Measurement of Thermally Cracked Gas

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Contents

Introduction

This document initiates improving thermally cracked gas (TCG) property calculation methods for measurement applications. It is a research report on TCG research work in progress. The methods presented here are for example illustration purposes only. They are not for use at this stage in the development work. Modifications will occur to the methods presented here and to other industry methods commonly used for TCG measurement once the research work is completed. The goal is to reduce TCG custody transfer uncertainty. TCG is not a naturally occurring natural gas mixture. It is produced as a by-product in the refining process of petroleum fluids.

The principal flow measurement method used to measure TCG is orifice measurement as applied in API *MPMS* Ch. 14.3/AGA Report No. 3/GPA 8185. These documents reference the use of API *MPMS* Ch. 14.2/AGA Report No. 8/GPA 8185 for compressibility factor calculations. The assumption in the current application of API *MPMS* Ch. 14.3/AGA Report No. 3/GPA 8185 is that the fluid sampling, measurement, and calculations conditions are in the single gas phase region and that the fluid components are consistent with API *MPMS* Ch. 14.2/AGA Report No. 8/GPA 8185. TCG mixtures contain significant quantities of olefins and hydrogen. These fluid mixtures are not natural gases and fall outside of natural gas measurement and operation practices.

No reference or inference is made in API *MPMS* Ch. 14.2/AGA Report No. 8/GPA 8185 to applying natural gas components as chemical analogs for olefinic compounds, or that high concentrations of hydrogen can be permitted in such mixtures. Nor do current industry measurement documents make statements regarding the uncertainty of such practices.

Current orifice measurement standards do not address the metering, operations, or physical properties of TCGs. Industry practice has been to substitute natural gas component analogs as a means to estimate TCG property values for custody transfer. This practice increases measurement uncertainties.

In order to address the issues associated with TCGs, API initiated a four-phase project on TCG measurement. Phase I evaluated current TCG measurement practices. The results suggested that component substitution methods produced mass density uncertainties of 0.3 % to 5 % for TCG mixtures. The uncertainty depends on operating conditions. Phase I identified experimental data gaps and the need for experimental reference data over custody transfer and common pipeline operating conditions. In order to initiate filling experimental data gaps for TCG mixture mixtures, a single gas mixture was prepared and measured during Phase II. The Gas Technology Institute (GTI) provided the experimental setup and measured data to support Phase II work. The experimental work measured gas phase measurements of density, sound speed, and capacitance for a synthetic TCG mixture over a narrow operating range. Measured data were compared to predicted values from API *MPMS* Ch. 14.2/AGA Report No. 8/GPA 8185, NIST14-DDMIX, GERG 2004/GERG 2008, and the Soave-Redlich-Kwong equations of state. Subsequent analysis was also made using ISO 20765-2 for extended range applications. This report completes the Phase III work. The final phase, Phase IV, will obtain data over a broad range of TCG operating conditions. Measured reference data for many key TCG mixtures are not available. The mixture data from the Phase IV lab work may be used to evaluate TCG mixture data and determine the applicability of various measurement equations to TCG mixtures.

Measurement of Thermally Cracked Gas

1 Scope

This technical report presents a method to compute the density, compressibility factor, and supercompressibility factor for thermally cracked gas (TCG) for custody transfer using orifice meters. It provides equations, parameters, computation flow diagrams, and example spreadsheet calculations.

This technical report applies to TCG mixtures after treatment. See Table 2 for more information on the types of gases covered. It applies for temperature from 90 °F to 120 °F (305 K to 322 K) at pressures up to 300 psig (2 MPa). It is limited to a specific operating region. The method is for the single gas phase only.

2 Normative References

The following referenced documents are indispensable for the application of this document or provide additional information pertinent to mass measurement of natural gas liquids. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

API *Manual of Petroleum Measurement Standards (MPMS)*, Chapter 14.2, *Compressibility Factors of Natural Gas and Other Related Hydrocarbon Gases* (AGA Report No. 8 [1]) (GPA 8185 [2])

3 Terms, Definitions, Abbreviations, and Symbols

3.1 Terms and Definitions

The quantities used in the equations in this document are defined when they are used.

3.2 Abbreviations and Symbols

For the purposes of this document, the following abbreviations and symbols apply.

B	second virial coefficient
B_{mix}	mixture second virial coefficient
b_{n}	constant in Table 4
C	third virial coefficient
C_{mix}	mixture third virial coefficient
c_{n}	constant in Table 4
d	mass density (mass per unit volume)
$\rho(T_\rho, P_\rho)$	molar density at reference condition T_ρ, P_ρ
F_{pv}	supercompressibility factor
M_{r}	molar mass (molecular weight)
M_{r} (air)	molar mass of air
M_{r_i}	molar mass of ith component
N	number of components in gas mixture
n	number of moles of gas

[1] American Gas Association, 400 N. Capitol Street, NW, Suite 450, Washington, DC 20001, www.aga.org.
[2] Gas Processors Association, 6526 E. 60th Street, Tulsa, Oklahoma 74145, www.gasprocessors.com.

P	absolute pressure
P_b	absolute pressure at base conditions
P_d	reference pressure for density
P_{gr}	reference pressure for relative density
R	gas constant
T	absolute temperature of gas
T_b	absolute temperature at base conditions
T_d	reference temperature for density
T_{gr}	reference temperature for relative density (specific gravity)
V	gas volume
x_i	mole fraction of component the ith in gas mixture
x_j	mole fraction of component j in the gas mixture
x_k	mole fraction of component j in the gas mixture
ρ	molar density (mass per unit volume)
$\rho(T_{gr}, P_{gr})$	molar density of gas mixture at T_{gr}, P_{gr}
$\rho(\text{air}, T_{gr}, P_{gr})$	molar density of air at T_{gr}, P_{gr}
ρ_b	mass density at contract reference base condition T_b, P_b
Z	compressibility factor
Z_b	compressibility factor at contract reference condition T_b, P_b

3.3 Units and Conversions

The units used in the basic formulation of the equations and in the associated computer subroutines are SI units.

The subroutines use the following units for the absolute temperature in kelvins (K), pressure in megapascals (MPa), and molar density in moles per cubic decimeter (mol/dm^3). The value of the gas constant is 0.008314472 KJ/mol-K.

Conversion factors are required for conversions to and from other units. Consistent conversion factors for use with the TCG method are given in Table 1. When possible, the conversion factors given in Table 1 correspond to international standards (GPA 2172-2009 and ISO 6976). Any differences in values used in this program and later values are within the experimental uncertainty in the validation data. Hence any unit conversion changes are unlikely to affect the uncertainty of the calculations. It is recommended that any subsequent changes be ignored unless the agency promoting the change provides a detailed cost impact of the change on industry.

4 Types of Gases Covered

This research document applies to TCG mixtures that may occur in refinery operations. Table 2 provides a simplified list of illustrative TCG mixture example components. A number of components have been excluded either because they were not present in the data or because of low concentration amounts. This shall not be construed to mean those components are not important for TCG calculations. It simply means those components were not available to the research stage data sets.

It is recommended that users obtain additional data to validate performance for their fluid mixtures for their operating conditions.

Table 1—Units Conversions

Quantity	Units Conversion
Length	1.0 in. = 0.0254 m
Length	12.0 in. = 1.0 ft
Mass	1.0 lbm = 0.4535924 kg
Moles	1.0 lb-mole = 0.4535924 kg-mole
Temperature	Temperature (in °R) = Temperature (in °F) + 459.67
Temperature	Temperature (in K) = Temperature (in °C) + 273.15
Temperature	1.8 °R = 1.0 K
Pressure	1.0 psia = 0.006894757 MPa
Pressure	1.0 bar = 0.10 MPa
Acceleration of Gravity	32.17405 ft/s^2 = 9.806650 m/s^2
Gas Constant	10.73164 psia ft^3/lbmol-R = 8.314510 J/mol-K
Gas Constant	1.985886 Btu/lbmol-R = 8.314472 J/mol-K

Table 2—Thermally Cracked Gas Characteristics

Component	CAS	Mole Percent
Ethylene	74-85-1	<14 %
Propylene	115-07-1	<4 %
Hydrogen	1333-74-0	<25 %
Methane	74-82-8	>35 %
Ethane	74-84-0	<14 %
Propane	74-98-6	<1 %
Butanes	106-97-8	<0.5 %
Olefins	NA	<0.5 %
Nitrogen	7727-37-9	<8 %
Carbon Dioxide	124-38-9	TBD
Carbon Monoxide	630-08-0	TBD
Water	7732-18-5	TBD
Hydrogen Sulfide	7783-06-4	TBD

5 Operating Conditions

Most TCG measurement operating conditions occur within a range from approximately 60 °F to 140 °F and pressures less than 1000 psia. The principal custody transfer measurement region occurs in the lower pressure and higher temperature range of this region [90 °F to 120 °F (305 K to 322 K) and less than 300 psia (2 MPa)]. This custody transfer region is well suited for the methods presented in this report. The broader operating region is beyond the scope of this work. It is expected that the broader region will be addressed by methods that are under development (e.g. GERG 2008).

This document applies only for the gas phase in a restricted range. Specifically, it is for low pressure TCG custody transfer conditions only. It can be applied for temperatures from 90 °F to 120 °F at pressures up to 300 psia.

Application and operation conditions should be verified by obtaining experimental data for other conditions. The calculation method should not be used outside of the specified boundaries without supporting experimental data, nor should it be used in the vicinity of the critical point. It cannot be used for two-phase calculations. It is recommended that methods be considered with broader applicability (e.g. API *MPMS* Ch. 14.2 or GERG 2008 methods) be applied to extended operating conditions until API completes its TCG mixture data work.

NOTE API *MPMS* Ch. 14.2 and GERG 2008 methods were not explicitly developed for TCG mixtures. These methods have unknown uncertainties for TCG mixtures at the time this technical report was produced.

In Section 1.3.2 of API *MPMS* Ch. 14.2/AGA Report No. 8/GPA 8185, no reference is made to the application of the equations to TCG mixtures. This section indicates that the performance for calculations for gas mixtures that do not fall in the normal range of gas mixtures should be verified by other means (i.e. measured data representing commercial TCG mixtures).

Figure 1 provides an overview of the custody transfer measurement and operating pressure and temperature region for TCGs.

6 TCG Calculation Method Overview

6.1 Overview of Requirements

The user of this report has to be aware of the custody transfer operating conditions and the applicability of the method over those conditions.

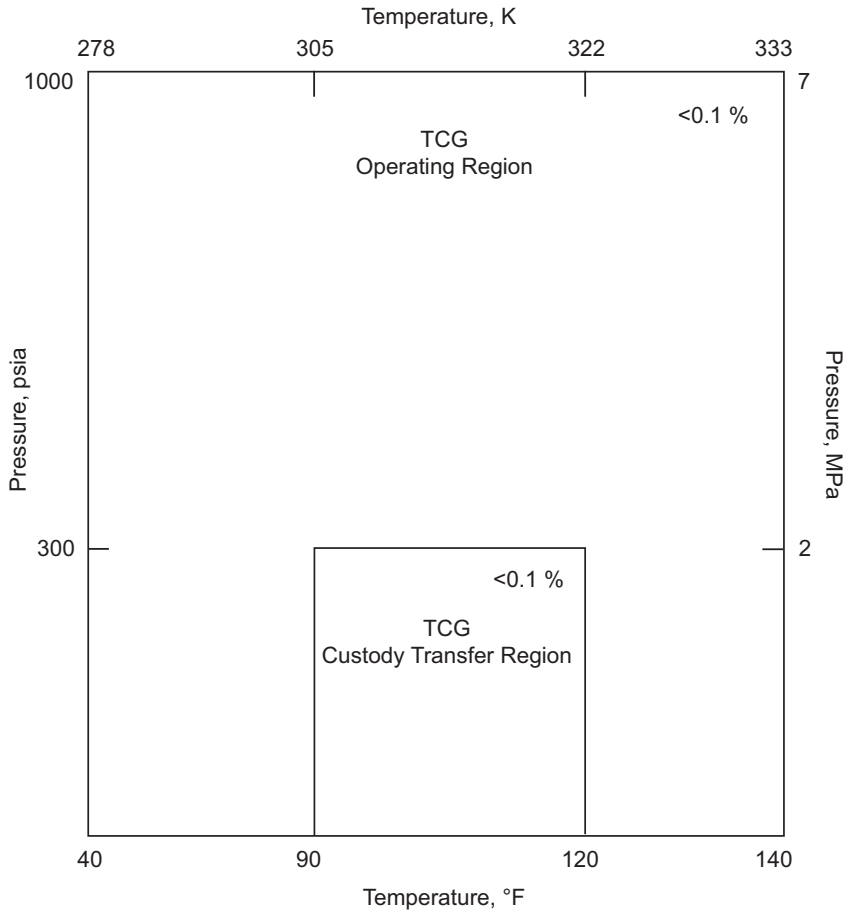

Figure 1—Targeted Uncertainty for Thermally Cracked Gas Mixture

The user is required to provide the operating temperature, pressure, and a detailed gas analysis as input for the method (i.e. the mole fractions or mole percentages of the components in the TCG mixture).

At present, an insufficient database is available for validating component substitutions for many olefinic compounds. Preliminary analysis for large mole fraction components suggests that uncertainties increase when component substitution is utilized. The effect of low mole fraction concentrations of heavy olefinic compounds and sour compounds has not been experimentally determined.

6.2 TCG Reference Mixture Data

The recommended methodology for evaluating mixture data uncertainty can be found in API *MPMS* Ch. 14.2/AGA Report No. 8/GPA 8185.

6.3 TCG Method Uncertainty

In general, the target uncertainty in the gas phase for any TCG method is the same as other industry measurement documents such as found in API *MPMS* Ch. 14.2. The target uncertainty for TCG custody transfer is illustrated in Figure 1 for gases having the normal range of gas characteristics identified in Table 3.

7 General Equations

The compressibility factor Z is defined by the equation:

$$Z = \frac{P}{\rho R T} \tag{1}$$

where

$$\rho = \frac{n}{V}.$$

The molar mass M_r of a mixture is calculated from the composition using:

$$M_\mathrm{r} = \sum_{i=1}^{N} x_\mathrm{i} M_{\mathrm{r_i}} \tag{2}$$

where the summation is over all components in the gas mixture.

The mass density d is related to the molar density ρ by the relation:

$$d = M_\mathrm{r}\rho$$

8 Reference Conditions

8.1 Mass Density at Contract Condition

The mass density d_b at the contract reference condition (i.e. base condition) T_b, P_b can be calculated using the following relation:

$$d_\mathrm{b} = \frac{M_\mathrm{r} P_\mathrm{b}}{Z_\mathrm{b} R T_\mathrm{b}} \tag{3}$$

8.2 F_{pv} Reference Condition

The supercompressibility factor F_{pv} is defined by the following relation:

$$F_{pv}^2 = \frac{Z(T_b, P_b)}{Z(T, P)} \tag{4}$$

where

$Z(T_b, P_b)$ is the compressibility factor at T = 60 °F, P = 14.73 psia;

$Z(T, P)$ is the compressibility factor at T, P.

The condition T = 60 °F, P = 14.73 psia is a reference condition.

The contract reference condition equals the reference condition for supercompressibility factor only when the contract reference condition is T = 60 °F, P = 14.73 psia.

8.3 Relative Density Reference Condition

The relative density (specific gravity) at the reference condition T_{gr}, P_g is defined by the relation:

$$G_r(T_{gr}, P_{gr}) = \frac{d(T_{gr}, P_{gr})}{d(\text{air}, T_{gr}, P_{gr})} \tag{5}$$

where

$G_r(T_{gr}, P_{gr})$ is the relative density of gas mixture at T_{gr}, P_{gr};

$d(T_{gr}, P_{gr})$ is the mass density of gas mixture at T_{gr}, P_{gr};

d(air, T_{gr}, P_{gr}) is the mass density of air at T_{gr}, P_{gr}.

9 TCG Method for Compressibility Factors

9.1 General

TCG calculations methods are in development. A virial equation is applied here for example purposes to simply illustrate a TCG mixture computation sequence. The method uses published and approximated virial coefficient values which are based on limited data sets. Other methods such as API *MPMS* 14.2 may use different computation sequences.

Virial coefficient values may be obtained from any number of published literature references. Those sources may derive the virial values from measurement data, theoretical estimates, correlations, substitution methods or approximations. A number of TCG mixture virial values do not exist due to the lack of experimental data. Consequently, the list included in this document is not a complete compilation of TCG mixture virial coefficients, rather it is approximate. Again, the purpose of the method in this document is to provide an example for illustration purposes only. TCG mixture measurement users must verify the applicability of any TCG mixture data and TCG methods to their TCG measurement applications.

In the TCG method, a virial equation method is applied to compute the density and compressibility factor. A TCG mixture is characterized by its composition. The pure and interaction virial coefficients (first and second order density

terms in the equation) of the components that make up the mixture are computed at the operating temperature. The calculated virial equation terms are adjusted by applying virial equation mixing rules. The adjusted values are summed to provide the mixture virial coefficients. A simple density search algorithm is applied to compute the density and compressibility factor. The density search converges on the operating pressure condition to obtain the density and compressibility factor for the mixture.

Care always has to be used when implementing such methods to validate that they apply in the user's range of application. A spreadsheet example is used to illustrate the computational sequence to compute the compressibility factor application of the method.

9.2 TCG Virial Method

$$Z_{TCG\_mix} = 1 + B_{mix}\rho + C_{mix}\rho^2 \quad (6)$$

TCG Second Virial Coefficient

$$B_{mix} = \sum_{i=1}^{n}\sum_{j=1}^{n} x_i x_j B_{ij} \quad (7)$$

where

B_{mix}	is the mixture second virial coefficient—summation;
B_{ij}	is $b_0 + b_1 T + b_2 T^2 + b_3 T^3$ and is the second virial coefficient for ith and jth pairs in the mixture;
x_i, x_j	is the ith, jth component mole fraction in mixture from gas analysis;
$\sum_{i=1}^{n}\sum_{j=1}^{n}$	is the simplified double summation over all i and j components in the mixture;
b_0, b_1, b_2, b_3	are the regression parameters for B_{ij} contributions—coefficients from Table 3.

Third Virial Coefficient

$$C_{mix} = \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} x_i x_j x_k C_{ijk} \quad (8)$$

where

C_{mix}	is the mixture third virial coefficient—summation;
C_{ijk}	is $c_0 + c_1 T + c_2 T^2 + c_3 T^3$ and is the second virial coefficient for ith and jth components in the mixture;
x_i, x_j, x_k	is the ith, jth, kth component mole fraction in TCG mixture from gas analysis;
$\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}$	is the simplified triple summation over i, j, k components in the mixture.
c_0, c_1, c_2, c_3	are the regression parameters for C_{ijk} contributions—coefficients from Table 4.

Table 3—Illustrative Example Terms for Equation (7)

For example illustration purposes only (partial list, not final coefficients).

B_id	BNid	Bid1	Bid2	b0	b1	b2
1	CH4-CH4	1	1	-3.04437E-01	1.36882E-03	-1.64768E-06
2	H2-H2	2	2	-5.44541E-04	7.89787E-05	-9.78422E-08
3	N2-N2	3	3	-1.31267E-01	6.51876E-04	-7.64212E-07
4	C2H6-C2H6	4	4	-1.11736E+00	4.93379E-03	-6.06390E-06
5	C2H4-C2H4	5	5	-8.34330E-01	3.65658E-03	-4.45419E-06
6	C3H8-C3H8	6	6	-2.48630E+00	1.12580E-02	-1.41434E-05
7	C3H6-C3H6	7	7	-2.20964E+00	9.99105E-03	-1.25670E-05
8	C4H10-C4H10	8	8	-5.15139E+00	2.41808E-02	-3.11105E-05
9	C5H12-C5H12	9	9	-9.44731E+00	4.53861E-02	-5.92058E-05
10	CH4-H2	1	2	-4.43405E-02	2.53684E-04	-2.76323E-07
11	CH4-N2	1	3	-1.87076E-01	8.72315E-04	-1.02392E-06
12	CH4-C2H6	1	4	-5.38347E-01	2.33717E-03	-2.79124E-06
13	CH4-C2H4	1	5	-4.69469E-01	2.04759E-03	-2.43818E-06
14	CH4-C3H8	1	6	-7.72934E-01	3.37406E-03	-4.05980E-06
15	CH4-C3H6	1	7	-6.59909E-01	2.79427E-03	-3.29052E-06
16	CH4-C4H10	1	8	-9.75547E-01	4.20042E-03	-4.98713E-06
17	CH4-C5H12	1	9	-1.02562E+00	4.24896E-03	-4.93994E-06
18	H2-N2	2	3	-2.52081E-02	1.92804E-04	-2.20136E-07
19	H2-C2H6	2	4	-7.48503E-02	3.56892E-04	-3.54485E-07
20	H2-C2H4	2	5	-7.48503E-02	3.56892E-04	-3.54485E-07
21	H2-C3H8	2	6	-1.20074E-01	5.15882E-04	-4.88974E-07
22	H2-C3H6	2	7	-1.20074E-01	5.15882E-04	-4.88974E-07
23	H2-C4H10	2	8	-1.42864E-01	6.35388E-04	-6.00598E-07
24	H2-C5H12	2	9	2.22916E-02	-1.12421E-04	3.71465E-07
25	N2-C2H6	3	4	-3.40604E-01	1.52278E-03	-1.79179E-06
26	N2-C2H6	3	5	-3.03312E-01	1.38068E-03	-1.62593E-06
27	N2-C3H8	3	6	-4.35053E-01	1.87391E-03	-2.13741E-06
28	N2-C3H6	3	7	-4.09086E-01	1.75100E-03	-2.00221E-06
29	N2-C4H10	3	8	-5.15485E-01	2.16573E-03	-2.42666E-06
30	N2-C5H12	3	9	-5.18406E-01	2.07624E-03	-2.23471E-06
31	C2H6-C2H4	4	5	-9.22106E-01	3.98481E-03	-4.78457E-06
32	C2H6-C3H8	4	6	-1.60514E+00	7.01753E-03	-8.55800E-06
33	C2H6-C3H6	4	7	-1.43513E+00	6.25422E-03	-7.61594E-06
34	C2H6-C4H10	4	8	-2.08318E+00	9.13479E-03	-1.11740E-05
35	C2H6-C5H12	4	9	-2.41352E+00	1.05621E-02	-1.29402E-05

Table 3—Illustrative Example Terms for Equation (7) (Continued)

For example illustration purposes only (partial list, not final coefficients).

B_id	BNid	Bid1	Bid2	b0	b1	b2
36	C2H4-C3H6	5	7	-1.23567E+00	5.41417E-03	-6.64563E-06
37	C2H4-C3H8	5	6	-1.28524E+00	5.64771E-03	-6.94444E-06
38	C3H8-C3H6	6	7	-2.31404E+00	1.04640E-02	-1.31475E-05
39	C3H8-C4H10	6	8	-3.47067E+00	1.59331E-02	-2.02137E-05
40	C3H8-C5H12	6	9	-4.12925E+00	1.90359E-02	-2.42352E-05
41	C3H6-C4H10	7	8	-3.45876E+00	1.62007E-02	-2.09603E-05
42	C4H10-C5H12	8	9	-6.86785E+00	3.25483E-02	-4.21281E-05

Table 4—Illustrative Example Terms for Equation (8)

For example illustration purposes only (partial list, not final coefficients).

C_id	CNid	Cid1	Cid2	Cid3	c0	c1	c2
1	CH4	1	1	1	1.06932E-02	-4.50800E-05	5.79578E-08
2	H2	2	2	2	5.77484E-04	-9.01467E-07	8.69670E-10
3	N2	3	3	3	3.71896E-03	-1.32639E-05	1.77041E-08
4	C2H6	4	4	4	3.07383E-02	-8.33658E-05	5.70631E-08
5	C2H4	5	5	5	7.09314E-03	3.02671E-05	-9.73383E-08
6	C3H8	6	6	6	2.13383E-02	-1.28455E-05	-3.95338E-09
7	C3H6	7	7	7	-2.55230E-01	1.65935E-03	-2.51191E-06
8	CH4-CH4-H2	1	1	2	2.33159E-04	1.02923E-05	-2.27208E-08
9	CH4-CH4-N2	1	1	3	8.89649E-03	-4.10784E-05	6.03723E-08
10	CH4-CH4-C2H6	1	1	4	1.60923E-02	-6.38586E-05	7.79273E-08
11	CH4-CH4-C2H4	1	1	5	1.60923E-02	-6.38586E-05	7.79273E-08
12	CH4-CH4-C3H8	1	1	6	8.92850E-03	1.90637E-05	-9.79363E-08
13	CH4-CH4-C3H6	1	1	7	8.92850E-03	1.90637E-05	-9.79363E-08
14	CH4-CH4-C4H10	1	1	8	2.27707E-01	-1.39926E-03	2.21564E-06
15	CH4-CH4-C5H12	1	1	9	3.20344E-02	-6.91674E-05	0.00000E+00
16	H2-H2-CH4	2	2	1	-3.08914E-03	2.54973E-05	-4.39625E-08
17	H2-H2-N2	2	2	3	-8.77711E-03	6.39925E-05	-1.07591E-07
18	H2-H2-C2H6	2	2	4	2.94870E-02	-1.97083E-04	3.34778E-07
19	H2-H2-C2H4	2	2	5	2.94870E-02	-1.97083E-04	3.34778E-07
20	H2-H2-C3H8	2	2	6	2.94870E-02	-1.97083E-04	3.34778E-07
21	H2-H2-C3H6	2	2	7	2.94870E-02	-1.97083E-04	3.34778E-07
22	N2-N2-CH4	3	3	1	8.74115E-03	-4.43880E-05	6.96584E-08
23	N2-N2-H2	3	3	2	-6.50954E-03	5.19104E-05	-8.87528E-08
24	N2-N2-C2H6	3	3	4	-1.36584E-02	1.06972E-04	-1.79369E-07
25	N2-N2-C2H4	3	3	5	-1.36584E-02	1.06972E-04	-1.79369E-07

Table 4—Illustrative Example Terms for Equation (8) (Continued)

For example illustration purposes only (partial list, not final coefficients).

C_id	CNid	Cid1	Cid2	Cid3	c0	c1	c2
26	N2-N2-C3H8	3	3	6	6.74630E-03	-3.65557E-06	-2.34530E-08
27	N2-N2-C3H6	3	3	7	6.74630E-03	-3.65557E-06	-2.34530E-08
28	N2-N2-C4H10	3	3	8	-1.01202E-01	7.23716E-04	-1.21618E-06
29	C2H6-C2H6-CH4	4	4	1	-8.27905E-03	1.21913E-04	-2.39958E-07
29	C2H4-C2H4-CH4	5	5	1	-8.27905E-03	1.21913E-04	-2.39958E-07
30	C2H6-C2H6-H2	4	4	2	8.43800E-03	-2.65166E-05	3.81345E-08
31	C2H4-C2H4-H2	5	5	2	8.43800E-03	-2.65166E-05	3.81345E-08
32	C2H6-C2H6-N2	4	4	3	-3.69750E-02	2.89620E-04	-4.94852E-07
33	C2H4-C2H4-N2	4	4	3	-3.69750E-02	2.89620E-04	-4.94852E-07
34	C2H6-C2H6-C2H4	4	4	4	-1.44234E-01	1.01275E-03	-1.63277E-06
35	C2H6-C2H6-C3H8	4	4	6	-1.44234E-01	1.01275E-03	-1.63277E-06
36	C2H6-C2H6-C3H6	4	4	6	-1.44234E-01	1.01275E-03	-1.63277E-06
37	C2H6-C2H4-C2H4	4	5	5	7.09314E-03	3.02671E-05	-9.73383E-08
38	C3H8-C3H8-CH4	6	6	1	-8.48395E-02	6.05618E-04	-9.54102E-07
39	C3H8-C3H8-N2	6	6	2	-8.59670E-02	5.79776E-04	-8.77215E-07
40	C3H8-C3H8-C2H6	6	6	4	-2.16734E-01	1.43604E-03	-2.21182E-06
41	C3H8-C3H8-C2H4	6	6	5	-2.16734E-01	1.43604E-03	-2.21182E-06
42	CH4-N2-H2	1	3	2	3.60589E-03	-1.45437E-05	2.04722E-08
43	CH4-N2-C2H6	1	3	4	4.49508E-03	5.30233E-07	-1.52576E-08
44	CH4-N2-C2H4	1	3	5	4.49508E-03	5.30233E-07	-1.52576E-08
45	CH4-N2-C3H8	1	3	6	-1.87767E-02	1.42145E-04	-2.21855E-07
46	CH4-N2-C3H6	1	3	7	4.49508E-03	5.30233E-07	-1.52576E-08
47	CH4-C2H6-H2	1	4	2	-1.16095E-03	2.63812E-05	-5.12600E-08
48	CH4-C2H6-C2H4	1	4	5	-1.89480E-01	1.39040E-03	-2.38860E-06
49	CH4-C2H6-C3H8	1	4	6	-1.89480E-01	1.39040E-03	-2.38860E-06
50	CH4-C2H6-C3H6	1	4	7	-1.89480E-01	1.39040E-03	-2.38860E-06
51	CH4-C2H6-C4H10	1	4	8	-1.89480E-01	1.39040E-03	-2.38860E-06
52	CH4-C2H6-C5H12	1	4	9	-1.89480E-01	1.39040E-03	-2.38860E-06
53	CH4-C2H4-H2	1	5	2	-1.16095E-03	2.63812E-05	-5.12600E-08
54	CH4-C2H4-C3H8	1	5	6	-1.89480E-01	1.39040E-03	-2.38860E-06
55	CH4-C2H4-C3H6	1	5	7	-1.89480E-01	1.39040E-03	-2.38860E-06
56	N2-C2H6-H2	3	4	2	-2.97743E-04	1.68641E-05	-3.30680E-08
57	N2-C2H4-H2	3	5	2	-2.97743E-04	1.68641E-05	-3.30680E-08
58	N2-C2H6-C2H4	3	4	5	-5.06529E-02	3.63400E-04	-5.77241E-07
59	N2-C2H6-C3H8	3	4	6	-5.06529E-02	3.63400E-04	-5.77241E-07
60	N2-C2H6-C3H6	3	4	7	-5.06529E-02	3.63400E-04	-5.77241E-07
61	C2H6-C2H4-H2	4	5	2	8.43800E-03	-2.65166E-05	3.81345E-08

Annex A
(informative)

Example Computation Flow Diagram

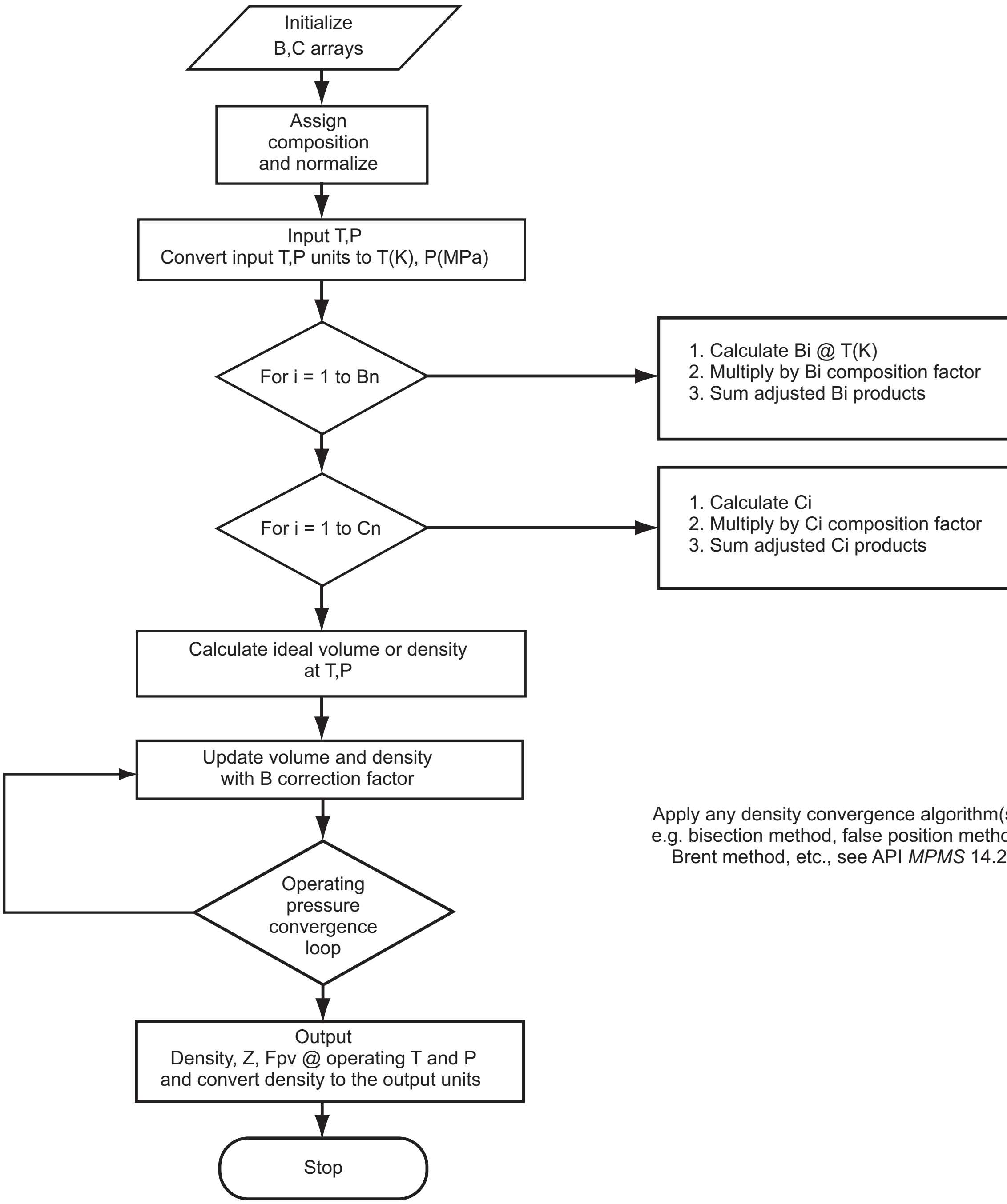

Figure A.1—Example Flow Diagram for Computing *Z* Using the Virial Method

Example Excel Macro Code

The following code is intended as a partial example for illustration purposes only.

```
Assign B and C virial equation coefficient parameter values to an array.
B and C methods follow Ref.3
Example of convergence methods to solve Eq.6 may be found in Ref. 1 and Ref. 3
Calculate B values and sum
        BSum = 0.
        For i = 1 TonBTerms
                If (XIB(BCID1(i, 1)) = 0 Or XIB(BCID2(i, 1)) = 0) Then GoTo Label2
                XIXJ = XIB(BCID1(i, 1)) * XIB(BCID2(i, 1))
                If (BCID1(i, 1) <> BCID2(i, 1)) Then
                XIXJ = 2 * XIXJ
                End If
                BT = BC2(i, 1) + BC2(i, 2) * TK + BC2(i, 3) * TK ^ 2  ‘ (example terms from Table 3)
                BT = XIXJ * BT
                BSUM = BSUM + BT
Label2: Next i
'Calculate C values and sum
        CSum = 0
        For i = 1 TonCTerms
                If (XIB(CCID1(i, 1)) = 0 Or XIB(CCID2(i, 1)) = 0 Or XIB(CCID3(i, 1)) = 0) Then GoToLabel3
                CT = CC3(i, 1) + CC3(I,2) * TK + CC3(i, 3) * TK ^ 2‘ (example terms from Table 4)
                If CCID1(i, 1) = CCID3(i, 1) Then GoTo Label4
                CT = 3# * CT
                If CCID2(i, 1) = CCID1(i, 2) Or CCID2(i, 1) = CCID3(i, 1) Then GoTo Label4
                CT = 2# * CT
Label4:   CT = CT * XIB(CCID1(i, 1)) * XIB(CCID2(i, 1)) * XIB(CCID3(i, 1 )
                CSum = CSum + CT
Label3:Next i
```

Table A.1—Example TCG Components and Mole Percents

ID	Component	Mole Percents
1	CH4	40
2	H2	25
3	N2	10
4	C2H6	10
5	C2H4	10

Table A.2—Example TCG *T* and *P* Conditions

Temperature, *T* K	Pressure, *P* MPa		
293.15	1	2	3

Table A.3—Illustrative Example Calculation—B Terms (@ 293.15 K)

For example illustration purposes only (partial list, not final coefficients).

Index	BName	Bid1	Bid2	x1	x2	b0	b1	b2	B_BName	Factor*x1x2*B	B Summation
1	CH4-CH4	1	1	0.45	0.45	-3.04437E-01	1.36882E-03	-1.64768E-06	-4.4763E-02	-9.0644E-03	-9.0644E-03
2	H2-H2	2	2	0.25	0.25	-5.44541E-04	7.89787E-05	-9.78422E-08	1.4200E-02	8.8749E-04	-8.1769E-03
3	N2-N2	3	3	0.1	0.1	-1.31267E-01	6.51876E-04	-7.64212E-07	-5.8431E-03	-5.8431E-05	-8.2354E-03
4	C2H6-C2H6	4	4	0.1	0.1	-1.11736E+00	4.93379E-03	-6.06390E-06	-1.9213E-01	-1.9213E-03	-1.0157E-02
5	C2H4-C2H4	5	5	0.1	0.1	-8.34330E-01	3.65658E-03	-4.45419E-06	-1.4518E-01	-1.4518E-03	-1.1609E-02
10	CH4-H2	1	2	0.45	0.25	-4.43405E-02	2.53684E-04	-2.76323E-07	6.2806E-03	1.4131E-03	-1.0195E-02
11	CH4-N2	1	3	0.45	0.1	-1.87076E-01	8.72315E-04	-1.02392E-06	-1.9350E-02	-1.7415E-03	-1.1937E-02
12	CH4-C2H6	1	4	0.45	0.1	-5.38347E-01	2.33717E-03	-2.79124E-06	-9.3078E-02	-8.3770E-03	-2.0314E-02
13	CH4-C2H4	1	5	0.45	0.1	-4.69469E-01	2.04759E-03	-2.43818E-06	-7.8748E-02	-7.0873E-03	-2.7401E-02
18	H2-N2	2	3	0.25	0.1	-2.52081E-02	1.92804E-04	-2.20136E-07	1.2395E-02	6.1973E-04	-2.6781E-02
19	H2-C2H6	2	4	0.25	0.1	-7.48503E-02	3.56892E-04	-3.54485E-07	-6.9087E-04	-3.4543E-05	-2.6816E-02
20	H2-C2H4	2	5	0.25	0.1	-7.48503E-02	3.56892E-04	-3.54485E-07	-6.9087E-04	-3.4543E-05	-2.6851E-02
25	N2-C2H6	3	4	0.1	0.1	-3.40604E-01	1.52278E-03	-1.79179E-06	-4.8182E-02	-9.6365E-04	-2.7814E-02
26	N2-C2H4	3	5	0.1	0.1	-3.03312E-01	1.38068E-03	-1.62593E-06	-3.8292E-02	-7.6585E-04	-2.8580E-02
31	C2H6-C2H4	4	5	0.1	0.1	-9.22106E-01	3.98481E-03	-4.78457E-06	-1.6513E-01	-3.3026E-03	-3.1883E-02

Table A.4—Illustrative example calculation - C terms (@ 293.15 K)

For example illustration purposes only (partial list, not final coefficients).

Index	CName	Cid1	Cid2	Cid3	X1	X2	X3	c0	c1	c2	C_CName	Factor*x1x2x3*C	C_Summation
1	CH4	1	1	1	0.45	0.45	0.45	1.06932E-02	-4.50800E-05	5.79578E-08	2.45868E-03	2.24048E-04	2.24048E-04
2	H2	2	2	2	0.25	0.25	0.25	5.77484E-04	-9.01467E-07	8.69670E-10	3.87956E-04	6.06181E-06	2.30109E-04
3	N2	3	3	3	0.1	0.1	0.1	3.71896E-03	-1.32639E-05	1.77041E-08	1.35208E-03	1.35208E-06	2.31461E-04
4	C2H6	4	4	4	0.1	0.1	0.1	3.07383E-02	-8.33658E-05	5.70631E-08	1.12035E-02	1.12035E-05	2.42665E-04
5	C2H4	5	5	5	0.1	0.1	0.1	7.09314E-03	3.02671E-05	-9.73383E-08	7.60098E-03	7.60098E-06	2.50266E-04
8	CH4-CH4-H2	1	1	2	0.45	0.45	0.25	2.33159E-04	1.02923E-05	-2.27208E-08	1.29779E-03	1.97102E-04	4.47368E-04
9	CH4-CH4-N2	1	1	3	0.45	0.45	0.1	8.89649E-03	-4.10784E-05	6.03723E-08	2.04257E-03	1.24086E-04	5.71454E-04
10	CH4-CH4-C2H6	1	1	4	0.45	0.45	0.1	1.60923E-02	-6.38586E-05	7.79273E-08	4.06898E-03	2.47191E-04	8.18645E-04
11	CH4-CH4-C2H4	1	1	5	0.45	0.45	0.1	1.60923E-02	-6.38586E-05	7.79273E-08	4.06898E-03	2.47191E-04	1.06584E-03
16	H2-H2-CH4	2	2	1	0.25	0.25	0.45	-3.08914E-03	2.54973E-05	-4.39625E-08	6.07392E-04	5.12487E-05	1.11708E-03
17	H2-H2-N2	2	2	3	0.25	0.25	0.1	-8.77711E-03	6.39925E-05	-1.07591E-07	7.36252E-04	1.38047E-05	1.13089E-03
18	H2-H2-C2H6	2	2	4	0.25	0.25	0.1	2.94870E-02	-1.97083E-04	3.34778E-07	4.81910E-04	9.03580E-06	1.13992E-03
19	H2-H2-C2H4	2	2	5	0.25	0.25	0.1	2.94870E-02	-1.97083E-04	3.34778E-07	4.81910E-04	9.03580E-06	1.14896E-03
22	N2-N2-CH4	3	3	1	0.1	0.1	0.45	8.74115E-03	-4.43880E-05	6.96584E-08	1.71504E-03	2.31530E-05	1.17211E-03
23	N2-N2-H2	3	3	2	0.1	0.1	0.25	-6.50954E-03	5.19104E-05	-8.87528E-08	1.08085E-03	8.10638E-06	1.18022E-03
24	N2-N2-C2H6	3	3	4	0.1	0.1	0.1	-1.36584E-02	1.06972E-04	-1.79369E-07	2.28602E-03	6.85807E-06	1.18708E-03
25	N2-N2-C2H4	3	3	5	0.1	0.1	0.1	-1.36584E-02	1.06972E-04	-1.79369E-07	2.28602E-03	6.85807E-06	1.19394E-03
29	C2H6-C2H6-CH4	4	4	1	0.1	0.1	0.45	-8.27905E-03	1.21913E-04	-2.39958E-07	6.83849E-03	9.23197E-05	1.28626E-03
30	C2H4-C2H4-CH4	5	5	1	0.1	0.1	0.45	-8.27905E-03	1.21913E-04	-2.39958E-07	6.83849E-03	9.23197E-05	1.37858E-03
31	C2H6-C2H6-H2	4	4	2	0.1	0.1	0.25	8.43800E-03	-2.65166E-05	3.81345E-08	3.94182E-03	2.95637E-05	1.40814E-03
32	C2H4-C2H4-H2	5	5	2	0.1	0.1	0.25	8.43800E-03	-2.65166E-05	3.81345E-08	3.94182E-03	2.95637E-05	1.43770E-03
33	C2H6-C2H6-N2	4	4	3	0.1	0.1	0.1	-3.69750E-02	2.89620E-04	-4.94852E-07	5.40105E-03	1.62031E-05	1.45391E-03
34	C2H4-C2H4-N2	4	4	3	0.1	0.1	0.1	-3.69750E-02	2.89620E-04	-4.94852E-07	5.40105E-03	1.62031E-05	1.47011E-03
35	C2H6-C2H6-C2H4	4	4	5	0.1	0.1	0.1	-1.44234E-01	1.01275E-03	-1.63277E-06	1.23384E-02	3.70153E-05	1.50712E-03
38	C2H6-C2H4-C2H4	4	5	5	0.1	0.1	0.1	7.09314E-03	3.02671E-05	-9.73383E-08	7.60098E-03	2.28029E-05	1.52993E-03

Table A.4—Illustrative example calculation - C terms (@ 293.15 K) (Continued)

For example illustration purposes only (partial list, not final coefficients).

Index	CName	Cid1	Cid2	Cid3	X1	X2	X3	c0	c1	c2	C_CName	Factor*x1x2x3*C	C_Summation
43	CH4-N2-H2	1	3	2	0.45	0.1	0.25	3.60589E-03	-1.45437E-05	2.04722E-08	1.10172E-03	7.43662E-05	1.60429E-03
44	CH4-N2-C2H6	1	3	4	0.45	0.1	0.1	4.49508E-03	5.30233E-07	-1.52576E-08	3.33933E-03	9.01618E-05	1.69446E-03
45	CH4-N2-C2H4	1	3	5	0.45	0.1	0.1	4.49508E-03	5.30233E-07	-1.52576E-08	3.33933E-03	9.01618E-05	1.78462E-03
48	CH4-C2H6-H2	1	4	2	0.45	0.1	0.25	-1.16095E-03	2.63812E-05	-5.12600E-08	2.16757E-03	1.46311E-04	1.93093E-03
49	CH4-C2H6-C2H4	1	4	5	0.45	0.1	0.1	-1.89480E-01	1.39040E-03	-2.38860E-06	1.28468E-02	3.46864E-04	2.27779E-03
54	CH4-C2H4-H2	1	5	2	0.45	0.1	0.25	-1.16095E-03	2.63812E-05	-5.12600E-08	2.16757E-03	1.46311E-04	2.42410E-03
57	N2-C2H6-H2	3	4	2	0.1	0.1	0.25	-2.97743E-04	1.68641E-05	-3.30680E-08	1.80421E-03	2.70631E-05	2.45117E-03
58	N2-C2H4-H2	3	5	2	0.1	0.1	0.25	-2.97743E-04	1.68641E-05	-3.30680E-08	1.80421E-03	2.70631E-05	2.47823E-03
59	N2-C2H6-C2H4	3	4	5	0.1	0.1	0.1	-5.06529E-02	3.63400E-04	-5.77241E-07	6.27149E-03	3.76290E-05	2.51586E-03
62	C2H6-C2H4-H2	4	5	2	0.1	0.1	0.25	8.43800E-03	-2.65166E-05	3.81345E-08	3.94182E-03	5.91273E-05	2.57499E-03

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