

FORTSCHRITT-
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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**

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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.

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

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in memory
of our friend and colleague
RUSSELL COULTHURST

Errata for GERG Monograph TM-2 (1988)

- verso - below ISBN - insert "also published as -
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- 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

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VIRIAL EQUATION - AN ALTERNATIVE MEANS OF COMPRESSIBILITY
FACTOR CALCULATION FOR NATURAL GASES AND SIMILAR MIXTURES

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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.