number" is synonymous with "Wobbe index"; "compressibility factor" is synonymous with "compression factor".

3 If the composition of the gas is known by volume fractions these must be converted to mole fractions (see annex C). Note, however, that the derived mole fractions will have uncertainties greater than those of the original volume fractions.

4 For the purposes of this International Standard, the sum of the mole fractions used must be unity to the nearest 0,000 1, and all components with mole fractions greater than 0,000 05 must be accounted for.

5 For the calorific value calculated on a volumetric basis, there are limitations on the amounts of components other than methane which may be present. It is impossible to be definitive on this matter, but the following guidelines may be useful:

N_2 should not be present in amounts exceeding 0,3 mole fraction;

CO_2 and C_2H_6 should each not exceed 0,15 mole fraction;

no other component should exceed 0,05 mole fraction.

Given these limits, the expected trueness of the calculation is within 0,1 %.

6 The effects of water vapour on the calorific value, either directly measured or calculated, are discussed in annex F.

7 For the methods of calculation described to be valid, the gas must be above its hydrocarbon dew-point at the prescribed reference conditions.

8 The values of basic physical property data are subject to revision as more accurate values become available from authoritative sources.

2 Definitions

For the purposes of this International Standard, the following definitions apply.

2.1 superior calorific value: The amount of heat which would be released by the complete combustion in air of a specified quantity of gas, in such a way that the pressure p_1 at which the reaction takes place remains constant, and all the products of combustion are returned to the same specified temperature t_1 as that of the reactants, all of these products being in the gaseous state except for water formed by combustion, which is condensed to the liquid state at t_1.

Where the quantity of gas is specified on a molar basis, the calorific value is designated as $\overline{H}_S(t_1,p_1)$; on a mass basis the calorific value is designated as $\hat{H}_S(t_1,p_1)$.

Where the quantity of gas is specified on a volumetric basis, the calorific value is designated as $\tilde{H}_S[t_1,p_1, V(t_2,p_2)]$, where t_2 and p_2 are the gas volume (metering) reference conditions (see figure 1).

2.2 inferior calorific value: The amount of heat which would be released by the complete combustion in air of a specified quantity of gas, in such a way that the pressure p_1 at which the reaction takes place remains constant, and all the products of combustion are returned to the same specified temperature t_1 as that of the reactants, all of these products being in the gaseous state.

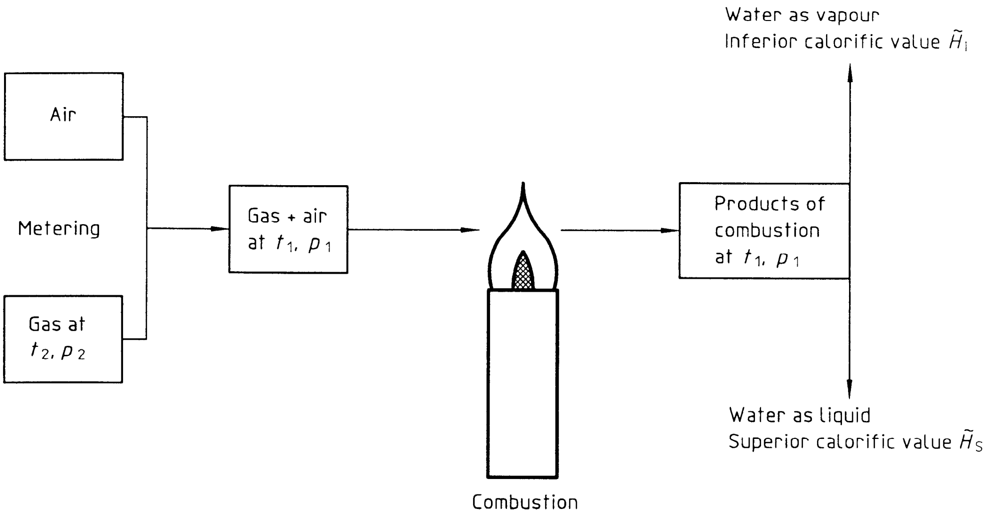
On molar, mass and volumetric bases, the inferior calorific value is designated respectively as $\overline{H}_I(t_1,p_1)$, $\hat{H}_I(t_1,p_1)$ and $\tilde{H}_I[(t_1, p_1),V(t_2,p_2)]$.

2.3 density: The mass of a gas sample divided by its volume at specified conditions of pressure and temperature.

2.4 relative density: The density of a gas divided by the density of dry air of standard composition (see annex B) at the same specified conditions of pressure and temperature. The term ideal relative density applies when both gas and air are considered as fluids which obey the ideal gas law (see 2.7); the term real relative density applies when both gas and air are considered as real fluids.

2.5 Wobbe index: The superior calorific value on a volumetric basis at specified reference conditions, divided by the square root of the relative density at the same specified metering reference conditions.

2.6 enthalpy of transformation: The enthalpy of transformation of a substance from state A to state B is thermodynamic terminology for the amount of heat release which accompanies the transformation between states. A **positive** heat release is taken by convention to be a numerically identical **negative** enthalpy increment. The quantities enthalpy of combustion and enthalpy of vaporization therefore have meanings which should be contextually self-evident; the term enthalpic correction refers to the (molar) enthalpy of transformation between the ideal and real states of a gas.



$$\frac{\text{Heat release}}{\text{Metered volume of gas}} = \text{Calorific value } \tilde{H}$$

Figure 1 — Calorific value on a volumetric basis — Metering and combustion reference conditions

2.7 ideal gas and real gas: An ideal gas is one which obeys the ideal gas law:

$$p \cdot V_m = R \cdot T \qquad \dots (1)$$

where

p is the absolute pressure;

T is the thermodynamic temperature;

V_m is the volume per mole of gas;

R is the molar gas constant, in coherent units.

No real gas obeys this law. For real gases, equation (1) must be rewritten as

$$p \cdot V_m = Z(T,p) \cdot R \cdot T \qquad \dots (2)$$

where $Z(T,p)$ is a variable, often close to unity, and is known as the compression factor (see 2.8 and E.2).

2.8 compression factor: The actual (real) volume of a given mass of gas at a specified pressure and temperature divided by its volume, under the same conditions, as calculated from the ideal gas law.

2.9 combustion reference conditions: The specified temperature t_1 and pressure p_1. These are the conditions at which the fuel is notionally burned (see figure 1).

2.10 metering reference conditions: The specified temperature t_2 and pressure p_2. These are the conditions at which the amount of fuel to be burned is notionally determined; there is no *a priori* reason for these to be the same as the combustion reference conditions (see figure 1).

NOTE 9 A range of reference conditions is in use throughout the world; appropriate data for the principal sets of metric reference conditions are given in tables in this International Standard.

2.11 dry natural gas: Gas which does not contain water vapour at a mole fraction greater than 0,000 05.

3 Principle

Methods are provided for the calculation of the calorific values, density, relative density and Wobbe index of any dry natural gas, natural gas substitute or other combustible gaseous fuel from a known composition. These methods use equations in which, for all individual molecular species of the gas mixture, the values of ideal-gas thermophysical properties (which are given) are weighted in accordance with the corresponding mole fraction, all the terms then being added together to obtain the "mole fraction average" of the property for the ideal-gas mixture. Values on a volumetric basis are then converted to values for the real-gas state by applying a volumetric correction factor.

NOTE 10 An enthalpic correction factor which is also, in principle, required in calorific value calculations is deemed to be negligible in all relevant cases.

In clause 10, values are given for the physical properties of the pure components of natural gas on molar, mass and volumetric bases for the commonly used reference conditions. Examples of calculations are given in annex D.

4 Behaviour of ideal and real gases

4.1 Enthalpy of combustion

The most fundamental physical quantities required in the calculation of calorific values from first principles are the ideal-gas (standard) molar enthalpies of combustion for the component gases of the mixture. These quantities are complex functions of temperature; thus, the values required depend upon the combustion reference temperature t_1. For practical reasons, it is not intended that the user himself carries out calculations which give the appropriate values at any arbitrary combustion reference temperature. Instead, tabulations are given for the temperatures $t_1 = 25$ °C, 20 °C, 15 °C and 0 °C. In clause E.1 the derivations of the values tabulated are discussed; the important point is that all four values for any substance are mutually consistent in a thermodynamic sense.

For the calorific value (on any of the three possible bases), a so-called enthalpic correction is, in principle, required in order to convert the ideal-gas enthalpy of combustion for the gas mixture to a value appropriate to the real gas. This, however, is generally small enough to be negligible. A discussion justifying such neglect is given in clause E.3.

4.2 Calculation of compression factor

For the volumetric-basis calorific value, a second real-gas correction is required to account for the deviation of the gas from volumetric ideality, and this is generally not negligible. This correction is also required in the calculation of density, relative density and, by implication, Wobbe index. Clause E.2 gives the background to the way in which corrections for volumetric non-ideality should be applied, discusses the principles involved, and justifies the simplifications employed which enable tractable calculations to be made without necessitating machine computation.

Such corrections for volumetric non-ideality are made using the compression factor Z_{mix}. The formulation to be used for Z_{mix} at the metering reference conditions, as required for the calculations described in clauses 5 to 9, is (equation E.17):

$$Z_{mix}(t_2,p_2) = 1 - \left[\sum_{j=1}^{N} x_j \cdot \sqrt{b_j}\right]^2 \qquad \ldots (3)$$

where the summation is taken over all N components of the mixture. Values of the so-called summation factor $\sqrt{b_j}$ are given in table 2 (clause 10) at the three metering reference conditions of common interest, for all of the components of natural gas and substitute natural gas considered in this International Standard. Values are also given for all pure component compression factors (or hypothetical compression factors) Z_j, from which the b_j's have generally been derived using the relationship $b_j = 1 - Z_j$. Any user requiring greater detail should consult clause E.2.

5 Calculation of calorific value on a molar basis

5.1 Ideal gas

The ideal-gas calorific value on a molar basis, at a temperature t_1, of a mixture of known composition is calculated from the equation

$$\overline{H}^{o}(t_1) = \sum_{j=1}^{N} x_j \cdot \overline{H}_j^{o}(t_1) \qquad \ldots (4)$$

where

$\overline{H}^{o}(t_1)$ is the ideal molar calorific value of the mixture (either superior or inferior);

$\overline{H}_j^{o}(t_1)$ is the ideal molar calorific value of component j (either superior or inferior);

x_j is the mole fraction of component j.

Numerical values of $\overline{H}_j^{o}$ for $t_1 = 25$ °C are given in table 3 (clause 10); the values for $(\overline{H}_j^{o})_S$ are taken from the original literature sources cited in annex M, and the values for $(\overline{H}_j^{o})_I$ derived using the accepted value of the standard enthalpy of vaporization of water at 25 °C (see annex B).

Values for $\overline{H}_j^{o}$ for other temperatures ($t_1 = 20$ °C, 15 °C and 0 °C) are also given in table 3; these values have been derived from the 25 °C values in accordance with the methods described in clause E.1.

NOTES

11 Values of $\overline{H}_j^{o}$ are independent of pressure; consequently the combustion reference pressure p_1 is irrelevant for the ideal-gas case and is omitted from the nomenclature adopted.

12 The ideal-gas calorific value on a molar basis of a gas or gas mixture is defined in this International Standard as a positive number. The values given in table 3 are numerically equal to the standard molar enthalpies of combustion, which are, however, conventionally expressed as negative quantities (see 2.6).

5.2 Real gas

For the purposes of this International Standard the real-gas calorific value on a molar basis is taken as numerically equal to the corresponding ideal-gas value.

NOTE 13 A rigorous approach to the calculation of the real-gas calorific value on a molar basis from the ideal-gas value would require the calculation of an enthalpic correction (see 4.1) for the mixture. In practice, this correction is very small for typical natural gases, and can usually be neglected with resultant errors not exceeding 50 J·mol^{-1} (approximately 0,005 %) (see clause E.3).

6 Calculation of calorific value on a mass basis

6.1 Ideal gas

The ideal-gas calorific value on a mass basis, at a temperature t_1, of a mixture of known composition is calculated from the equation

$$\hat{H}^{o}(t_1) = \frac{\overline{H}^{o}(t_1)}{M} \qquad \ldots (5)$$

where

M is the molar mass of the mixture, and is calculated from the equation

$$M = \sum_{j=1}^{N} x_j \cdot M_j \qquad \ldots (6)$$

x_j being the mole fraction of component j;

M_j being the molar mass of component j;

$\hat{H}^{\circ}(t_1)$ is the ideal calorific value on a mass basis of the mixture (either superior or inferior).

Table 1 (clause 10) lists values of the molar mass for all components considered in this International Standard.

Use of equations (5) and (6) represents the definitive method for calculating $\hat{H}^{\circ}$. An alternative method uses the equation

$$\hat{H}^{\circ}(t_1) = \sum_{j=1}^{N}\left(x_j \times \frac{M_j}{M}\right)\hat{H}_j^{\circ}(t_1) \qquad \ldots (7)$$

where $\hat{H}_j^{\circ}(t_1)$ is the ideal calorific value on a mass basis of component j (either superior or inferior).

For convenience, values of $\hat{H}_j^{\circ}$ for four values of t_1 (25 °C, 20 °C, 15 °C and 0 °C) are given in table 4 (clause 10), in order that the user may avoid the necessity of using values of $\bar{H}_j^{\circ}$ as the starting point of a calculation.

Numerical values obtained from either method will be concordant to within 0,01 MJ·kg^{-1}, which is within the limits of significance for the current state-of-the-art.

6.2 Real gas

For the purposes of this International Standard, the real-gas calorific value on a mass basis is taken as numerically equal to the corresponding ideal-gas value.

NOTE 14 See 5.2 for clarification and justification.

7 Calculation of calorific value on a volumetric basis

7.1 Ideal gas

The ideal-gas calorific value on a volumetric basis, for a combustion temperature t_1, of a mixture of known composition, metered at a temperature t_2 and pressure p_2, is calculated from the equation

$$\tilde{H}^{\circ}[t_1,V(t_2,p_2)] = \bar{H}^{\circ}(t_1) \times \frac{p_2}{R\cdot T_2} \qquad \ldots (8)$$

where

$\tilde{H}^{\circ}[t_1,V(t_2,p_2)]$ is the ideal calorific value on a volumetric basis of the mixture (either superior or inferior);

R is the molar gas constant (= 8,314 510 J·mol^{-1}·K^{-1}, see clause B.1);

$T_2 (= t_2 + 273{,}15)$ is the absolute temperature, in kelvins.

The use of equation (8) represents the definitive method for calculating $\tilde{H}^{\circ}$. An alternative method uses the equation

$$\tilde{H}^{\circ}[t_1, V(t_2,p_2)] = \sum_{j=1}^{N} x_j\cdot\tilde{H}_j^{\circ}[t_1,V(t_2,p_2)] \qquad \ldots (9)$$

where $\tilde{H}_j^{\circ}[t_1,V(t_2,p_2)]$ is the ideal calorific value on a volumetric basis of component j (either superior or inferior).

For convenience, values of $\tilde{H}_j^{\circ}$ for a variety of combustion and metering reference conditions are given in table 5 (clause 10), in order that the user may avoid the necessity of using values of $\bar{H}_j^{\circ}$ as the starting point of a calculation.

Numerical values obtained from either method will be concordant to within 0,01 MJ·m^{-3}, which is within the limits of significance for the current state-of-the-art.

7.2 Real gas

The real-gas calorific value on a volumetric basis, for combustion at temperature t_1 and pressure p_1 of a gas mixture metered at a temperature t_2 and pressure p_2 is calculated from the equation

$$\tilde{H}[t_1,V(t_2,p_2)] = \frac{\tilde{H}^{\circ}[t_1,V(t_2,p_2)]}{Z_{\mathrm{mix}}(t_2,p_2)} \qquad \ldots (10)$$

where

$\tilde{H}[t_1,V(t_2,p_2)]$ is the real-gas calorific value on a volumetric basis (either superior or inferior);

$Z_{\mathrm{mix}}(t_2,p_2)$ is the compression factor at the metering reference conditions.

The compression factor $Z_{\mathrm{mix}}(t_2,p_2)$ is calculated from equation (3), using values of the summation factor $\sqrt{b_j}$ given for individual pure substances in table 2 (clause 10).

NOTE 15 See 5.2 for clarification and justification of the practical approach to real-gas calorific values. Since no enthalpic correction is made to the ideal-gas calorific value on a volumetric basis in this calculation, the combustion reference pressure p_1 is irrelevant and is omitted from the nomenclature adopted.