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Analiza plinov - Pretvorba podatkov o sestavi plinskih zmesi (ISO/DIS 14912:2023)

Gas analysis - Conversion of gas mixture composition data (ISO/DIS 14912:2023)

Gasanalyse - Umrechnung von Zusammensetzungsangaben für Gasgemische (ISO/DIS 14912:2023)

Analyse des gaz - Conversion des données de composition de mélanges gazeux (ISO/DIS 14912:2023)

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Gas analysis — Conversion of gas mixture composition data

Analyse des gaz — Conversion des données de composition de mélanges gazeux

ICS: 71.040.40

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Foreword

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The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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This document was prepared by Technical Committee ISO/TC 158 *Analysis of gases*.

This second edition cancels and replaces the first edition (ISO 14912:2003 and Cor.1:2006), which has been technically revised.

The main changes compared to the previous edition are as follows:

— update of the molar mass data for mixture components in Annex C according to the 2019 IUPAC/CIAAW atomic mass data

— update of the value of the gas constant according to the 2018 revision of the SI System

— update of the bibliography and the corresponding references in the text

— update of the information in Annex E on the computer programme CONVERT

— correction of formulae (37) and (39)

— recalculation of the examples in Annex D

— addition of a table of molar mass data for the relevant elements from which the molar mass data for mixture components were calculated

— addition of information concerning data for synthetic air

— editorial amendments

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

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Introduction

The composition of a gas mixture is given by the identity of the mixture components and their proportion in the mixture. For the purpose of expressing component proportions, different quantities are in use, the most common ones being mass concentration, amount fraction and volume fraction. This diversity is due to the fact that in different applications different quantities have decisive advantages. Therefore procedures for conversion between different quantities are required.

As far as these quantities involve volumes, their value depends on the state conditions, i.e. pressure and temperature, of the gas mixture. For these quantities, therefore, procedures for conversion between different state conditions are required.

As a crude approximation, all of the conversions referred to above can be performed on the basis of the Ideal Gas Law. In most cases, however, an accurate conversion has to take into account the real gas volumetric behaviour of the components and of the entire gas mixture. These calculations require values of the compression factor (or of the density) of the components concerned and the entire gas mixture.

This document provides conversion procedures which fully account for real gas behaviour of pure gases and gas mixtures. In addition to these, approximate procedures for practical applications are described, designed for different levels of accuracy and available data. These procedures are based on approximate calculations (i) of pure gas compression factors using virial coefficients and (ii) of mixture compression factors using component data. Uncertainty estimates are given which account for the uncertainty due to approximations in the conversion procedures and the uncertainty of the input data.

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Gas analysis — Conversion of gas mixture composition data

1   Scope

This document defines the following quantities commonly used to express the composition of gas mixtures:

— amount fraction,

— mass fraction,

— volume fraction,

and

— amount concentration,

— mass concentration,

— volume concentration.

For these quantities of composition, this Document provides methods for

— conversion between different quantities, and

— conversion between different state conditions.

Conversion between different quantities means calculating the value of the content of a specified component in terms of one of the quantities listed above from the value of the same content, at the same pressure and temperature of the gas mixture, given in terms of another of these quantities. Conversion between different state conditions means calculating the value of the content of a specified component, in terms of one of the quantities listed above, under one set of state conditions from the value of the same quantity under another set of state conditions, i.e. pressure and temperature, of the gas mixture. Gas mixture composition can be converted simultaneously between different quantities of composition and different state conditions by combination of the two types of conversion.

This document is applicable only to homogeneous and stable gas mixtures. Therefore any state conditions (pressure and temperature) considered need to be well outside the condensation region of the gas mixture. In addition, the use of volume concentrations requires that the component under consideration is completely gaseous, and for the use of volume fractions even all components shall be completely gaseous. Further restrictions of state conditions apply for approximations of compression factors using virial coefficients (see Annex A).

2   Normative references

There are no normative references in this document.

3   Terms and definitions

For the purposes of this document, the following terms and definitions apply.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

— ISO Online browsing platform: available at https://www.iso.org/obp

— IEC Electropedia: available at https://www.electropedia.org/

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3.1 Quantities for the expression of gas mixture composition

Note 1 to entry   Further information concerning the terms defined in this subclause is given in 5.1.

Note 2 to entry The definitions are consistent with those in ISO 7504 and ISO 80000-9. In case of different symbols (3.1.5) a note is added to the respective entry.

3.1.1
amount fraction
amount-of-substance fraction
x
quotient of the amount of substance of a specified component and the sum of the amounts of substance of all components of a gas mixture

Note 1 to entry: The amount fraction is independent of the pressure and the temperature of the gas mixture.

3.1.2
mass fraction
w
quotient of the mass of a specified component and the sum of the masses of all components of a gas mixture

Note 1 to entry: The mass fraction is independent of the pressure and the temperature of the gas mixture.

3.1.3
volume fraction
ϕ
quotient of the volume of a specified component and the sum of the volumes of all components of a gas mixture before mixing, all volumes referring to the pressure and the temperature of the gas mixture

Note 1 to entry: The volume fraction is not independent of the pressure and the temperature of the gas mixture. Therefore the pressure and the temperature have to be specified.

Note 2 to entry: The volume fraction can only be used at state conditions where all mixture components are completely gaseous.

3.1.4
amount concentration
amount-of-substance concentration
c
quotient of the amount of substance of a specified component and the volume of a gas mixture

Note 1 to entry: The amount concentration is not independent of the pressure and the temperature of the gas mixture. Therefore the pressure and the temperature have to be specified.

3.1.5
mass concentration
β
quotient of the mass of a specified component and the volume of a gas mixture

Note 1 to entry: The mass concentration is not independent of the pressure and the temperature of the gas mixture. Therefore the pressure and the temperature have to be specified.

Note 2 to entry: In ISO 7504 and ISO 80000-9 the symbol γ is used for the mass concentration.

3.1.6
volume concentration
σ

quotient of the volume of a specified component before mixing and the volume of a gas mixture, both volumes referring to the same pressure and the same temperature

Note 1 to entry: The volume concentration is not independent of the pressure and the temperature of the gas mixture. Therefore the pressure and the temperature have to be specified.

Note 2 to entry: The volume concentration can only be used at state conditions where the specified component is completely gaseous.

Note 3 to entry: The *volume fraction* ([3.1.3](#)) and *volume concentration* ([3.1.6](#)) take the same value if, at the same state conditions, the sum of the component volumes before mixing and the volume of the mixture are equal. However, because the mixing of two or more gases at the same state conditions is usually accompanied by a slight contraction or, less frequently, a slight expansion, this is not generally the case.

3.2   Additional quantities involved in conversions of gas mixture composition

3.2.1
compression factor
Z

quotient of the volume of an arbitrary amount of gas at specified pressure and temperature and the volume of the same amount of gas, at the same state conditions, as calculated from the ideal gas law

Note 1 to entry: This definition is applicable to pure gases and to gas mixtures, therefore the term "gas" is used as a general term to be understood to cover pure gases as well as gas mixtures.

Note 2 to entry: By definition, the compression factor of an ideal gas is 1. At room temperature and atmospheric pressure, for many gases the compression factor differs only moderately from 1.

3.2.2
mixing factor
f

quotient of the volume of an arbitrary amount of a gas mixture at specified pressure and temperature and the sum of the volumes of all mixture components, before mixing, at the same state conditions

Note 1 to entry: If the component volumes are strictly additive, i.e. if the sum of the component volumes before mixing is the same as the volume after mixing, the mixing factor is 1. At room temperature and atmospheric pressure, for many gas mixtures the mixing factor differs only slightly from 1.

3.2.3
density
ρ

quotient of the mass of an arbitrary amount of gas and its volume at specified pressure and temperature

Note 1 to entry: This definition is applicable to pure gases and to gas mixtures, therefore the term "gas" is used as a general term to be understood to cover pure gases and gas mixtures.

3.2.4
molar volume
V_{mol}

quotient of the volume of an arbitrary amount of gas at specified pressure and temperature and its amount of substance

Note 1 to entry: This definition is applicable to pure gases and to gas mixtures, therefore the term "gas" is used as a general term to be understood to cover pure gases and gas mixtures.

Note 2 to entry: The amount of substance of a mixture is given by the sum of the amounts of substance of the components.

Note 3 to entry: In ISO 80000-9 the symbol V_m is used for the molar volume.

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3.2.5
virial coefficients
coefficients in the expansion of the compression factor in terms of powers of a quantity of state

Note 1 to entry: In practice, only two virial expansions are used, where the quantity of state is either the pressure, p, or the inverse molar volume, $1/V_{\text{mol}}$, as follows.

$$Z(V_{\text{mol}},T)=1+\frac{B(T)}{V_{\text{mol}}}+\frac{C(T)}{V_{\text{mol}}^2}+\dots \tag{1}$$

$$Z(p,T)=1+B'(T)p+C'(T)p^2+\dots \tag{2}$$

3.2.5.1
second molar-volume virial coefficient
B
coefficient of $1/V_{\text{mol}}$ in the expression of the compression factor as a series of inverse powers of the molar volume, V_{mol}

3.2.5.2
third molar-volume virial coefficient
C
coefficient of $1/V_{\text{mol}}^2$ in the expression of the compression factor as a series of inverse powers of the molar volume, V_{mol}

3.2.5.3
second pressure virial coefficient
B'
coefficient of p in the expression of the compression factor as a series of powers of the pressure p

3.2.5.4
third pressure virial coefficient
C'
coefficient of p^2 in the expression of the compression factor as a series of powers of the pressure p

4   Symbols and units

Symbol	Quantity	SI unit
α	$= p/(RT)$	mol/m^3
B	second molar-volume virial coefficient	m^3/mol
B'	second pressure virial coefficient	$1/\text{Pa}$
B	mass concentration	kg/m^3
c	amount concentration	mol/m^3
C	third molar-volume virial coefficient	m^6/mol^2
C'	third pressure virial coefficient	$1/\text{Pa}^2$
D	dilution factor	1
f	mixing factor	1
ϕ	volume fraction	m^3/m^3
m	mass	kg
M	molar mass	kg/mol
n	amount of substance	mol
N	number of gas mixture components	1
p	pressure	Pa
p_{vap}	saturation vapour pressure	Pa

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Symbol	Quantity	SI unit
p_{dew}	dew pressure	Pa
R	gas constant (8,314 462 618 153 24)	J/(mol·K)
ρ	density	kg/m^3
σ	volume concentration	m^3/m^3
t	Celsius temperature	°C
T	thermodynamic temperature	K
V	volume	m^3
V_{mol}	molar volume	m^3/mol
w	mass fraction	kg/kg
W	mass of a gas cylinder	kg
x	amount fraction	mol/mol
X_{ref}	reference value of state conditions ($X = p, T$)	same as for X
X_{crit}	critical property of a pure gas ($X = p, T, V, Z$)	same as for X
X_{pscrit}	pseudo-critical property of a gas mixture ($X = p, T$)	same as for X
Z	compression factor	1

Symbol	Index
i, j, k	for gas mixture components ($i, i, k = 1, ..., N$)
S	(sample of) gas mixture

In addition to the symbols specified above, the following symbols are used to denote objects of generic mathematical expressions.

Symbol	Quantity
F	mathematical function expressing a conversion
I	input quantity of composition
O	output quantity of composition
Ω	conversion factor
K,L,P,Q,Y	general variables or quantities
$\partial F/\partial P$	partial derivative (sensitivity coefficient)
$r(P,Q)$	correlation coefficient of quantities P,Q
$\boldsymbol{R}$	correlation matrix
$u(P)$	standard uncertainty of quantity P
$u^2(P)$	variance of quantity P
$u(P,Q)$	covariance of quantities P,Q
$\boldsymbol{U}$	variance-covariance matrix
$v(P)$	relative standard uncertainty of quantity P
	$v(P) = u(P)/|P|$

5 Basic Principles

5.1 Expression of gas mixture composition

The generic term for the proportion of a component in a mixture is "content". This term is intended for use only in a purely descriptive or qualitative sense, and is, without further qualification, inappropriate and insufficient to express quantitatively the proportion of a component.

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Quantitative statements require the expression of content as a value (the product of a number and a unit) of a "quantity of composition".

For the purposes of this Document, six quantities of composition, subdivided into two distinct conceptual families, called fractions and concentrations, are defined in 3.1. The terms "fraction" and "concentration" are themselves incomplete, and shall not be used in quantitative statements of content without further qualification by one of the modifiers "amount", "mass" or "volume".

In quantitative expressions of gas mixture composition, the applicable quantity, for example the amount fraction or the mass concentration, shall be used in conjunction with the name or the chemical symbol of the component.

EXAMPLE 1   The hydrogen content in a hydrogen/nitrogen mixture, expressed as amount fraction, is $x(\mathrm{H}_2) = 0,1$.

EXAMPLE 2   The sulfur dioxide content in air at 101,325 kPa and 25 °C, expressed as mass concentration, is $\beta(\mathrm{SO}_2) = 1\ \mathrm{mg/m^3}$.

Gas mixture composition may either relate to the preparation of gas mixtures or to the analysis of gas mixtures. In the first case, the composition expresses the formulation of a prepared mixture. Here the components are the parent gases that were mixed. These can be technically pure gases or specified gas mixtures. In the second case, the composition expresses the results of analysis. Here the components are the analytes (i.e. the distinct chemical substances determined quantitatively) and the matrix (i.e. the complementary gas).

Fractions are often used in the expression of results of gas mixture preparation. If a gas mixture consists of N components, 1, 2, ..., N, and if the amounts of these components in the mixture are quantified by amount of substance, $n_1, n_2, ..., n_N$, the amount fraction x_i of any component i is given by

$$x_i = \frac{n_i}{\sum\limits_k n_k} \tag{3}$$

If the amounts of the mixture components are quantified by mass, $m_1, m_2, ..., m_N$, the mass fraction w_i of any component i is given by

$$w_i = \frac{m_i}{\sum\limits_k m_k} \tag{4}$$

If the amounts of the mixture components are quantified by volume, $V_1, V_2, ..., V_N$, the volume fraction ϕ_I of any component i is given by

$$\phi_i = \frac{V_i}{\sum\limits_k V_k} \tag{5}$$

Concentrations are often used to express the results of chemical analysis of a mixture. If the amount of a specified component, i, found in the analysed sample is quantified by amount of substance, n_i, and if

V_S is the sample volume at specified pressure and temperature, the amount concentration (amount-of-substance concentration) c_i is given by

$$c_i = \frac{n_i}{V_S} \tag{6}$$

If the amount of the component is quantified by mass, m_i, the mass concentration β_i is given by

$$\beta_i = \frac{m_i}{V_S} \tag{7}$$

If the amount of the component is quantified by volume, V_i, the volume concentration σ_i is given by

$$\sigma_i = \frac{V_i}{V_S} \tag{8}$$

In all the above expressions, it shall be noted that the sample volume depends on pressure and temperature. In the expression for the volume concentration, the volume of the component also depends on pressure and temperature. For both volumes, the state conditions shall be the same.

The quantities of composition exhibit different behaviour concerning the dependence on pressure and temperature, as follows:

— amount concentration and mass concentration depend strongly on state conditions,

— volume fraction and volume concentration depend weakly on state conditions,

— amount fraction and mass fraction are strictly independent of state conditions.

Given the application to homogeneous gas mixtures only (see Scope), the state conditions (pressure and temperature) shall be such that the mixture is completely gaseous. In addition,

a) the volume concentration is only applicable if the state conditions are such that the individual component under consideration, before mixing, is completely gaseous, and

b) the volume fraction is only applicable if the state conditions are such that all components, before mixing, are completely gaseous.

The expression "completely gaseous" means, for an individual component, that the pressure is well below the saturation pressure at the given temperature or that the temperature is well above the critical temperature. For a mixture, the equivalent condition is that the pressure is well below the dew pressure at the given temperature or that the temperature is well above the cricondentherm. Thus, the state conditions are to be well outside the relevant condensation regions. Methods for assessing whether, at specified state conditions, gas mixtures and their components are completely gaseous are described in Annex A.

5.2 Conversion between different quantities

The conversion between different quantities of composition uses the basic relations between the following quantities, which apply both to pure gases and to gas mixtures:

— amount of substance, n

— mass, m

— volume, V