

# **AGA Report No. 8**

## **Part 1**

### **Thermodynamic Properties of Natural Gas and Related Gases**

#### **DETAIL and GROSS Equations of State**

**Third Edition**

**April 2017**

**(A revision of AGA Report No. 8, 2nd edition, 1994)**

**Prepared by  
Transmission Measurement Committee**



**American Gas Association**

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## FOREWORD

AGA Report No. 8, Part 1, is designated as the third edition of the revised 1994 second edition of AGA Report No. 8. As in the second edition, the third edition provides the technical information necessary to compute thermodynamic properties including compressibility factors and densities of natural gas and related gases for states in the gas phase only. Additionally, equations for calculating speeds of sound and other thermodynamic properties are given. Historical information on this document is given in Section 1.2, Background. Analyses of the calculation of uncertainties are provided for various gas temperatures, pressures, and compositions. It is based on research managed and sponsored by the then Gas Research Institute (GRI) in cooperation with AGA and the *Groupe Europeen de Recherches Gazieres* (GERG). Because the equations of state contained within International Standards Organization documents ISO 12213: *Natural Gas – Calculation of Compression Factor*, Part 2: *Calculation Using Molar-Composition Analysis*, 2006 edition, and ISO 20765: *Natural Gas – Calculation of Thermodynamic Properties*, Part 1: *Gas Phase Properties for Transmission and Distribution Applications*, 2005 edition, are based on the same equations in this revision, calculated properties should have the same values.

This revised edition, now designated as AGA Report No. 8, Part 1, uses the same DETAIL and GROSS equations of state as in the 1994 edition of AGA Report No. 8. However, the temperature, pressure, and gas composition limits have been modified in this edition; and therefore, it will be necessary to ensure that the temperature, pressure, and gas composition fall within the new limits for the desired uncertainty. The users are advised to verify the applicability/acceptability of the program for the new limits based on the 1994 edition of AGA 8.

The documentation of programs for calculating properties from the methods described in this document is available as supplementary material in Appendix C. Examples are available in Fortran, VB, and C++ code. The supplementary material also contains a Microsoft Excel spreadsheet for property calculations. This can be used to determine if, for a particular temperature, pressure, and composition, the property values calculated from the equations in Part 1 are within the desired uncertainty (by comparing with those in Part 2) even though one or more of these inputs may be outside the ranges given in Part 1. A file containing calculated points at different compositions (not necessarily related to typical natural gas) is included, which can be used to verify that programs or equipment have been implemented or upgraded correctly to produce values that are in agreement with the equations in this document.

**The user is encouraged to compare property values obtained through the use of the software provided in this edition with those obtained from the user's existing software and determine if the differences are within the uncertainty limits of their respective calculation methods. The Excel spreadsheet provided in the supplementary material can be used to determine if property values are within the acceptable uncertainty limits even though the state point may be outside the ranges given in this revision. If the property values are not within the uncertainty limits, the user should consider implementing AGA Report No. 8, Part 2, noted below.**

AGA Report No. 8, Part 2, published separately, is based on the GERG-2008 equation of state, and is applicable for temperature, pressure, and composition ranges outside those in Part 1, with uncertainties in density, compressibility factor, and speed of sound still within 0.1 %. Part 2 can also be used for operating conditions and compositions that are applicable for Part 1, with differences in the calculated values within the uncertainty limits of each equation, where uncertainties are given with a 95 % level of confidence ( $k=2$ ). **While adoption of the equations in Part 2 is encouraged, the decisions to upgrade existing installations to use AGA Report No. 8, Part 2, are left to the discretion of the parties involved.**

Some material described in Part 1 also applies to Part 2, and vice versa, and is not repeated in both parts. For example, Part 1 describes an algorithm for obtaining densities through an iterative procedure that can also be used with the equations in Part 2 (and which is applied for this purpose to the GROSS, DETAIL, and GERG-2008 equations of state in the programs in the supplementary material). Similarly, Part 2 outlines the method for reporting calculated results and uncertainties from the equations in both parts, and also describes the experimental

database available for natural gas mixtures (both binary and multicomponent systems), much of which was used in the development of the equations in Part 1. Some information, however, is repeated in both parts, such as the material in Sections 2 and 3. **The combination of Parts 1 & 2 gives a wider overview of the equations of state and their appropriate application to natural gas.**

The publication AGA Report No. 10: *Speed of Sound in Natural Gas and Other Related Hydrocarbon Gases* has been discontinued with the release of this AGA Report No. 8, Part 1. The calculation of the speed of sound no longer requires integration of the compressibility factor equation, as was done in AGA Report No. 10, but is implemented through differentiation of the fundamental Helmholtz energy equation of state. This results in faster calculations through direct computation of the required derivatives.

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### Individuals who made substantive contributions are:

Ian Bell, NIST, USA  
Ilia Bluvshstein, Union Gas Ltd., Canada  
David Bromley, BP Pipelines, USA  
Greg Dunn, Eagle Research Corporation, USA  
Juan Escobar, ARAMCO, Saudi Arabia  
Volker Heinemann, Honeywell, Germany  
Randy Herman, Flow-Cal Measurement Applications, USA  
Gurwinder Kamboz, Krohne Oil & Gas, The Netherlands  
Jason Lu, Thermo Fisher Scientific, USA  
Ian McDavid, Flow-Cal Measurement Applications, USA  
Warren Peterson, Alliance Pipeline, Canada  
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Daniel Harris, Columbia Pipeline Group–TransCanada Corp., USA  
Masahiro Ishibashi, Research Institute for Engineering Measurement, Japan  
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Christina Sames  
Vice President, Operations & Engineering

Ali Quraishi  
Director, Operations & Engineering Services

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# 1 INTRODUCTION

## 1.1 Scope

Part 1 presents information for the computation of thermodynamic properties (*e.g.*, compressibility factor, density, and speed of sound) of natural gas and related gases with the DETAIL and GROSS equations of state. Uncertainty estimations for different compositions, pressures, and temperatures are given. The computations are valid for single-phase gaseous states only. For mixed or liquid phases, refer to Part 2.

## 1.2 Background

Research in 1928 and 1929 under the direction of Mr. Howard S. Bean of the National Bureau of Standards provided the natural gas industry with its initial compressibility factor data covering pressures up to 600 psia (4 MPa). However, it was not until 1954 that extensive tables of natural gas supercompressibility factors were published, based on tests supervised by Professor Samuel R. Beitler of Ohio State University. The natural gas supercompressibility factor tables were extended and an equation of state was developed in 1956-1962 under the direction of Mr. R. H. Zimmerman of Ohio State University. The results of this project, designated PAR Project NX-19, appear in AGA's *Manual for Determination of Supercompressibility Factors for Natural Gas*, published in 1962.

The research leading to the 1985 and 1992 reports was initiated in 1981 under the sponsorship of GRI in close liaison with the AGA Transmission Measurement Committee. This research, carried out under the direction of Professor Kenneth E. Starling of the University of Oklahoma, was aimed at extending capabilities for accurate computation of compressibility factors beyond the temperature, pressure, and composition ranges of PAR Project NX-19. The results for pipeline-quality natural gas, which were completed in 1984, provided the basis for the 1985 report.

The initial 1981-1984 research used data ranging in pressures up to approximately 900 psia (6 MPa) obtained from the literature and provided by GERG. However, the GERG data bank was extended considerably over the period 1985-1990. The new data showed that the original equation of state, developed in the period 1981-1984, needed to be improved. In addition, speed of sound data obtained under GRI sponsorship during 1985-1989 showed calculations for rich gases were not sufficiently accurate for critical flow applications.

Although the 1992 and 1994 AGA 8 publications of the equation of state are explicit in the compressibility factor  $Z$ , the formulation was originally developed with an equation of state explicit in the Helmholtz energy  $a$  with independent variables of molar density  $d$  and temperature  $T$ . The Helmholtz energy equation was not given in the 1992 and 1994 AGA 8 documents, where only equations explicit in pressure and compressibility factor were reported. The Helmholtz energy is a fundamental thermodynamic property from which all other thermodynamic properties can be calculated as derivatives with respect to density or temperature. For example, the expression for calculating pressure is

$$P = d^2 \left( \frac{\partial a}{\partial d} \right)_T. \quad (1-1)$$

When starting from the pressure explicit equation, the calculation of other properties, including the speed of sound, requires not only derivatives of the compressibility factor with respect to density and temperature, but also integration of  $Z$  over density, which can be quite complicated. Equations are presented in this revision that start with the Helmholtz energy form, and allow access to other thermodynamic properties such as heat capacities, enthalpies, and entropies by differentiation of this fundamental property. Formulations explicit in the Helmholtz energy have been used heavily over the last two decades to represent the properties of pure fluids and mixtures due to the ease of calculating all other thermodynamic properties.

Work began in the 1990's at the Ruhr University in Bochum, Germany, under the direction of Wolfgang Wagner to develop even more sophisticated models to represent not only the gas phase, as in the case of AGA 8, but also the liquid phase and retrograde region. The first version was released in 2004 for 18 fluids, and then updated in 2008 with three additional fluids. These 21 fluids are identical to the fluids available in this document.

Because the calculation of dew points requires knowledge of the liquid phase as well as the gas phase, the DETAIL equation of state presented in Part 1 is not able to determine the state where liquids will condense from a natural gas stream. With the addition of accurate liquid calculations in the GERG-2008 equation, dew points, as well as bubble points and saturation states in the retrograde region can now be evaluated for any temperature or pressure input state. The equations required to do so are covered in Part 2.

### 1.3 Overview of Properties from Equations of State

This report provides recommended equations of state to compute accurate compressibility factors, densities, and other thermodynamic properties for natural gas. The information in this report can be used for calculations of compressibility factors and densities for pure methane, ethane, nitrogen, carbon dioxide, hydrogen, and hydrogen sulfide, and for gas mixtures of up to twenty-one components. Compressibility factors, supercompressibility factors, and density values can be applied directly in calculations of gas volume and gas flow rate. These computations can also be used in other instances where the relationship between the temperature, pressure, and volume of a gas is important.

Other thermodynamic properties that can be calculated with the information in this report include the heat capacity, enthalpy, entropy, sonic velocity, critical flow factor (see Appendix E of ASME/ANSI MFC-7M-1987), and component chemical potentials. Applications that use these properties include calculations for sonic nozzles, compressors, heat exchangers, gas mixture reaction equilibrium, and gas mixture component fugacities (for use in vapor-liquid equilibrium calculations).

Two equations of state are provided in Part 1. All information needed to efficiently implement the appropriate equation of state as a function of the natural gas composition (*i.e.*, a gas analysis) is contained in this report, except the molar heating values, which can be obtained from AGA Report No. 5, *Natural Gas Energy Measurement*. The two equations differ by their complexity and the range over which calculations can be made. The equation of state with a wider range of conditions is referred to as the "DETAIL Equation of State." See References [1] and [2]. The equation of state with a limited range of conditions, herein referred to as the "GROSS Equation of State," uses second and third virial coefficients to compute the compressibility factor. See References [3] and [4]. Although gas properties are best calculated through the use of the natural gas composition, they can also be obtained with an aggregate or gross knowledge of the gas (given by heating value and/or relative density, and diluent gas content information).

#### 1.3.1 DETAIL Equation of State

The DETAIL equation of state was developed to accurately describe the gas-phase pressure-temperature-density behavior of natural gas mixtures. This equation of state reduces the uncertainties of compressibility factor and density calculations for natural gas, which can contain mole percentages of hexanes plus heavier hydrocarbons greater than 1 %. Equations of the density behavior of pure hydrogen sulfide and binary mixtures of hydrogen sulfide with methane, ethane, nitrogen, and carbon dioxide were developed to reduce the calculation uncertainty for natural gas containing hydrogen sulfide (sour gas). Second virial equations were developed for water and binary mixtures of water with methane, ethane, nitrogen, and carbon dioxide to reduce the calculation uncertainty for natural gas containing water vapor. Section 4 presents complete information for the DETAIL equation of state.

Part 1 is only valid for the gas phase. For the liquid phase, mixed phase, and saturation properties (including dew points), see Part 2. The DETAIL equation of state can be applied, as shown in Figure 1, for temperatures above  $-200^{\circ}\text{F}$  ( $-130^{\circ}\text{C}$ ) and at pressures up to 40,000 psia (280 MPa). The upper temperature limit is the onset of decomposition of the components in the gas [which is generally above  $350^{\circ}\text{F}$  ( $180^{\circ}\text{C}$ )]. For applications outside these ranges of temperature and pressure, refer to Part 2 or experimental verification. Use of the DETAIL equation of state is not recommended within the vicinity of the critical point or liquid-like states.

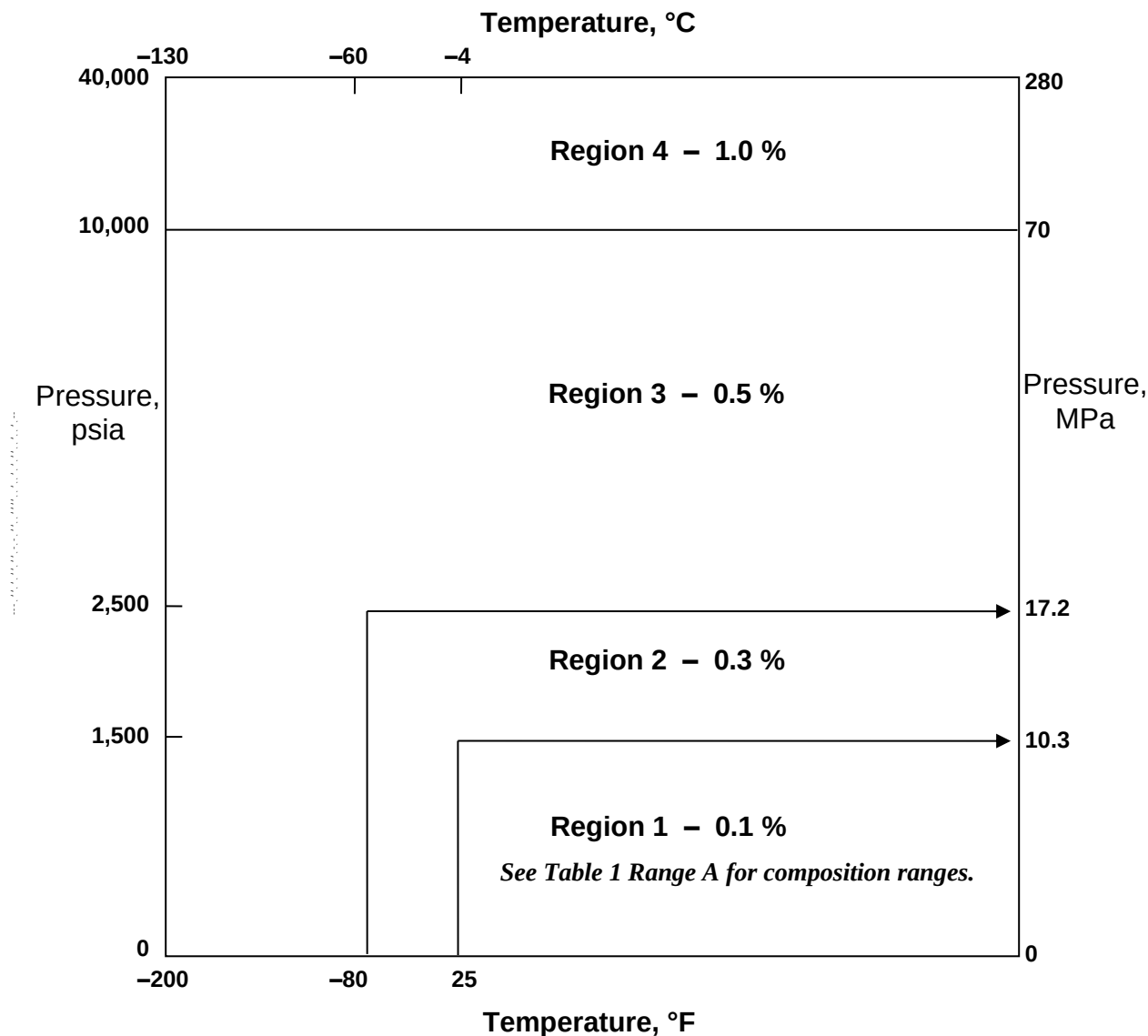


Figure 1. Overview of uncertainties for natural gas compressibility factors with the DETAIL equation of state (not to scale). The upper temperature limit is the onset of decomposition of the components in the gas.

**Note:** *This figure is not intended for contractual use. Table 1 should be consulted for specific uncertainty information.*

A database for mixtures with water, heavy hydrocarbons, or hydrogen sulfide in natural gas is not presently available for the determination of uncertainties of calculated gas properties. Therefore, as a practical matter, the only limitation is that the calculation is for the gas phase. Thus, the limits are the water dew point for mole percent water and the hydrocarbon dew point for mole percent heavy hydrocarbons.

Figure 1 gives a simple overview of typical uncertainties for the DETAIL equation of state, but should not be used as a basis to estimate the uncertainties in calculated properties. Rather, Table 1 lists comprehensive ranges for which the uncertainties are less than 0.1 % (details are given in Reference [5]). Three different sets of ranges are defined below, each having its own range of validity for temperature, pressure, and component fractions.

**Range A** in Table 1 shows the limits of the mole percent of components in a natural gas mixture in which the uncertainties in compressibility factors are less than 0.1 % for temperatures above 25 °F (−4 °C), pressures less than 1500 psia (10.3 MPa), heating values from 630 to 1200 Btu/scf, and relative densities from 0.554 to 0.91. However, a mixture with compositions near the upper limits of every component in this range, except methane and nitrogen, will have an uncertainty higher than 0.1 %. Most typical natural gases do not fall under such a condition. This was verified through the use of the 200 gas compositions available in the supplementary material. Deviations between the DETAIL and GERG equations of state were compared for each gas composition – those that met the 0.1 % uncertainty limit fell within the ranges listed in Range A of Table 1, or were slightly outside this range at the lower temperature limit with pressures slightly below the upper pressure limit. Several of the limits listed in this range have been modified from those given in Reference [5] to give better results. The regions in Figure 1 with uncertainty limits of 0.3 %, 0.5 %, and 1.0 % are also based on the Range A compositions. However, it is important to make use of a phase diagram to ensure that states are not in the 2-phase or in the critical region. The DETAIL equation of state should not be used for states at pressures exceeding the dew or bubble point (including 2-phase states). This applies for Ranges B and C as well.

**Range B** in Table 1 shows the maximum allowable mole percent composition for temperatures above 25 °F (−4 °C), but with pressures less than 300 psia (2 MPa), heating values from 680 to 1500 Btu/scf, and relative densities from 0.47 to 0.91. Range B allows higher upper range values of the compositions for operations below 300 psia.

**Range C** in Table 1 has a composition range that is much smaller than the other ranges, but allows temperatures down to 17 °F (−8 °C) and pressures up to 3000 psia (21 MPa).

In this AGA 8, Part 1, document the upper pressure limit for 0.1 % uncertainty has been changed from 1750 psia to 1500 psia (12 MPa to 10.3 MPa), and the lower temperature limit has been changed from 17 °F (−8 °C) to 25 °F (−4 °C) based on work presented in Reference [5]. However, uncertainties in the DETAIL equation of state are often below 0.1 % far outside the ranges listed in Table 1, especially at temperatures above 40 °F. For continued use of the DETAIL equation of state outside the ranges listed in Table 1, comparisons can be made between this and the GERG-2008 equation of state. When the difference is less than 0.1 %, the DETAIL equation of state can be used with a stated uncertainty of 0.1 %. The Excel application given in the supplementary material will calculate the difference between the DETAIL and GERG-2008 equations for any gaseous state. Other tools can also be used (*e.g.*, Reference [6]) to ascertain the differences in the calculations between the two equations. When exceeding the limits of Table 1 but claiming the 0.1 % uncertainty, users should specify the method or software used to arrive at this claim.

Table 1 – Ranges for Temperature, Pressure, Heating Value, and Relative Density with Uncertainties Less than 0.1 % in Compressibility Factors of Natural Gas Calculated with the DETAIL Equation of State

|                                         | Range A               | Range B             | Range C             |
|-----------------------------------------|-----------------------|---------------------|---------------------|
| Lower temperature limit                 | 25 °F<br>–4 °C        | 25 °F<br>–4 °C      | 17 °F<br>–8 °C      |
| Upper pressure limit                    | 1500 psia<br>10.3 MPa | 300 psia<br>2.1 MPa | 3000 psia<br>21 MPa |
| Gross heating value <sup>†</sup>        |                       |                     |                     |
| Btu/scf                                 | 630 to 1200           | 680 to 1500         | 960 to 1090         |
| MJ/m <sup>3</sup>                       | 23.5 to 44.7          | 25.3 to 56          | 35.8 to 40.6        |
| Relative density <sup>†</sup>           | 0.554 to 0.91         | 0.47 to 0.91        | 0.554 to 0.64       |
| Upper composition limits (mole percent) |                       |                     |                     |
| Methane                                 | 100.0                 | 100.0               | 100.0               |
| Nitrogen                                | 50.0                  | 50.0                | 3.0                 |
| Carbon dioxide                          | 30.0 <sup>‡</sup>     | 80.0                | 3.0                 |
| Ethane                                  | 10.0                  | 25.0                | 4.0                 |
| Propane                                 | 4.0                   | 6.0                 | 2.0                 |
| Isobutane                               | 0.4                   | 1.5                 | 0.1                 |
| <i>n</i> -Butane                        | 0.6                   | 6.0                 | 0.4                 |
| Isopentane                              | 0.3                   | 2.0                 | 0.1                 |
| <i>n</i> -Pentane                       | 0.3                   | 2.0                 | 0.1                 |
| Total pentanes                          | 0.3                   | 2.0                 |                     |
| <i>n</i> -Hexane                        | 0.12                  | 0.2                 | 0.03                |
| <i>n</i> -Heptane                       | 0.04                  | 0.2                 | 0.01                |
| <i>n</i> -Octane                        | 0.03                  | 0.2                 | 0.003               |
| <i>n</i> -Nonane                        | 0.03                  | 0.2                 | 0.003               |
| <i>n</i> -Decane                        | 0.03                  | 0.2                 | 0.003               |
| Total hexanes plus                      | 0.15                  |                     |                     |
| Total heptanes plus                     | 0.04                  |                     |                     |
| Hydrogen                                | 5.0                   | 100.0               | 1.0                 |
| Oxygen                                  | 0.2                   | 1.0                 | 0.2                 |
| Carbon monoxide                         | 1.0                   | 10.0                | 1.0                 |
| Water                                   | 0.05                  | 1.4                 | 0.005               |
| Hydrogen sulfide                        | 0.1                   | 4.0                 | 0.1                 |
| Helium                                  | 0.4                   | 5.0                 | 0.4                 |
| Argon                                   | 0.2                   | 3.0                 | 0.2                 |

**Note:** The above table provides component mole percent limits under the specified ranges of pressure, temperature, Btu value, and relative density for states with an uncertainty in density generally less than 0.1 %. The composition limits for different pressures, temperatures, Btu values, and relative densities outside of these ranges can be determined from the Excel spreadsheet provided in the supplementary material.

<sup>†</sup>Values are based on a methane lower limit composition of 60 mole percent. Reference conditions in U.S. customary units are (60 °F, 14.73 psia; density at 60 °F, 14.73 psia) and in SI units are (15 °C, 0.101325 MPa; density at 0 °C, 0.101325 MPa).

<sup>‡</sup>The upper limit for the mole percent of CO<sub>2</sub> is reduced under the following conditions:

|                                                                     |                                                                       |
|---------------------------------------------------------------------|-----------------------------------------------------------------------|
| $x_{\text{CO}_2, \text{max}} = 20 \%$ when $x_{\text{N}_2} > 7 \%$  | $x_{\text{CO}_2, \text{max}} = 5 \%$ when $x_{\text{C}_3} > 2 \%$     |
| $x_{\text{CO}_2, \text{max}} = 10 \%$ when $x_{\text{N}_2} > 15 \%$ | $x_{\text{CO}_2, \text{max}} = 10 \%$ when $x_{\text{iC}_4} > 0.1 \%$ |
| $x_{\text{CO}_2, \text{max}} = 7 \%$ when $x_{\text{C}_3} > 1 \%$   | $x_{\text{CO}_2, \text{max}} = 10 \%$ when $x_{\text{nC}_4} > 0.3 \%$ |

See the discussion in Section 1.3.1 for further information.

### 1.3.2 GROSS Equation of State

The GROSS equation of state was developed for dry, sweet natural gas to calculate compressibility factors. The limits for this method are listed in Table 2. For some gases at the upper limits of the allowed compositions, with temperatures below 80 °F (27 °C) or at pressures above 800 psia (5.5 MPa), the uncertainty of the GROSS equation of state can exceed 0.1 %. The maximum composition limits were therefore significantly reduced from the 1994 edition of AGA 8 so as to meet the 0.1 % uncertainty level. When exceeding the bounds listed in Table 2, the procedure given at the end of Section 1.3.1 for validating the uncertainty of a particular state should be followed.

Section 5 and Appendix A present information for this equation of state. Optimally, natural gas property calculations from the GROSS equation require the gas composition, *i.e.*, the mole fractions of the components in the mixture. When this information is not available, methods given in Appendix A can be used as a substitute to obtain the molar ideal gross heating value  $H_{CH}$  of the mixture of hydrocarbon components present in the natural gas along with the compositions of nitrogen and carbon dioxide in the mixture.

Table 2 – Ranges for Temperature, Pressure, Heating Value, and Relative Density with Uncertainties Less than 0.1 % in Compressibility Factors of Natural Gas Calculated with the GROSS Equation of State

| Quantity                                | Range 1                                               | Range 2                                             |
|-----------------------------------------|-------------------------------------------------------|-----------------------------------------------------|
| Temperature                             | 25 °F to 143 °F (–4 °C to 62 °C)                      | 17 °F to 143 °F (–8 °C to 62 °C)                    |
| Maximum pressure                        | 1500 psia (10.3 MPa)                                  | 600 psia (4.1 MPa)                                  |
| Relative density                        | 0.554 to 0.63                                         | 0.554 to 0.89                                       |
| Gross heating value <sup>†</sup>        | 930 to 1040 Btu/scf<br>34.7 to 38.7 MJ/m <sup>3</sup> | 665 to 1100 Btu/scf<br>24.8 to 41 MJ/m <sup>3</sup> |
| Upper composition limits (mole percent) |                                                       |                                                     |
| Nitrogen                                | 7                                                     | 20                                                  |
| Carbon dioxide                          | 3                                                     | 25                                                  |
| Ethane                                  | 2                                                     | 8                                                   |
| Propane                                 | 0.5                                                   | 4                                                   |
| Total butanes                           | 0.3                                                   | 0.5                                                 |
| Total pentanes                          | 0.2                                                   | 0.3                                                 |
| Hexanes plus                            | 0.04                                                  | 0.08                                                |
| Hydrogen <sup>‡</sup>                   | 0.2                                                   | 2                                                   |
| Oxygen <sup>‡</sup>                     | 0.2                                                   | 0.5                                                 |
| Carbon monoxide <sup>‡</sup>            | 0.4                                                   | 1                                                   |
| Water <sup>‡</sup>                      | 0.03                                                  | 0.2                                                 |
| Hydrogen sulfide <sup>‡</sup>           | 0.08                                                  | 0.2                                                 |
| Helium <sup>‡</sup>                     | 0.05                                                  | 0.3                                                 |
| Argon <sup>‡</sup>                      | 0.1                                                   | 0.2                                                 |

<sup>†</sup>Values are based on a methane lower composition limit of 60 mole percent. Reference conditions in U.S. customary units are (60 °F, 14.73 psia; density at 60 °F, 14.73 psia) and in SI units are (15 °C, 0.101325 MPa; density at 0 °C, 0.101325 MPa).

<sup>‡</sup>The nonhydrocarbon species listed in this table (except nitrogen and CO<sub>2</sub>) are considered here as impurities for use in the GROSS equation of state, and should be added to the equivalent hydrocarbon mole fraction as explained in Section 5.2. The SGERG-88 equation contains additional parameters for hydrogen and carbon monoxide, and Reference [3], ISO 12213:3, or GERG TM 5 (1991) should be consulted when the mixture contains these fluids.

## 1.4 Uncertainty

The uncertainties of compressibility factors or densities (relative deviations calculated in terms of  $Z$  or in terms of  $d$  are nearly identical but with an opposite sign) calculated with either the DETAIL equation of state or the GROSS equation of state depend upon the natural gas composition and the operating temperature and pressure conditions. Evaluations of the uncertainties of calculated compressibility factors for natural gas were made by comparing to the GRI and GERG compressibility factor reference databases. The reference databases have similar natural gas physical characteristics as those listed in Table 1. Comparisons were also made with data for pure fluids and binary mixtures. Lastly, comparisons were made with experimental speed-of-sound data to access derived thermodynamic property capabilities of the DETAIL equation of state. Uncertainty analyses are available in Appendix B.

### 1.4.1 DETAIL Equation of State Uncertainty

The GRI and GERG compressibility factor reference databases and comparisons with the GERG-2008 equation of state have verified the expected uncertainties given in Table 1 and within Region 1 and parts of Regions 2, 3, and 4 of Figure 1. The boundaries in Table 1 can often be exceeded at lower temperatures or higher pressures than those given. The last paragraph of Section 1.3.1 explains the procedure that can be used to determine if a particular gas or operating condition still resides within the 0.1 % uncertainty limit.

### 1.4.2 GROSS Equation of State Uncertainty

In general, the expected uncertainty in density of the GROSS equation of state is 0.1 % for natural gas having compositions and operating conditions identified in Table 2. The GRI and GERG compressibility factor reference databases and comparisons with the GERG-2008 equation of state have verified the expected uncertainties given in Table 2. ***The equation was not designed for and should not be used outside of these limits, unless comparisons as described in the last paragraph of Section 1.3.1 have been made.***

## 1.5 Recommendations

Two different equations for the compressibility factor, the DETAIL equation of state and the GROSS equation of state, are provided in Part 1. The choice of a particular equation of state depends on the natural gas composition and operating conditions, and the uncertainty expectation. See Part 2 for liquid phase and vapor-liquid equilibrium phases, or for applications outside the uncertainty ranges given in Figure 1 and Tables 1 and 2.

The GERG-2008 equation of state given in Part 2 is the most accurate in the calculation of compressibility factors and densities, but also has the most complex form. The DETAIL equation of state is more accurate than the GROSS equation. The GROSS equation of state is only recommended when simplicity is needed for calculations of natural gas compressibility factors and densities, provided the natural gas compositions and operating conditions are within the ranges given in Table 2.

Use of the GERG-2008 equation of state may be considered due to its higher accuracy and for maintaining consistency for operating conditions that may lie either within or outside the ranges in Table 1. Switching between the GERG-2008 and DETAIL equations based on the operating state will lead to discontinuities in calculated values at the point of overlap. For conditions that never exceed the ranges in Table 1, the DETAIL equation of state may be the most practical for certain applications based on the operator's needs.

## 2 DEFINITIONS AND GENERAL EQUATIONS

### 2.1 Definitions of Phase Regions

This AGA 8, Part 1, puts forth a new approach to define the gas phase, dense phase, and liquid phase of a mixture. Figure 2 shows the phase boundary of a natural gas mixture with about 83 % methane. The heaviest hydrocarbons are heptane with a mole percent composition of 0.027 %, octane with 0.017 %, and nonane with 0.0009 %, where these three components play the largest role in the upper temperature and pressure limits of the saturation boundaries.

Although a fluid transitions smoothly from vapor to liquid without discontinuities when the path is such that it does not cross the phase boundary, defined regions are useful to give a general indication of the fluid's state. Most definitions of the phase regions use pressure and temperature parameters for bounding the gas, liquid, and dense regions, resulting in different parsing techniques with varying degrees of complexity depending on a group's point of view. Most of these bounding techniques result in some inappropriately labeled areas, *e.g.*, more gas-like than dense-like or vice-versa, due to the extent to which a certain bounding box extends into a temperature or pressure space.

As shown in Figure 2, the three phase regions are now defined in terms of the critical density only. (The critical point is the state where the co-existing liquid and vapor phases have the same density and composition.) The gas phase is the region with densities less than 50 % of the critical density. Liquids are defined as states with densities greater than 125 % of the critical density. The dense phase of a fluid is any single-phase state between these two areas, *i.e.*, a state with a density greater than 50 % and less than 125 % of the critical density. Other points or curves are also shown in Figure 2, including the cricondentherm (maximum 2-phase temperature), the cricondenbar (maximum 2-phase pressure), the bubble point curve, the dew point curve, and the retrograde curve.

In the dense phase region near the critical point for any pure fluid or mixture, the properties change rapidly as the state approaches the critical point. For example, for a pure fluid the isobaric heat capacity increases to infinity and the speed of sound approaches zero. For temperatures near the critical point, the area between 50 % and 125 % of the critical density represents states where property changes become more significant.

There are various approaches that can be used to determine the critical density of a mixture, such as the tools available in Reference [6] that use the GERG-2008 equation of state (given in Part 2) to locate the critical point. The use of cubic equations of state (PR, SRK, *etc.*), though not as accurate as the GERG-2008, will determine a state point that is in the general vicinity of the true critical point of the mixture when volume translation is applied. The simplest but least accurate approach is to use a mole fraction average of the critical volumes of the pure fluids (the critical density would then be the reciprocal of the critical volume). The approach taken depends on the needs of a particular application.

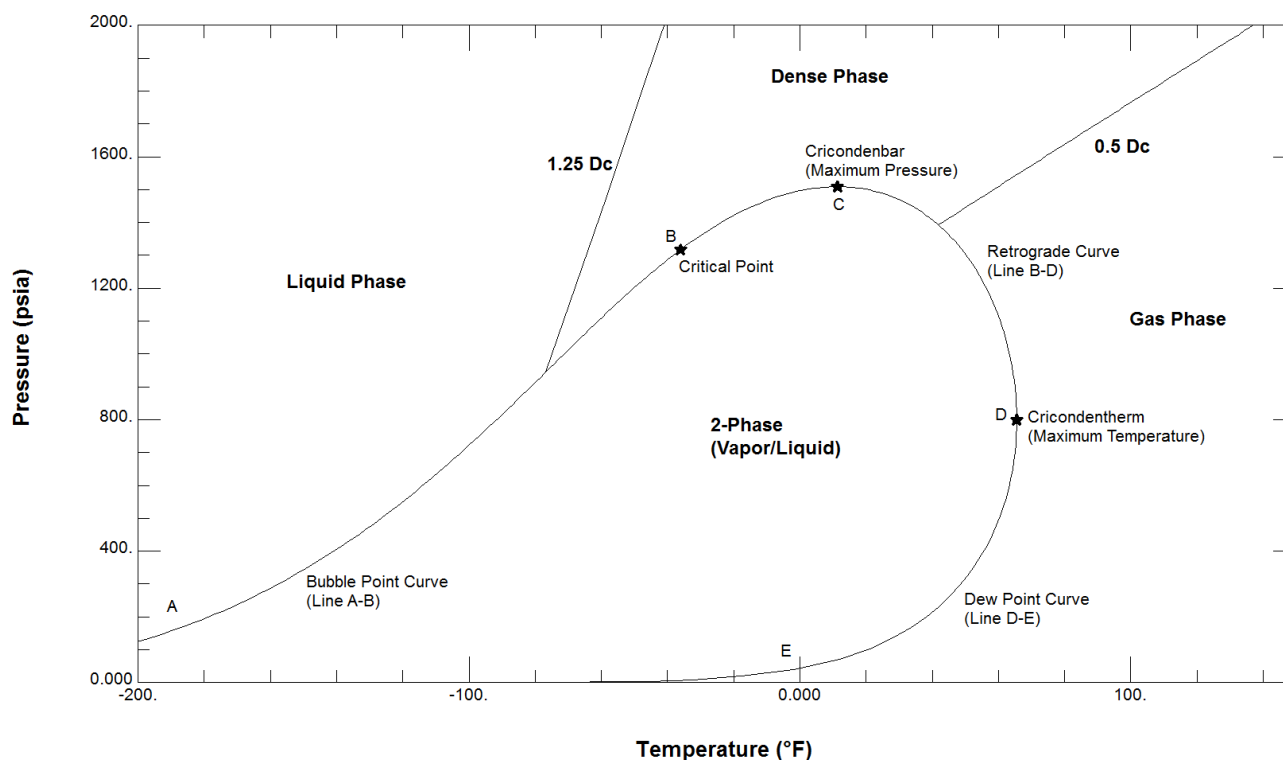


Figure 2. Example of gas, liquid, and dense phase regions of a natural gas mixture.

## 2.2 Nomenclature

The symbols used in this publication are generally specific to thermodynamics, although those specific to flow measurement have been used as a convenience to the reader. General symbols that do not refer to a specific equation of state are given below. Symbols that are specific in the equations of state are given in Sections 4 and 5.

|                 |                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------|
| $d$             | Molar density (mol/dm <sup>3</sup> )                                                        |
| $D_c$           | Critical density (mol/dm <sup>3</sup> )                                                     |
| $F_{pv}$        | Supercompressibility factor                                                                 |
| $M$             | Molar mass (molecular weight) (g/mol)                                                       |
| $M_i$           | Molar mass of the component $i$ in the mixture (g/mol)                                      |
| $n$             | Number of moles of a gas (mol)                                                              |
| $N$             | Number of components in the mixture                                                         |
| $P$             | Absolute pressure (MPa)                                                                     |
| $R$             | Gas constant [J/(mol·K)]                                                                    |
| $T$             | Absolute temperature (K)                                                                    |
| $V$             | Gas volume (dm <sup>3</sup> )                                                               |
| $x_i$           | Mole fraction of component $i$ in the mixture                                               |
| $Z(T, P)$       | Compressibility factor at $T$ and $P$                                                       |
| $Z_b(T_b, P_b)$ | Base compressibility factor at $T_b$ and $P_b$ (generally 60 °F and 14.73 psia in the U.S.) |
| $\rho$          | Mass density (mass per unit volume) (kg/m <sup>3</sup> )                                    |