This document is not an ASTM standard and is intended only to provide the user of an ASTM standard an indication of what changes have been made to the previous version. Because it may not be technically possible to adequately depict all changes accurately, ASTM recommends that users consult prior editions as appropriate. In all cases only the current version of the standard as published by ASTM is to be considered the official document.



Designation: D8221 - 18 D8221 - 18a

Standard Practice for Determining the Calculated Methane Number (MN_c) of Gaseous Fuels Used in Internal Combustion Engines¹

This standard is issued under the fixed designation D8221; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This practice covers the method to determine the calculated methane number (MN_C) of a gaseous fuel used in internal combustion engines. The basis for the method is a dynamic link library (DLL) suitable for running on computers with Microsoft Windows operating systems.

1.2 This practice pertains to commercially available natural gas products that have been processed and are suitable for use in internal combustion engines. These fuels can be from traditional geological or renewable sources and include pipeline gas, compressed natural gas (CNG), liquefied natural gas (LNG), liquefied petroleum gas (LPG), and renewable natural gas (RNG) as defined in Section 3.

1.3 The calculation method within this practice is based on the MWM Method as defined in EN 16726, Annex A.² The calculation method is an optimization algorithm that uses varying sequences of ternary and binary gas component tables generated from the composition of a gaseous fuel sample.³ Both the source code and a Microsoft Excel-based calculator are available for this method.

1.4 This calculation method applies to gaseous fuels comprising of hydrocarbons from methane to hexane and greater (C6+); carbon monoxide; hydrogen; hydrogen sulfide; nitrogen; and carbon dioxide. The calculation method addresses pentanes (C5) and higher hydrocarbons and limits the individual volume fraction of C5 and C6+ to $\frac{3\%}{3\%}$ each and a combined total of $\frac{5\%}{5\%}$. (See EN 16726, Annex A.) The calculation method is performed on a dry, oxygen-free basis.

1.5 Units—The values stated in SI units are to be regarded as standard. Other units of measurement included in this standard practice are for reference only.provided for information only and are not considered standard.

1.6 This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety, health, and environmental practices and determine the applicability of regulatory limitations prior to use.

1.7 This international standard was developed in accordance with internationally recognized principles on standardization established in the Decision on Principles for the Development of International Standards, Guides and Recommendations issued by the World Trade Organization Technical Barriers to Trade (TBT) Committee.

2. Referenced Documents

2.1 ASTM Standards:⁴

E29 Practice for Using Significant Digits in Test Data to Determine Conformance with Specifications

2.2 CEN Standard:⁵

EN 16726 Gas infrastructure—Quality of gas—Group H, Annex A—Calculation of methane number of gaseous fuels for engines

¹ This practice is under the jurisdiction of ASTM Committee D03 on Gaseous Fuels and is the direct responsibility of Subcommittee D03.03 on Determination of Heating Value and Relative Density of Gaseous Fuels.

Current edition approved Sept. 1, 2018 Dec. 1, 2018. Published October 2018 April 2019. Originally approved in 2018. Last previous edition approved in 2018 as D8221-18. DOI: 10.1520/D8221-18.10.1520/D8221-18A.

² European Standards (ENs) are documents that have been ratified by one of the three European Standardization Organizations (ESOs), CEN, CENELEC or ETSI; recognized as competent in the area of voluntary technical standardization as for the EU Regulation 1025/2012. EN16726 was developed by the Technical Committee CEN/TC 234.

³ Leiker, M., Christoph, K., Rankl, M., Cartellieri, W., and Pfeifer, U., "Evaluation of Antiknocking Property of Gaseous Fuels by Means of Methane Number and its Practical Application to Gas Engines," ASME, 72-DGP-4, 1972.

⁴ For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For Annual Book of ASTM Standards volume information, refer to the standard's Document Summary page on the ASTM website.

⁵ Available from European Committee for Standardization (CEN), Avenue Marnix 17, B-1000, Brussels, Belgium, http://www.cen.eu.



2.3 ISO Standard:⁶
ISO 14912 Gas analysis—Conversion of gas mixture composition data
2.4 ASTM Adjuncts:⁷
ASTM_D8221_mzdll_ver2.32.0.dll
ASTM_D8221_MNc_Method_ver1.32.0.xlsb

NOTE 1-The adjuncts listed above are the Microsoft Office 32-bit version.

ASTM_D8221_mzdll_ver2.64.0.dll ASTM_D8221_MNc_Method_ver1.64.0.xlsb

NOTE 2-The adjuncts listed above are the Microsoft Office 64-bit version.

3. Terminology

3.1 Definitions:

3.1.1 *compressed natural gas (CNG), n*—natural gas that has been compressed after processing for storage or transportation purposes.

3.1.1.1 Discussion-

CNG is primarily used as a fuel for vehicles, typically compressed up to 24 821 kPa in the gaseous state.

3.1.2 liquefied natural gas (LNG), n-natural gas that has been liquefied after processing for storage or transportation purposes.

3.1.2.1 Discussion-

Liquefied natural gas is revaporized and introduced into pipelines for transmission and distribution as natural gas and may be used as a fuel for internal combustion engines.

3.1.3 liquefied petroleum gas (LPG), n—a gaseous fuel that has been liquefied after processing for storage or transportation purposes composed primarily of propane, propene (propylene), butane, and mixtures of these gases.

3.1.3.1 Discussion—

This special mixture of gases was specifically developed for use as a fuel in spark ignited internal combustion engines. Limits are applied to propene and butane, which are used to adjust the vaporization pressure. When used in vehicles, LPG is specified as HD-5 propane or HD-10 propane.

3.1.4 *methane number (MN), n*—an experimental determination of a gaseous fuel's resistance to knock based on a Cooperative Fuel Research (CFR) Motor Octane Number (MON) test engine and indicated by the volume of methane in a blend with hydrogen.

3.1.4.1 Discussion—

Methane has a value of $\frac{MN=100}{MN=100}$ MN = 100 and hydrogen has a value of $\frac{MN=0}{MN=0}$.

3.1.5 methane number, calculated (MN_c) , n—a calculation of a rating index, indicating the resistance to knock of a gaseous fuel when compared to a reference methane/hydrogen mixture.

3.1.5.1 Discussion-

Multiple methods have been developed in the past for providing this analytical estimate based on gas composition. A MN_C is determined using volumetric fuel composition. Sometimes MN_C is described as "methane index (MI)."

3.1.6 natural gas, n—a naturally occurring mixture of hydrocarbon and nonhydrocarbon gases found in porous geological formations (reservoirs) beneath the earth's surface, often in association with petroleum. The principal component of natural gas is methane.

3.1.7 pipeline gas, n-gas that is refined to high quality levels and transported in natural gas pipeline systems.

⁶ Available from American National Standards Institute (ANSI), 25 W. 43rd St., 4th Floor, New York, NY 10036, http://www.ansi.org.

⁷ Available from ASTM International Headquarters. Order Adjunct No. ADJD822118-EA. Original adjunct produced in 2018.

🕼 D8221 – 18a

3.1.8 renewable natural gas (RNG), n—a pipeline-quality gas that is all or in part from renewable sources, and is fully interchangeable with geological natural gas.

3.1.8.1 Discussion—

RNG can be biogas or biomethane (the gaseous product of the decomposition of organic matter) that has been processed to purity standards and thus can be used as a fuel for internal combustion engines.

3.1.8.2 Discussion—

Like geological natural gas, RNG can be used for transportation purposes in the form of compressed natural gas (CNG) or liquefied natural gas (LNG).

3.2 Definitions of Terms Specific to This Standard:

3.2.1 *commercially available, adj*—a natural gas product from more than one non-governmental entity that may be distributed to more than one user.

3.2.1.1 Discussion-

Examples of commercially available natural gas products are pipeline gas from a utility, CNG from a fueling station, and so forth.

3.2.1.2 Discussion-

Examples of natural gas that is not commercially available include well-head gas, landfill gas, methane digester gas, and so forth.

4. Summary of Calculation Method

4.1 The application of analytical methods to groups of ternary and binary mixtures of gas components with known methane numbers that reflect the makeup of the gaseous fuel mixture is the basis for this calculated methane number method.

4.2 This calculation method originates with the data of a research program performed by AVL Deutschland GmbH for FVV and was updated and revised by MWM GmbH and then finally published for global use in EN16726, EN 16726, Annex A.

5. Significance and Use

5.1 The methane number (MN) is a measure of the resistance of the gaseous fuel to autoignition (knock) when used in an internal combustion engine. The relative merits of gaseous fuels from different sources and having different compositions can be compared readily on the basis of their methane numbers. Therefore, the calculated methane number (MN_C) is used as a parameter for determining the suitability of a gaseous fuel for internal combustion engines in both mobile and stationary applications.

CALCULATION METHOD

6. Scope

6.1 This calculation method applies to gaseous fuels as defined by the Scope, and defined in Section 3, and listed in Procedure 8.1, Table 2.

TABLE 1 Error Messages

Error Message	Comment
"The input sample total must be from 99 % to 101 %, inclusive; please correct!"	No MN _C value displayed
"The input sample total must be from 99 % to 101 %, inclusive; please correct!"	<u>No MN_c value displayed</u>
"The MNc calculation is not possible due to internal program errors!"	No MN_C value displayed
"A valid MNc value cannot be calculated!"	No MN_C value displayed
"A MNc value with reasonable certainty is not possible due to high C5+ content!"	No MN_C value displayed



	TABL	.E 2	Com	ponents
--	------	------	-----	---------

Component	Formula	Component	Formula
Methane	CH₄	Hexane	C_6H_{14}
Ethylene	C_2H_4	Heptane	C_7H_{16}
Ethane	C ₂ H ₆	Octane	C ₈ H ₁₈
Propylene	C_3H_6	Nonane	C ₉ H ₂₀
Propane	C ₃ H ₈	Decane	C ₁₀ H ₂₂
Butadiene	C_4H_6	Hydrogen	H ₂
Butylene	C₄H ₈	Hydrogen Sulfide	H ₂ S
<i>i</i> -Butane	C_4H_{10}	Carbon Monoxide	CO
n-Butane	C_4H_{10}	Nitrogen	N ₂
<i>i</i> -Pentane	C ₅ H ₁₂	Oxygen	0 ₂
n-Pentane	C ₅ H ₁₂	Carbon Dioxide	CO ₂
Neopentane	C ₅ H ₁₂	Water Vapor	H ₂ O

7. Significance and Use

7.1 The methane number of a gaseous fuel can be calculated based on its composition by various analytical methods which can give different results. The results of the method described in this practice match measured methane numbers (see X1.1 and X2.1) with reasonable certainty for the fuels as defined in this practice.

7.2 The method requires input of composition in the form of volume fractions at reference conditions of $\frac{15.55 \text{ °C}}{15.55 \text{ °C}}$ and $\frac{101.325 \text{ kPa}}{15.55 \text{ °C}}$ and $\frac{101.325 \text{ kPa}}{101.325 \text{ kPa}}$ and expressed as a percentage. Compositions available as either mole fraction or mass fraction are to be converted to volume fraction using the methods cited in ISO 14912. For general use, it may be assumed that mole fraction and volume fraction are equivalent.

7.3 The final result, the calculated methane number, is expressed as an integer per Practice E29.

7.4 While this calculation method will provide results for gaseous fuel compositions outside the scope of this practice, the results may have a higher degree of uncertainty.

7.5 *Errors*—This calculation method may not apply to certain gas compositions based on the component inputs violating input limit requirements or due to the method's internal calculations and regressions being unable to develop a calculated methane number value. Error messages are provided to the user and are listed in Table 1 and described in 7.5.1 to 7.5.4.

7.5.1 "The input sample total must be from 99 % to 101 %, 99 % to 101 %, inclusive; please correct!"—The calculated methane number program requires a gas sample composition that totals 99 % to 101 %, 99 % to 101 %, inclusive. Please correct the gas component inputs manually or normalize the gas sample composition.

7.5.2 "The MN_C calculation is not possible due to internal program errors!"—A calculated methane number is not possible for the given gas sample because the internal program iteration routines failed. During the program's internal optimization processes, the differences between calculated methane numbers for various ternary mixtures used within the program were outside allowable internal program limits and a reasonable MN_C value could not be generated. An example of a gas sample causing this error would be a high CH_4 composition with the rest of the sample containing H_2 and CO components (for example, 98 % CH_4 , $\frac{1.8 \% - 1.8 \%}{1.8 \%}$ H_{22} and $\frac{0.2 \% - 0.2 \% - 0.2 \%}{CO}$.

7.5.3 "A valid MN_C value cannot be calculated!"—A calculated methane number is not possible for the given gas sample because internal program data is not available to support the calculation method or the internal program processes were unable to complete the calculation. An example of a gas sample causing this error would be a N_2 free composition with low CH_4 content and high CO_2 content (for example, $39 \% - 39 \% - CH_4$ and $61 \% - 61 \% - CO_2$).

7.5.4 "A MN_C value with reasonable certainty is not possible due to high C5+ content!"—The calculation method limits the volume fraction of C5 and C6+ to 3-%-3-% each and a total of 5 % for a given gas sample and will not provide a calculated methane number if these limits are exceeded due to the high uncertainty in the result (for example, 94-%-94% CH₄, 3-%-3% C₅H₁₂, and 3% C₆H₁₄).

7.6 The basis for this method is a dynamic link library $(DLL)^8$ suitable for running on computers with 32-bit or 64-bit Microsoft Windows operating systems.

7.7 An Excel Virtual Basic for Applications (VBA) macro is available for a user to tailor their calculations for a specific application (see <u>A1.1A1.2</u>). The DLL file is currently supported by only an Excel 32-bit platform and not an Excel 64-bit platform.files currently support either Excel 32-bit or Excel 64-bit versions of Microsoft Office. An Excel program (see A1.1) using the VBA macro (see <u>A1.1A1.2</u>) has been developed allowing for either individual or multiple gas samples (see samples. <u>A1.2</u>).

⁸ The sole source of the calculation method is a dynamic link library suitable for running on computers and was created by ASTM based on the FORTRAN code developed by MWM GmbH. ASTM will update the DLL file associated with this practice as revisions are published. If you are aware of any revisions that should be made to the calculation method and the DLL file, please provide this information to ASTM International Headquarters. Your comments will receive careful consideration at a meeting of the responsible technical committee,¹ which you may attend.



It also provides conversions for mass or mole fractions to volume fraction per ISO 14912 as well as a normalization routine. A graphical user interface (GUI) could also be developed by a user to use the dynamic link library file.⁹

8. Procedure

8.1 Determine the volume composition of the gaseous fuel in accordance with any ASTM or GPA method (see X2.2.1 and X2.2.2) that yields the complete composition in component amounts of 0.1 % - 0.1 % or more, in terms of the components listed in Table 2. Not all components listed in Table 2 must be input for a MN_C value to be calculated. Several of the components are not typically included in a standard gas chromatograph analysis of natural gas, for example, oxygen, water, hydrogen sulfide, carbon monoxide, and hydrogen. However, these components can be quantified by other techniques if their concentrations are considered significant.

8.2 Conversion from a mass-based composition or a molar-based composition and/or at different pressure or temperature conditions should be done in accordance with ISO 14912. All significant inputs should be in the form of volume fractions expressed as percentages at reference conditions of 101.325 kPa, 15.55 °C except H₂S, which is in ppmv. All measured hexane and higher hydrocarbons are combined and input as hexane in the calculation regardless if their individual component amounts are less than $0.1 \% \cdot 0.1 \%$. If the measurement reported a value for hexane-plus hydrocarbons, then that value should be input as hexane. If the measurement reported as a single nitrogen-oxygen value, then that value may be input as nitrogen with little impact to the MN_C value. Oxygen and water vapor component amounts may be input as part of the overall gaseous fuel composition, but they are later removed by the calculation method which is performed on a dry, oxygen-free basis.

8.3 An Excel program, augmenting the VBA macro described in A1.2, is executed after numerical values of the gaseous fuel composition (Table 2) are input. A calculated methane number (MN_C) is provided and possible warning or error messages may also be provided as described in 7.5, Table 1. See A1.1.

8.4 Alternatively, an Excel VBA macro has been developed allowing a user to develop their own Excel program. See A1.2.

9. Report

9.1 A calculated methane number (MN_C) should be reported as "per Practice D8221."

10. Precision and Bias

10.1 The determination of calculated methane number (MN_c) described by this practice is exact and is reported as an integer value per Practice E29.

10.2 *Precision*—The precision of the calculated methane number (MN_c) method described by this practice is dependent on the precision of the original gaseous fuel components that are entered into the method.

10.3 Bias—No general statement is made on bias of this calculation method since no agreed upon reference values are available.

11. Keywords

11.1 gaseous fuels; methane number; motor vehicle fuel; natural gas

ANNEX

(Mandatory Information)

A1. CALCULATED METHANE NUMBER (MN_C) METHOD

A1.1 Microsoft Excel Program

A1.1.1 Save the Excel file "ASTM_D8221_MNe_Method_ver2.32.0.xlsb" (ASTM_D8221_MNc_Method_ver1.32.0.xlsb") and the dynamic link library file "ASTM_D8221_mzdll_ver2.32.0.dll"¹⁰ to the same directory/folder in a local drive.drive for use with Excel 32-bit software. Alternatively, save the Excel file "ASTM_D8221_MNc_Method_ver1.64.0.xlsb" and the Dynamic Link Library file "ASTM_D8221_mzdll_ver2.64.0.dll"¹⁰ to the same directory/folder in a local drive for use with Excel 64-bit software.

⁹ Support of this calculation tool for use on current and future computer systems is important. An updated interface for the calculation is being planned for broader software compatibility.

¹⁰ Available from ASTM International Headquarters. Order Adjunct No. ADJD822118-EA. Original adjunct produced in 2018.

🕼 D8221 – 18a

A1.1.1.1 The .dll file cannot be renamed to other names or extensions.

A1.1.1.2 If the .xlsb and .dll files are saved to a network drive or remote server, avoid spaces from the path name.

A1.1.2 Include the "Solver Add-in" in Excel, if not already there.

A1.1.2.1 File > Options > Add-ins > Manage: Excel Add-ins "Go...".

A1.1.2.2 From the list of "Add-Ins available", check the box for "Solver Add-in" and click OK.

A1.1.2.3 Resave the Excel file.

A1.1.3 For the "Single Gas Sample" worksheet:

A1.1.3.1 Select the form of sample composition inputs; Vol %, Mass %, or Mol %.

A1.1.3.2 Input the percentage of the gas components in cells "C6" to "C29". "C29." Note that the H₂S component input is in ppmv, ppmm, or ppm(mol) per A1.1.3.1.

A1.1.3.3 Cell "C31" provides a running total of the gas component inputs.

A1.1.3.4 Clicking the "Calculate" button will execute the program and display the calculated methane number (MN_C) value in cell "116" if the input components total from 99 % to 101 %, inclusive.

A1.1.3.5 The "Vol % (Normalized)" values for the input components are displayed in cells "E6" to "E29" if the input components were Mass % or Mol %.

A1.1.3.6 If the input components do not total from 99 % to 101 %, inclusive, an error message will be displayed and an opportunity to normalize the data will be offered. Alternatively, there is a "Normalize" button that when clicked will normalize the sample input. The normalized values overwrite the input values in cells "C6" to "C29"."C29."

ASTM D8221-18a

A1.1.3.7 The status or error message associated with the MN_C value is displayed in cell "I20" (see Table 1).

A1.1.3.8 The "Clear Input" button resets the input cells "C6" to "C29". "C29."

A1.1.3.9 The "Clear Output" button resets the output cell "I16" and also the "Vol % (Normalized)"data shown in cells "E6" to "E29". "E29."

A1.1.4 For the "Multiple Gas Samples" worksheet:

A1.1.4.1 Input a sample name in the next available cell in Column B (for example, "B7"). (1) This automatically generates a next sample number in Column A.

A1.1.4.2 Select the type of sample composition input components; Vol %, Mass %, or Mol % in Column D (for example, "D7").

A1.1.4.3 Input the percentage of the gas components in the row associated with the sample name in cells Gn to ADn (for example, "G7" to "AD7"). Note that the H_2S component input is in ppm.

A1.1.4.4 Select "Yes" or "No" in Column E, (for example, "E7") if you want the input normalized.

A1.1.4.5 Either of the two available "Calculate MN_C " buttons executes the calculations.

A1.1.4.6 A running total of the gas component inputs for the sample is displayed in column AE (for example, "AE7").

A1.1.4.7 The calculated methane number (MN_C) value for the sample is displayed in column AG (for example, "AG7").