

FORTSCHRITT-
BERICHTE

VDI

Dr. rer. nat. Manfred Jaeschke, Dorsten
Federal Republic of Germany

Dr. Anthony E. Humphreys, London
United Kingdom

Standard GERG Virial Equation for Field Use

Simplification of the Input Data Requirements
for the GERG Virial Equation —
An Alternative Means of Compressibility
Factor Calculation for Natural Gases and
Similar Mixtures

Reihe **6**: Energieerzeugung

Nr. **266**

VDI VERLAG

Dr. rer. nat. Manfred Jaeschke, Dorsten
Federal Republic of Germany

Dr. Anthony E. Humphreys, London
United Kingdom

Standard GERG Virial Equation for Field Use

Simplification of the Input Data Requirements
for the GERG Virial Equation —
An Alternative Means of Compressibility
Factor Calculation for Natural Gases and
Similar Mixtures

Reihe **6**: Energieerzeugung

Nr. **266**

Jaeschke, Manfred, and Anthony E. Humphreys

STANDARD GERG VIRIAL EQUATION FOR FIELD USE
Simplification of the Input Data Requirements for the GERG Virial Equation —

An Alternative Means of Compressibility Factor Calculation for Natural Gases and Similar Mixtures

Fortschr.-Ber. VDI Reihe 6 Nr. 266. Düsseldorf: VDI-Verlag 1992.
188 pages, 42 figures, 33 tables.

Keywords: Calorific Value — Carbon Dioxide — Coke-Oven Gas — Compressibility Factor — FORTRAN Program — GERG Virial Equation — Hydrogen — Natural Gas — Relative Density

This Monograph provides a detailed account of the concept, development, performance and use of the Standard (or Simplified) GERG-88 Virial Equation for the accurate calculation of compressibility factors for natural gases. The equation has been developed from the Master (or Molar) GERG-88 Virial Equation — described fully in Fortschritt-Berichte VDI, Reihe 6 — and utilises a restricted set of input variables in place of the detailed (13 component) composition analyses required for the Master equation. The simplified input data requirement comprises any three from superior (gross) calorific value, relative density, carbon dioxide content (the usual set) and nitrogen content, together with pressure and temperature. Even with this minimal information, the equation predicts the compressibility factor $Z(p,T)$ within the respective pressure and temperature ranges of 0 to 12 MPa (0 to 120 bar) and 265 to 335 K (–8 to 62 °C) with an expectation accuracy which, at about 0.1%, matches that of the master equation. For mixtures containing manufactured (coke-oven) gas, the amount of hydrogen must also be known. The method is currently being prepared as a draft international standard for ISO TC 193/SC 1.

Die Reihen der FORTSCHRITT-BERICHTE VDI:

- | | |
|--|---|
| 1 Konstruktionstechnik/Maschinenelemente | 12 Verkehrstechnik/Fahrzeugtechnik |
| 2 Fertigungstechnik | 13 Fördertechnik |
| 3 Verfahrenstechnik | 14 Landtechnik/Lebensmitteltechnik |
| 4 Bauingenieurwesen | 15 Umwelttechnik |
| 5 Grund- und Werkstoffe | 16 Technik und Wirtschaft |
| 6 Energieerzeugung | 17 Biotechnik |
| 7 Strömungstechnik | 18 Mechanik/Bruchmechanik |
| 8 Meß-, Steuerungs- und Regelungstechnik | 19 Wärmetechnik/Kältetechnik |
| 9 Elektronik | 20 Rechnerunterstützte Verfahren
(CAD, CAM, CAE, CAP, CAQ, CIM, ...) |
| 10 Informatik/Kommunikationstechnik | 21 Elektrotechnik |
| 11 Schwingungstechnik | |

© VDI-Verlag GmbH · Düsseldorf 1992

Alle Rechte, auch das des auszugsweisen Nachdruckes, der auszugsweisen oder vollständigen Wiedergabe (Photokopie, Mikrokopie), der Speicherung in Datenverarbeitungsanlagen und das der Übersetzung, vorbehalten.

Als Manuskript gedruckt. Printed in Germany.

ISSN 0178-9414

ISBN 3-18-146606-9

GERG TECHNICAL MONOGRAPH 5 (1991)

STANDARD GERG VIRIAL EQUATION FOR FIELD USE

SIMPLIFICATION OF THE INPUT DATA REQUIREMENTS FOR THE
GERG VIRIAL EQUATION - AN ALTERNATIVE MEANS OF
COMPRESSIBILITY FACTOR CALCULATION FOR NATURAL GASES
AND SIMILAR MIXTURES

prepared by

M.JAESCHKE Ruhrgas A.G., Federal Republic of Germany
 (Convenor, GERG Working Group 1.1 (1987-88))

and

A.E.HUMPHREYS British Gas plc, United Kingdom

on behalf of

GERG Working Group 1.1

P.VAN CANEGHEM Distrigaz S.A., Belgium
M.FAUVEAU Gaz de France, France
R.JANSSEN-VAN ROSMALEN N.V.Nederlandse Gasunie, Netherlands
Q.PELLEI S.N.A.M. S.p.A., Italy

and

Programme Committee No.1
- Production, Supply and Gas Properties -
GRUPE EUROPEEN DE RECHERCHES GAZIERES (GERG)

GERG

GERG TM-5 (1991)

Published for GERG and printed in Germany by

Verlag des Vereins Deutscher Ingenieure
Düsseldorf, 1991

Reprinted from FORTSCHRITT-BERICHTE VDI
Reihe 6 Nr. 266 (1992)
ISBN 3-18-146606-9

in memory
of our friend and colleague
RUSSELL COULTHURST

Errata for GERG Monograph TM-2 (1988)

- verso - below ISBN - insert "also published as - Fortschritt-Berichte VDI series 6 number 231"
- page iii - page number list - "6" should read "5"
"41" should read "40"
"45" should read "44"
- page iv - page number list - "92" should read "94"
"113" should read "112"
"114" should read "113"
- page v - first line - "IMPLEMENTATION" is misspelled
- page 17 - ref [25] date - "1966" should read "1965"
ref [60] date - "1935" should read "1936"
- page 23 - data counts - "73" should read "72"
"493" should read "492"
- page 36 - ref [60] date - "1935" should read "1936"
- page 57 - penultimate line - first "is" should read "are"
- page 61 - fifth line down - delete second "in"
- page 75 - fourth line down - "80" should read "8"
- page 77 - 18th line down - insert "the" before "GERG"
- page 88 - 15th line down - "(N37)" should read "(N37,
N79)"
- page 92 - 18th line down - "factor" should read "factors"
- page 97 - figure 5.16 - faulty printing of data point for 280 K at 11 MPa
- page 112 - fifth line up - insert "," before "firstly"
- page 148 - reference 33(a) - run together lines 2 and 3
- page 149 - reference 45 - "1251" should read "1250"
- page 158 - first definition of N - incorrect line spacing of text

GERG TECHNICAL MONOGRAPH 5 (1991)STANDARD GERG VIRIAL EQUATION FOR FIELD USE

SIMPLIFICATION OF THE INPUT DATA REQUIREMENTS FOR THE GERG
VIRIAL EQUATION - AN ALTERNATIVE MEANS OF COMPRESSIBILITY
FACTOR CALCULATION FOR NATURAL GASES AND SIMILAR MIXTURES

Errata for GERG TM-2 (1988)	page ...	iv
Contents		v
Abstract		viii
Zusammenfassung		ix
Acknowledgements		xi
1 - <u>INTRODUCTION</u>		1
1.1 Compressibility Factor Calculation in the Natural Gas Industry		1
1.2 Current Restricted Input Methods		2
1.3 Specification for the Standard GERG Virial Equation		6
2 - <u>PRINCIPLES AND METHODOLOGY</u>		9
2.1 Basic Concepts: The Three-Component Truncated Virial Equation		9
2.2 The Equivalent Hydrocarbon and its Characterisation		11
2.3 Natural Gases with Hydrogen or Carbon Monoxide Admixture		13
2.4 Temperature Dependence of Virial Coefficients		15
3 - <u>EVALUATION OF VIRIAL COEFFICIENTS</u>		17
3.1 GERG Contract with the van der Waals Laboratory		17
3.2 Pure Component Second and Third Virial Coefficients		17
3.3 Unlike Interaction Second and Third Virial Coefficients of Systems containing Nitrogen, Carbon Dioxide, Hydrogen and Carbon Monoxide		18
3.4 Virial Coefficients for the Equivalent Hydrocarbon Gas		21
3.4.1 The GERG N-File of Natural Gas Compressibility Factors		21
3.4.2 Calculation of Calorific Value and Relative Density for N-File Natural Gases		26
3.4.3 Evaluation of Virial Coefficients for the Equivalent Hydrocarbon Gas		32
3.5 Unlike Interaction Virial Coefficients for the Equivalent Hydrocarbon Gas		37
3.5.1 Equivalent Hydrocarbon plus Carbon Dioxide or Nitrogen: Second Virial Coefficients		37

3.5.2	Equivalent Hydrocarbon plus Carbon Dioxide or Nitrogen: Third Virial Coefficients	39
3.5.3	Equivalent Hydrocarbon plus Hydrogen and Carbon Monoxide	40
4	<u>NUMERICAL VALUES</u>	42
4.1	Second Virial Coefficients and Coefficients of the Expansion in Temperature	42
4.2	Third Virial Coefficients and Coefficients of the Expansion in Temperature	45
5	<u>CALCULATIONAL PROCEDURES</u>	48
5.1	Relation between Molar Heating Value and Molar Mass	48
5.2	General Description of Iterative Procedures	48
5.3	Details of Procedures to Determine Compressi- bility Factor using the Standard Input Variables	53
5.4	Procedure when Hydrogen and Carbon Monoxide are Present	57
5.5	Procedures using Alternative Input Variables	59
5.5.1	Calorific Value, Relative Density and Mole Fraction of Nitrogen	59
5.5.2	Calorific Value, Mole Fractions of Carbon Dioxide and Nitrogen	59
5.5.3	Relative Density, Mole Fractions of Carbon Dioxide and Nitrogen	60
6	<u>PERFORMANCE OF THE STANDARD GERG-88 VIRIAL EQUATION</u>	61
6.1	Test Data and Input Parameters	61
6.2	Global Comparison against Test Data	62
6.3	Statistical Analysis of the Standard GERG Virial Equation by Pressure-Temperature Domains	72
6.4	Accuracy of the Standard GERG Virial Equation for Six Groups of Natural Gases	76
6.4.1	Group 1 - Natural Gases with $N_2 \geq 0.095$	76
6.4.2	Group 2 - Natural Gases with $CO_2 \geq 0.040$	80
6.4.3	Group 3 - Natural Gases with $C_2H_6 \geq 0.080$	82
6.4.4	Group 4 - Natural Gases with $H_2 \geq 0.020$	84
6.4.5	Group 5 - Natural Gases with N_2 and C_2H_6 each ≥ 0.040	86
6.4.6	Group 6 - Natural Gases with $CH_4 \geq 0.940$	87
6.5	Performance for Specific Natural Gases	87
6.6	Performance for Liquefied Natural Gas and Simulated Natural Gases	93
6.7	Expected Accuracy of the Standard GERG Equation	96
6.8	Comparison with Alternative Simplified Input Methods	96

7 - <u>DISCUSSION AND CONCLUSIONS</u>	101
7.1 General Comments on Overall Performance	101
7.2 Recommendations - Use and Misuse of the Standard GERG Virial Equation	102
7.2.1 Extrapolation beyond Pressure and Temperature Limits	104
7.2.2 Extrapolation beyond Specified Composition and Quality Limits	105
7.3 Sensitivity to Input Variables	110
7.3.1 Inbuilt Uncertainties	110
7.3.2 Calorific Value	111
7.3.3 Relative Density	113
7.3.4 Concentrations of Inerts	114
7.3.5 Temperature and Pressure	116
7.3.6 Overall Sensitivity to Input Variables	116
7.4 Use of Alternative Input Variables	120
8 - <u>COMPUTER IMPLEMENTATION OF THE STANDARD GERG-88 VIRIAL EQUATION</u>	123
8.1 Calculation of Compressibility Factor	123
8.1.1 Input Data Requirements	123
8.1.2 Calorific Value Reference Conditions	124
8.1.3 Units and Conversion Factors for Pressure and Temperature	126
8.1.4 Conversion between Reference Conditions	126
8.2 Basic Implementation - the Program ZGERG-88	128
8.3 Fortran Implementation - the Subroutine SGERG	129
8.4 Example Calculations	130
8.5 Program Availability	130
9 - <u>REFERENCES</u>	167
10 - <u>NOMENCLATURE</u>	170

Abstract

This Monograph provides a detailed account of the concept, development, performance and use of the Standard (or Simplified) GERG-88 Virial Equation for the accurate calculation of compressibility factors for natural gases. The equation has been developed from the Master (or Molar) GERG-88 Virial Equation - described fully in GERG Technical Monograph TM2 - and utilises a restricted set of input variables in place of the detailed (13 component) composition analysis required for the Master equation. The simplified input data requirement comprises any three from superior (gross) calorific value, relative density, carbon dioxide content (the usual set) and nitrogen content, together with pressure and temperature. Even with this minimal information, the equation predicts the compressibility factor $Z(p,T)$ within the respective pressure and temperature ranges of 0 to 12 MPa (0 to 120 bar) and 265 to 335 K (-8 to 62 °C) with an expectation accuracy which, at about 0.1%, matches that of the Master equation. For mixtures containing manufactured (coke-oven) gas, the amount of hydrogen must also be known.

The principle involved in the new development is to consider any natural gas as a 3-component mixture containing carbon dioxide, nitrogen and an "equivalent hydrocarbon" CH which represents all of the alkane hydrocarbons collectively as a single pseudo-component. Given the mole fraction of either inert component, it turns out that both the mole fraction and the virial coefficients of the equivalent hydrocarbon may be inferred through knowledge of the superior calorific value and relative density of the whole natural gas, i.e. these two properties are sufficient to characterise the gas uniquely.

Coefficients used in the Standard GERG-88 Virial Equation have either been taken directly from those used in the Master equation or, for the equivalent hydrocarbon, derived from available data for actual natural gases. The resulting equation describes the set of some 4,500 data points, for natural gases in the GERG databank of compressibility factors, with a root-mean-square error of 0.049%.

Numerical values for all coefficients needed to implement the equation are given, together with flow diagrams showing the iterative structure of an efficient calculational procedure; computer program listings are provided.

The Standard GERG-88 Virial Equation was developed at the van der Waals Laboratorium of the University of Amsterdam, under contract to, and with specific guidance from, the Groupe Européen de Recherches Gazières.

Zusammenfassung

In dieser Monographie werden im Detail das Konzept, die Entwicklung, die Güte und der Gebrauch der Standard (oder Vereinfachten) GERG-88 Virial-Gleichung zur genauen Berechnung der Realgasfaktoren von Erdgasen beschrieben. Die Gleichung ist von der Master (oder Molaren) GERG-88 Virial-Gleichung, die ausführlich im GERG Technical Monograph TM2 beschrieben worden ist, abgeleitet worden. Sie benutzt nur einen reduzierten Satz von Eingabegrößen anstelle einer detaillierten Gasanalyse (13 Komponenten), die von der Master-Gleichung benötigt wird. Als vereinfachter Eingabedatensatz kommen dabei drei der folgenden Größen in Frage: der Brennwert, die relative Dichte, der Kohlendioxid-Anteil (dies sind die üblichen Eingabegrößen) und der Stickstoff-Anteil zusammen mit dem Druck und der Temperatur. Selbst mit dieser minimalen Information ist es möglich, mit der Gleichung den Realgasfaktor $Z(p,T)$ innerhalb der Druck- und Temperaturbereiche von 0 bis 12 MPa (0 bis 120 bar) und 265 bis 335 K (-8 bis 62 °C) mit einer Voraussagegenauigkeit von etwa 0,1% zu bestimmen. Damit ist diese Gleichung der Master-Gleichung ebenbürtig. Für Gemische, die Zumischungen von künstlich hergestellten Gasen (Kokereigas) enthalten, muß zusätzlich der Wasserstoffanteil bekannt sein.

Das wesentliche Prinzip dieser Neuentwicklung ist, jedes Erdgas als ein Drei-Komponenten-Gemisch zu betrachten, welches Kohlendioxid, Stickstoff und ein "äquivalentes Kohlenwasserstoffgas" CH enthält. Hierbei werden alle vorhandenen, gesättigten Kohlenwasserstoff gemeinsam durch diese einzelne Pseudokomponente, das CH-Gas, repräsentiert. Ist der Molanteil eines der inerten Gase bekannt, so läßt sich sowohl der Molanteil als auch die Virialkoeffizienten des äquivalenten Kohlenwasserstoffgases allein aus der Kenntnis des Brennwertes und der relativen Dichte für das ganze Erdgas ableiten; d.h., diese beiden Eigenschaften reichen aus, um das Gas vollständig zu charakterisieren.

Die Virialkoeffizienten, die in der Standard GERG Virial-Gleichung benutzt werden, sind entweder direkt von der Master GERG Virial-Gleichung übernommen oder für das äquivalente Kohlenwasserstoffgas aus den vorhandenen Daten für tatsächliche Erdgase abgeleitet worden. Die so aufgebaute Gleichung beschreibt die Realgasfaktoren für Erdgase aus der GERG-Datenbank von etwa 4500 Punkten mit einem mittleren quadratischen Fehler (rms-error) von 0,049%.

Alle Zahlenwerte für die Koeffizienten der Gleichung, die zur Implementierung notwendig sind, sind zusammen mit den Fließdiagrammen, die die iterative Struktur für eine effiziente Berechnungsprozedur aufzeigen, aufgeführt; die Listings der Computerprogramme werden mitgeliefert.

Die Standard GERG-88 Virial-Gleichung wurde vom Van der Waals Laboratorium der Universität von Amsterdam im Auftrag und unter der Leitung der "Groupe Européen de Recherches Gazières" entwickelt.

Acknowledgements

Once again it is our pleasure to record our thanks to GERG Programme Committee No.1, and especially to its former chairman Dr Alec Melvin, for recognising and responding to the urgent need of the international community of natural gas engineers (and others) for a new, accurate and reasonably simple method with which to predict compressibility factors for natural gas and similar mixtures, and for supporting the consequent efforts of GERG Working Group 1.1 in this area. Both the timeliness of the developments described in this and previous GERG Monographs from WG-1.1, and their success, are evidenced by the intention of the International Organization for Standardization (ISO) to incorporate the Standard GERG-88 Virial Equation into a new international standard method for the calculation of compressibility factor.

The Working Group could not have achieved its success without the detailed correlational work carried out under contract to GERG at the University of Amsterdam by Dr Jan Schouten and Dr Jan Michels.

Manfred Jaeschke

Tony Humphreys

August 1991

The main part (pages 1 to 173) of Fortschritt- Bericht VDI Reihe 6: Energieerzeugung Nr. 266 is identical with and may be found in the corresponding GERG Technical Monograph TM5 1991.