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Gas analysis — Conversion of gas mixture composition data

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

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This document was prepared by Technical Committee ISO/TC 158, *Analysis of gases,* in collaboration with the European Committee for Standardization (CEN) Technical Committee CEN/TC 238, *Test gases, test pressures, appliance categories and gas appliance types*, in accordance with the Agreement on technical cooperation between ISO and CEN (Vienna Agreement).

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

The main changes are as follows:

— update of the molar mass data for mixture components in Annex C according to the 2019 to 2021 IUPAC/CIAAW atomic mass data;

— update of the value of the gas constant according to the 2018 revision of the International System of Units (SI);

— 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 corrections.

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.

The composition of a gas mixture is given by the identity of the mixture components and their content in the mixture. For the purpose of expressing component contents, 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 needed.

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 needed.

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 shall take into account the real gas behaviour of the components and of the entire gas mixture. These calculations use values of the compression factor (or 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 of a) pure gas compression factors using virial coefficients and b) 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.

Recently, advanced compression factor calculations for pure gases and gas mixtures, based on multi-parameter equations of state became publicly available (see e.g. NIST Reference Fluid and Transport Properties Database (REFPROP))[17] and were even standardized (see e.g. ISO 20765-2). Concerning accuracy and uncertainty, these tools clearly outperform the simple approach used in ISO 14912 (truncated virial expansion, linear interpolation of virial coefficient data). However, for the intended use of ISO 14912, the performance is sufficent and the simplicity is beneficial for many users.