ISO/TR 29922:2017-03 (E)

Natural gas - Supporting information on the calculation of physical properties according to ISO 6976

Contents

Page

Foreword vi

Introduction vii

1 Scope 1

2 Normative references 1

3 Termsanddefinitions 1

4 Symbols, units and abbreviated terms 1
4.1 Quantities 1
4.2 Subscripts 3
4.3 Superscripts 3
4.4 Abbreviated terms 3

5 Enthalpy of combustion of the ideal gas and its variation with temperature 4
5.1 Preamble 4
5.2 Standard enthalpy of combustion at 25 °C 4
5.3 Standard enthalpy of combustion at other temperatures 5
5.4 Formulation of the ideal-gas enthalpy 6
5.5 Illustrative examples 7
5.6 Uncertainty in enthalpy of combustion 8

6 Non-ideality: Variation of real-gas enthalpy of combustion with pressure 9
6.1 Preamble 9
6.2 Formulation of the enthalpic correction 10
6.3 Estimation of the enthalpic correction 12
6.4 Conclusion 13

7 Non-ideality:Compressionfactoreffectonvolume-basiscalorificvalues 13
7.1 Compression factor 13
7.2 Virial equation of state 14
7.3 Estimation of mixture compression factor 15
7.4 Limitations of the modified IGT-32 method 17
7.5 Uncertainty in compression factor 18

8 Quantitation of volumetric non-ideality 18
8.1 Second virial coefficients of pure components 18
8.1.1 Preliminary procedures 18
8.1.2 Improved procedure 19
8.2 Summation factors of pure components 21
8.2.1 Overview 21
8.2.2 Major components of natural gas 21
8.2.3 Hydrogen and helium 22
8.3 Compression factors of the permanent gases 23
8.4 Pure component uncertainties 25
8.4.1 Uncertainty of second virial coefficients 25
8.4.2 Truncation error 25
8.4.3 Linearization error 27
8.4.4 Berlin versus Leiden 28

8.4.5 Hydrogen and helium 29
8.4.6 Water 30
8.4.7 Combination of uncertainties 31
8.5 Mixture uncertainty 31

9 Miscellaneous data 31
9.1 Atomic weights of the elements 31
9.1.1 Atomic weights 2007 31
9.1.2 Atomic weights 2009 and 2011 32
9.1.3 Discussion 34
9.2 Composition and molecular weight of dry air 35

10 Effectsofwatervapouroncalorificvalue 36
10.1 Preamble 36
10.2 Excluded volume effect 37
10.3 Latent heat (enthalpic) effect 38
10.4 Compression factor effect 39
10.5 Combination of effects 39
10.6 Spectator water 40
10.7 Effect of humid air 41
10.7.1 Preamble 41
10.7.2 Stoichiometric combustion with oxygen 42
10.7.3 Combustion of dry gas with excess dry air 42
10.7.4 Combustion of wet gas with excess dry air 43
10.7.5 Combustion of wet gas with excess humid air 43

11 Summary,discussionandselectionofthecalorificvalueofmethane 45
11.1 Standard enthalpy of combustion 45
11.1.1 Background 45
11.1.2 Selection of data 45
11.1.3 Recalculation of Rossini values 46
11.1.4 Evaluation of selected data 48
11.1.5 Selected value and uncertainty 52
11.2 Derived calorific values 52
11.3 Comparisons between calorimetric methodologies 54

12 Calorificvaluesonamassbasis 56
12.1 Calorific values on a mass basis for components of natural gas 56
12.2 Alternative (non-normative) method of calculation for mass-basis calorific values 57

13 Calorificvaluesonavolumebasis 60
13.1 Calorific values on a volume basis for components of natural gas 60
13.2 Alternative (non-normative) method of calculation for volume-basis calorific values 60

14 Approximate conversion between reference conditions 63
14.1 Factors for conversion between metric reference conditions 63
14.2 Equations for conversion between metric reference conditions 65
14.3 Expression of non-SI reference (base) pressures in metric units 65

15 Mathematical and methodological issues relating to estimation of uncertainty 66
15.1 Principles 66
15.2 Input data 68
15.2.1 Preamble 68
15.2.2 Reference conditions 68
15.2.3 Composition data 68
15.2.4 Physical property data 69
15.3 Uncertainty of the calculational method 70
15.4 Evaluation of sensitivity coefficients 70
15.4.1 Preamble 70
15.4.2 Analytical method 71
15.4.3 Finite difference method 73

15.4.4 Monte Carlo method 73

16 Detailed derivation of uncertainty equations in ISO 6976:2016 73
16.1 Principles and assumptions 73
16.2 General formulation 74
16.3 Effects of correlations 75
16.3.1 Correlation between mole fractions 75
16.3.2 Correlation between molar masses 76
16.3.3 Correlation between physical properties 78
16.4 Uncertainty equations for basic properties 78
16.4.1 Molar mass 78
16.4.2 Molar-basis gross calorific value 79
16.4.3 Molar-basis net calorific value 79
16.4.4 Summation factor 80
16.4.5 Compression factor 80
16.5 Uncertainty equations for compound properties 81
16.5.1 Mass-basis gross calorific value 81
16.5.2 Mass-basis net calorific value 82
16.5.3 Volume-basis gross calorific value 83
16.5.4 Volume-basis net calorific value 84
16.5.5 Density 86
16.5.6 Relative density 87
16.5.7 Gross Wobbe index 88
16.5.8 Net Wobbe index 89
16.6 Repeatability and reproducibility 91

17 Computer implementation of recommended methods 92
17.1 Compiled BASIC shareware program 92
17.2 Spreadsheet implementation 94

Bibliography 97