

MWM MN calculation program

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1. Disclaimer

This .exe version of the Methane number calculation of natural gas mixtures program includes some improvements compared to the published EN 16726 standard. EUROMOT believes that with the given information, the Source Code and the description in Annex A specialists should be able to analyse, replicate and recompile the calculation program if needed.

The source code can also be downloaded along with some of the background documentation. This program is free software intended for information purposes only, and copyright is 2017, EUROMOT (www.euromot.eu).

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2. Preamble

The here published *.exe version of the MWM MN calculation program includes some improvements compared to the published EN 16726 standard and these are discussed in chapter “**Description of the program, corrections Annex A**”. A corrigendum or an amendment to Annex A is in discussion and will be published after finalization.

With the given information from the Source Code and the description in Annex A specialists would be able to replicate the calculation program with a very high effort. Even with selecting the same triangle diagrams and using the given polynomials from Annex A there might be differences in the resulting MN due to different iteration routines. **In order to ensure the most accurate results, we recommend to use only the original programme.**

3. Installation

- Unzip the file MN.zip in the folder C:\MN
- Rename “mn.exe_” to “mn.exe”

Remark: The file extension is temporarily changed because most email and file transfer systems block *.exe files.

The executable “mn.exe” together with the dynamic link library “mzdll.dll” can be installed in a user defined folder. The help file “readme.pdf” must remain in the folder C:\MN

4. Requirements for the computer:

- Processor x86 or x86-64.
- 3 MB free disk space
- Windows NT or higher

5. User Guide for “mn.exe”

a) Start the executable file “mn.exe”. The MN- calculation will be displayed:

Methane Number Calculation

Input

Gas composition: Volume-%

Gas composition	Value
CO2.....Carbon dioxide.....[%]	.000
N2.....Nitrogen.....[%]	.000
O2.....Oxygen.....[%]	.000
H2.....Hydrogen.....[%]	.000
CO.....Carbon monoxide.....[%]	.000
CH4.....Methane.....[%]	.000
C2H4.....Ethylene.....[%]	.000
C2H6.....Ethane.....[%]	.000
C3H6.....Propylene.....[%]	.000
C3H8.....Propane.....[%]	.000
C4H6.....Butadiene.....[%]	.000
C4H8.....Butene.....[%]	.000
C4H10.....Butane.....[%]	.000
C5H12.....Pentane.....[%]	.000
C6+.....Hexanes+.....[%]	.000
H2S.....Hydrogen sulphide.....[%]	.000
H2O.....Water vapour.....[%]	.000
Total [%]	.000

Output

Mw/M

Methane Number [-]

mzdl-Version: 2.0.0

Buttons: Clear, Calculate, Help, Exit

b) Select the unit for the gas composition: Volume-%, Mol-% or Mass-%

Methane Number Calculation

Input

Gas composition: Volume-%

Dropdown menu options: Volume-%, Mol-%, Mass-%

Output

Mw/M

Methane Number [-]

mzdl-Version: 2.0.0

After this selection, input the numerical values of the gas composition.

A dot or period must be used to separate the decimal place of the values!

Use TAB to move to the next input box of the gas components.

Use SHIFT+TAB to move to the previous input box of the gas components.

You can also use the mouse to move to an input box of the gas components.

- c) After the input of the data has been completed, select **Calculate** and receive the calculation result:
 The “Output” section in the bottom right corner of the window shows the calculated MN data based on the gas composition.

Methane Number Calculation

Input

Gas composition Volume-% ▾

CO2.....Carbon dioxide.....[%]	1.000
N2.....Nitrogen.....[%]	2.000
O2.....Oxygen.....[%]	.000
H2.....Hydrogen.....[%]	.000
CO.....Carbon monoxide.....[%]	.000
CH4.....Methane.....[%]	85.000
C2H4.....Ethylene.....[%]	.000
C2H6.....Ethane.....[%]	7.000
C3H6.....Propylene.....[%]	.000
C3H8.....Propane.....[%]	5.000
C4H6.....Butadiene.....[%]	.000
C4H8.....Butene.....[%]	.000
C4H10.....Butane.....[%]	.000
C5H12.....Pentane.....[%]	.000
C6+.....Hexanes+.....[%]	.000
H2S.....Hydrogen sulphide.....[%]	.000
H2O.....Water vapour.....[%]	.000
Total [%]	100.000

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mn-Version : 2.0.0

Clear

Calculate

Help

Exit

Output

MWM
 Methane Number [-] **71**

mzdl-Version: 2.0.0

d) The button deletes the previous gas composition.

Methane Number Calculation

Input

Gas composition

CO2.....Carbon dioxide.....[%]	.000
N2.....Nitrogen.....[%]	.000
O2.....Oxygen.....[%]	.000
H2.....Hydrogen.....[%]	.000
CO.....Carbon monoxide...[%]	.000
CH4.....Methane.....[%]	.000
C2H4.....Ethylene.....[%]	.000
C2H6.....Ethane.....[%]	.000
C3H6.....Propylene.....[%]	.000
C3H8.....Propane.....[%]	.000
C4H6.....Butene.....[%]	.000
C4H8.....Butane.....[%]	.000
C4H10.....Butane.....[%]	.000
C5H12.....Pentane.....[%]	.000
C6+.....Hexanes+.....[%]	.000
H2S.....Hydrogen sulphide..[%]	.000
H2O.....Water vapour.....[%]	.000
Total [%]	.000

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mn-Version : 2.0.0

MN-calculation

Do you really want to clear your whole input?

Output

Mw/M

Methane Number [-]

mzdll-Version: 2.0.0

Acknowledge with to delete previous input data.

Remark: You can also change the actual input data inside each of the boxes for the next calculation, it is not necessary to always clear all of the input values.

e) With the button you can display the “README.PDF” information

6. Messages, Descriptions:

- a) If the Total is <95% or >105% of the gas composition (100%), a manual correction or re-check of the input data is required. No calculation is possible, as shown in the message. Acknowledge with and revise the input data manually.

The screenshot displays the 'Methane Number Calculation' software window. The main window has a title bar 'Methane Number Calculation' and a logo for 'MWM Energy. Efficiency. Environment. A Caterpillar Company' with 'mn-Version : 2.0.0'. The interface is divided into 'Input' and 'Output' sections. The 'Input' section lists various gas components with their respective percentages: CO2 (Carbon dioxide) at 2.100%, N2 (Nitrogen) at 3.000%, O2 (Oxygen) at .000%, H2 (Hydrogen) at .000%, CO (Carbon monoxide) at .000%, CH4 (Methane) at .000%, C2H4 (Ethylene) at .000%, C2H6 (Ethane) at .000%, C3H6 (Propylene) at .000%, C3H8 (Propane) at .000%, C4H6 (Butadiene) at .000%, C4H8 (Butene) at .000%, C4H10 (Butane) at .000%, C5H12 (Pentane) at .000%, C6+ (Hexanes+) at .000%, H2S (Hydrogen sulphide) at .000%, and H2O (Water vapour) at .000%. The 'Total [%]' is calculated as 105.100. The 'Output' section shows 'M/W/M Methane Number [-]' as an empty field and 'mzdll-Version: 2.0.0'. A modal dialog box titled 'MN-calculation' is overlaid on the input section, displaying a yellow warning triangle icon and the message: 'The Total is < 95% or > 105%; correct the input please!'. The dialog has an 'OK' button.

Gas composition	Volume-%
CO2.....Carbon dioxide.....[%]	2.100
N2.....Nitrogen.....[%]	3.000
O2.....Oxygen.....[%]	.000
H2.....Hydrogen.....[%]	.000
CO.....Carbon monoxide.....[%]	.000
CH4.....Methane.....[%]	.000
C2H4.....Ethylene.....[%]	.000
C2H6.....Ethane.....[%]	.000
C3H6.....Propylene.....[%]	.000
C3H8.....Propane.....[%]	.000
C4H6.....Butadiene.....[%]	.000
C4H8.....Butene.....[%]	.000
C4H10.....Butane.....[%]	.000
C5H12.....Pentane.....[%]	.000
C6+.....Hexanes+.....[%]	.000
H2S.....Hydrogen sulphide.....[%]	.000
H2O.....Water vapour.....[%]	.000
Total [%]	105.100

Output

M/W/M
Methane Number [-]

mzdll-Version: 2.0.0

MN-calculation

The Total is < 95% or > 105%; correct the input please!

- b) If the Total is $\geq 95\%$ or $\leq 105\%$ of the gas composition (100%) a correction to 100% will be offered to the user. Select to revise the input data manually or for automatic apportionment to 100%.

Methane Number Calculation

Input

Gas composition

CO ₂Carbon dioxide.....[%]	2.00
N ₂Nitrogen.....[%]	3.000
O ₂Oxygen.....[%]	.000
H ₂Hydrogen.....[%]	.000
CO.....Carbon monoxide...[%]	.000
CH ₄Methane.....[%]	97.000
C ₂ H ₄Ethylene.....[%]	
C ₂ H ₆Ethane.....[%]	
C ₃ H ₆Propylene.....[%]	
C ₃ H ₈Propane.....[%]	
C ₄ H ₆Butene.....[%]	
C ₄ H ₈Butane.....[%]	
C ₄ H ₁₀Butane.....[%]	.000
C ₅ H ₁₂Pentane.....[%]	.000
C ₆ +.....Hexanes+.....[%]	.000
H ₂ S.....Hydrogen sulphide..[%]	.000
H ₂ O.....Water vapour.....[%]	.000
Total [%]	97.000

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mn-Version : 2.0.0

MN-calculation

The Total is not equal to 100% !
Would you like to apportion the gas components to 100%?

Output

MWM
Methane Number [-]

mzdll-Version: 2.0.0

After selection of you receive the adjusted gas composition and calculated results.

Displayed on the left is the corrected composition to 100%, and displayed on the right is the calculated MN based on the apportioned composition.

Methane Number Calculation

Input

Gas composition	Volume-%
CO2.....Carbon dioxide.....[%]	2.062
N2.....Nitrogen.....[%]	3.093
O2.....Oxygen.....[%]	.000
H2.....Hydrogen.....[%]	.000
CO.....Carbon monoxide...[%]	.000
CH4.....Methane.....[%]	89.691
C2H4.....Ethylene.....[%]	.000
C2H6.....Ethane.....[%]	5.155
C3H6.....Propylene.....[%]	.000
C3H8.....Propane.....[%]	.000
C4H6.....Butadiene.....[%]	.000
C4H8.....Butene.....[%]	.000
C4H10.....Butane.....[%]	.000
C5H12.....Pentane.....[%]	.000
C6+.....Hexanes+.....[%]	.000
H2S.....Hydrogen sulphide...[%]	.000
H2O.....Water vapour.....[%]	.000
Total [%]	100.000



mn-Version : 2.0.0

Clear

Calculate

Help

Exit

Output

MWM

Methane Number [-] 89

mzdll-Version: 2.0.0

- c) If the deviation for the calculated MN is >5 , the following message will be displayed:

The screenshot displays the 'Methane Number Calculation' software window. The 'Input' section on the left lists gas compositions with their respective percentages. The 'Output' section on the right shows the calculated Methane Number. A modal error dialog box titled 'MN-calculation' is centered on the screen, displaying a warning icon and the message 'MN not confident due to delta MN > 5 !' with an 'OK' button.

Input	
Gas composition	Volume-%
CO2.....Carbon dioxide.....[%]	.000
N2.....Nitrogen.....[%]	.000
O2.....Oxygen.....[%]	.000
H2.....Hydrogen.....[%]	10.000
CO.....Carbon monoxide.....[%]	20.000
CH4.....Methane.....[%]	
C2H4.....Ethylene.....[%]	
C2H6.....Ethane.....[%]	
C3H6.....Propylene.....[%]	
C3H8.....Propane.....[%]	
C4H6.....Butadiene.....[%]	
C4H8.....Butene.....[%]	.000
C4H10.....Butane.....[%]	.000
C5H12.....Pentane.....[%]	.000
C6+.....Hexanes+.....[%]	.000
H2S.....Hydrogen sulphide.....[%]	.000
H2O.....Water vapour.....[%]	.000
Total [%]	100.000

Methane Number Calculation

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mn-Version : 2.0.0

MN-calculation

! MN not confident due to delta MN > 5 !

OK

Output	
Mw/M	
Methane Number [-]	
mzdl-Version:	2.0.0

The iteration process failed with the given gas composition.
The calculated MN is not confident.

After acknowledgement with the calculated MN will be displayed with a question mark.

Methane Number Calculation


OK

Methane Number Calculation

Input

Gas composition Volume-% ▾

CO2.....Carbon dioxide.....[%]	<input type="text" value=".000"/>
N2.....Nitrogen.....[%]	<input type="text" value=".000"/>
O2.....Oxygen.....[%]	<input type="text" value=".000"/>
H2.....Hydrogen.....[%]	<input type="text" value="10.000"/>
CO.....Carbon monoxide...[%]	<input type="text" value="20.000"/>
CH4.....Methane.....[%]	<input type="text" value="70.000"/>
C2H4.....Ethylene.....[%]	<input type="text" value=".000"/>
C2H6.....Ethane.....[%]	<input type="text" value=".000"/>
C3H6.....Propylene.....[%]	<input type="text" value=".000"/>
C3H8.....Propane.....[%]	<input type="text" value=".000"/>
C4H6.....Butadiene.....[%]	<input type="text" value=".000"/>
C4H8.....Butene.....[%]	<input type="text" value=".000"/>
C4H10.....Butane.....[%]	<input type="text" value=".000"/>
C5H12.....Pentane.....[%]	<input type="text" value=".000"/>
C6+.....Hexanes+.....[%]	<input type="text" value=".000"/>
H2S.....Hydrogen sulphide..[%]	<input type="text" value=".000"/>
H2O.....Water vapour.....[%]	<input type="text" value=".000"/>
Total [%]	



mn-Version : 2.0.0

Output

MWM

Methane Number [-]

mzdll-Version: 2.0.0

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- d) For gas compositions with a content of hydrocarbons $C_5 > 3\%$ or $C_5 + C_6 > 5\%$ the following message will be displayed.

Methane Number Calculation

Input

Gas composition: Volume-%

CO ₂Carbon dioxide.....[%]	.000
N ₂Nitrogen.....[%]	.000
O ₂Oxygen.....[%]	.000
H ₂Hydrogen.....[%]	.000
CO.....Carbon monoxide...[%]	.000
CH ₄Methane.....[%]	83.9000
C ₂ H ₄Ethylene.....[%]	
C ₂ H ₆Ethane.....[%]	
C ₃ H ₆Propylene.....[%]	
C ₃ H ₈Propane.....[%]	
C ₄ H ₆Butadiene.....[%]	
C ₄ H ₈Butene.....[%]	
C ₄ H ₁₀Butane.....[%]	2.000
C ₅ H ₁₂Pentane.....[%]	3.100
C ₆ +.....Hexanes+.....[%]	.000
H ₂ S.....Hydrogen sulphide. [%]	.000
H ₂ O.....Water vapour.....[%]	.000
Total [%]	100.000


MW/M
Methane Number [-]

mzdl-Version: 2.0.1

mn-Version : 2.0.1

Clear
Calculate
Help
Exit

MN-calculation

 MN not confident,
due to high content of C>C₄ !

OK

After acknowledgement with the calculated MN will be displayed with a question mark.

Methane Number Calculation

Input

Gas composition

Volume-%

CO2.....Carbon dioxide.....[%]

.000

N2.....Nitrogen.....[%]

.000

O2.....Oxygen.....[%]

.000

H2.....Hydrogen.....[%]

.000

CO.....Carbon monoxide...[%]

.000

CH4.....Methane.....[%]

83.900

C2H4.....Ethylene.....[%]

.000

C2H6.....Ethane.....[%]

8.000

C3H6.....Propylene.....[%]

.000

C3H8.....Propane.....[%]

3.000

C4H6.....Butadiene.....[%]

.000

C4H8.....Butene.....[%]

.000

C4H10.....Butane.....[%]

2.000

C5H12.....Pentane.....[%]

3.100

C6+.....Hexanes+.....[%]

.000

H2S.....Hydrogen sulphide..[%]

.000

H2O.....Water vapour.....[%]

.000

Total [%]

100.000

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mn-Version : 2.0.1

Clear

Calculate

Help

Exit

Output

MWM

Methane Number [-]

47 ?

mzdll-Version: 2.0.1

- e) For unrealistic or out-of-range compositions the following message will be displayed:

The screenshot displays the 'Methane Number Calculation' software window. The main window has a title bar 'Methane Number Calculation' and a subtitle 'Methane Number Calculation'. It features a logo for 'MWM Energy. Efficiency. Environment. A Caterpillar Company' and 'mn-Version : 2.0.0'. The interface is divided into 'Input' and 'Output' sections. The 'Input' section includes a 'Gas composition' dropdown set to 'Volume-%' and a list of gas components with their respective percentages. The 'Output' section shows 'Mw/M' and 'Methane Number [-]' fields, along with 'mzdl-Version: 2.0.0'. A modal error dialog box titled 'MN-calculation' is open, displaying a yellow warning triangle icon and the text 'MN invalid !' with an 'OK' button.

Gas composition	Volume-%
CO2.....Carbon dioxide.....[%]	65.000
N2.....Nitrogen.....[%]	.000
O2.....Oxygen.....[%]	.000
H2.....Hydrogen.....[%]	.000
CO.....Carbon monoxide.....[%]	.000
CH4.....Methane.....[%]	
C2H4.....Ethylene.....[%]	
C2H6.....Ethane.....[%]	
C3H6.....Propylene.....[%]	
C3H8.....Propane.....[%]	
C4H6.....Butadiene.....[%]	
C4H8.....Butene.....[%]	.000
C4H10.....Butane.....[%]	.000
C5H12.....Pentane.....[%]	.000
C6+.....Hexanes+.....[%]	.000
H2S.....Hydrogen sulphide.....[%]	.000
H2O.....Water vapour.....[%]	.000
Total [%]	100.000

Output:

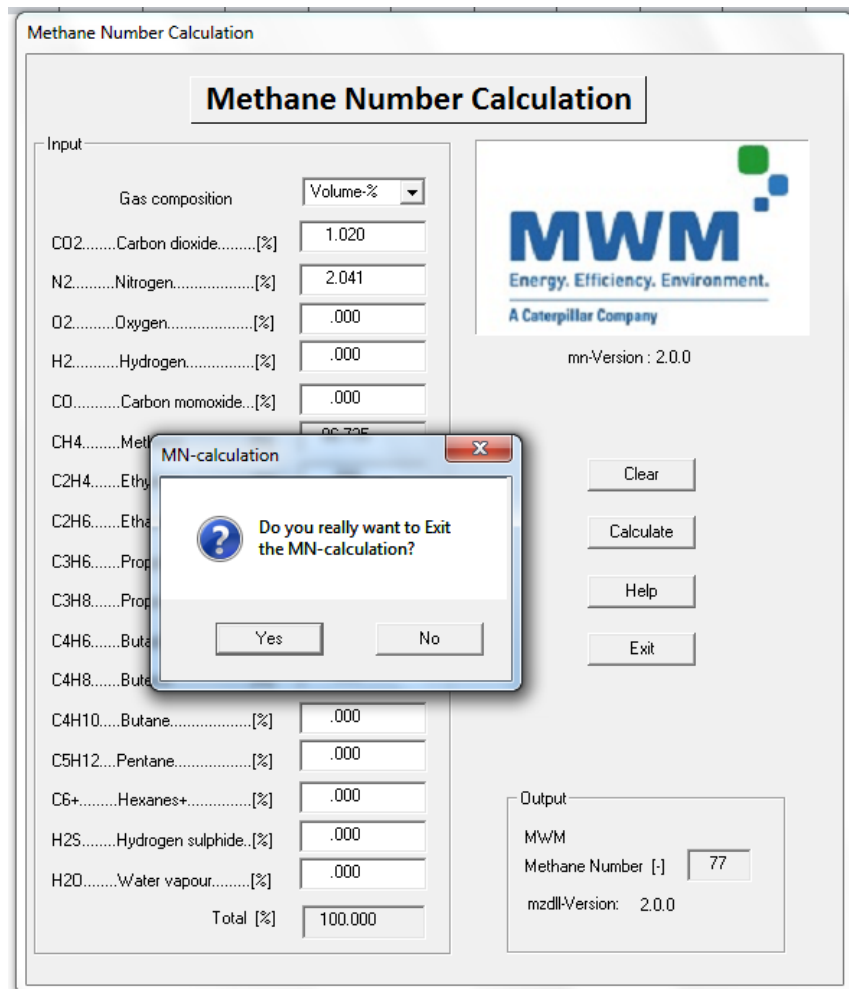
Mw/M

Methane Number [-]

mzdl-Version: 2.0.0

No calculation is possible because there are no data available for the calculation. This gas composition data are out of the range of the available data in the MN calculation.

- f) To exit the program, use the button .
The following message will be displayed:



Acknowledge with if you would like to exit the calculation program or if you would like to continue with calculations.

7. Description of the program, corrections Annex A

- The calculation of the MN is based on the data from the FVV report: “Erweiterung der Energieerzeugung durch Kraftgase, Teil 3” (Heft 120, 1971) The program can be used for a broad range of gas compositions.
- Corrections for gas compositions with Nitrogen, C5 and C6+ were implemented from MWM based on own measurements. The calculation of compositions with C5 and C6+ is limited to a content of C5 and C6+ of 3 Vol- % each and a total of 5 Vol-%.
- The complete description of the program is available in the EN 16726 in “Annex A”, but there is a need for some corrections, see below:

1. A.3.2 Selection of the ternary systems:

Systems A17 and A18 should be deleted from the selection list, because “*Butadiene and butylene are replaced with an equivalent amount of butanes by multiplying their quantities by 1*”, see **A.3.1 Simplification of the composition of the gaseous fuel**. Therefore A17 and A18 are not used for the selection process.

2. In **Table A.2 (continued)** in column A9, A10, A11, A20 the tolerances for x(min), y(max), z(max) are added for better understanding. The formulation in the Annex A may be misleading because it is only described for the calculation of the fitness for V_{sum_i} in **Table A.3**. But these boundary conditions are also valid during the optimization by varying the quantity of each gas component of the partial ternary system for the final calculation of the MN.
3. In **Table A.2 (continued)** is a typing error: a(2,2) in column A20 must be corrected to (minus!) -1.3816990E-06.
4. In **Table A.10**— Additional numerical examples for software validation purposes. In this original **Table A.10** only the selected systems are listed which are valid for the calculation. This may result in some confusion for specialists replicating the code. Following the described code in Annex A there are in some cases additional ternary systems selected. Some ternary systems may not be used for the final calculation of the MN, because with that ternary system(s) the criteria “minimize the (MN_{max} – MN_{min})” cannot be fulfilled (criteria see bullet point 6).
5. Changes in **Table A.10(modified)** are here described in detail:
 - i. Mix 8: selected systems changed, result for final MN also slightly changed (changes are marked in **green color** in **Table A.10(modified)** see below).
 - ii. Mix 10 and Mix 12: selected systems were added according described code for the selection process (**red color**). These red marked ternary systems are not used for the final calculation of the MN (criteria see bullet point 6)
 - iii. Mix 12: minor change in the calculated MN (**green color** in **Table A.10(modified)** see below)
 - iv. Mix 16: selected systems changed (**A7** selected instead of **A3**). The red marked system (**A7**) was not used for the final calculation of the MN (criteria see bullet point 6). The calculated MN changed (**green color** in **Table A.10(modified)**, see below)
6. Criteria for not using ternary systems for final calculation of the MN:
 - i. The MN from a partial ternary system does not match with the „target MN“. *The „target MN“ is the temporarily (during optimization) arithmetic average of all MNs calculated from each partial ternary system weighted according the volume content of the ternary system from the total gas composition. Example: there are 3 ternary systems selected, 1st system has 80% of the quantity of the gas components, 2nd has 15%, 3rd has 5%. The calculated MNs are: 1st 70.3, 2nd 70.2, 3rd 70. Therefore the “target MN” results in: $(70.3*0.8+70.2*0.15+70*0.05) = 70.27$*
 - ii. The content in these not used ternary systems after optimization is less than **0.05%** of the total quantity of the gas components in the composition.
7. Additional information with calculation results

During the calculation a temporary file mzdll.txt is automatically created. The file is stored in the folder: C:\Users\xxxx\AppData\Local\Temp (xxxx is the user ID). This file will be updated during every calculation. The file shows the gas composition, the selected ternary systems and optimization steps. After successful optimization the results for the calculated MN for each partial ternary system is displayed, and the result for the MN. This file is only available in German language, but at least self-explaining, see below:

```
mzdll-METHANZAHL-BERECHNUNG
-----
mzdll-Version: 2.0.1

INTERNAL REQUEST      25.07.16  12:00:01

GAS-ANALYSE IN VOLUMEN-PROZENTEN
H2.....WASSERSTOFF.....: 90.0000
C3H8.....PROPAN.....: 2.0000
C2H6.....AETHAN.....: 2.0000
C4H10....BUTAN.....: 2.0000
CH4.....METHAN.....: 4.0000

VERLAUF OPTIMIERUNG

  1  8.3  2.016  7.3  *****  7.4  7.1  26.8  30.7  *****
  2  9.0  1.598  7.7  *****  9.6  7.6  25.7  23.4  *****
  3  9.3  1.275  8.6  ***** 10.1  8.0  16.5  23.4  *****
  4  9.5  .922  9.2  ***** 10.0  8.3  15.8  19.6  *****
  5  9.4  .742  9.3  *****  9.9  8.1  14.3  16.2  *****
  6  9.3  .838  9.8  *****  9.7  7.8  13.2  13.6  *****
  7  9.4  .624  9.9  *****  9.6  8.2  12.7  11.6  *****
  8  9.5  .379  9.9  *****  9.5  8.8  11.5  11.0  *****
  9  9.5  .298  9.8  *****  9.5  8.9  10.5  10.7  *****
 10  9.6  .220  9.8  *****  9.5  9.2  10.5  10.3  *****
 11  9.6  .162  9.8  *****  9.6  9.4  10.3  10.0  *****
 12  9.6  .122  9.8  *****  9.6  9.5  10.2  9.9  *****
 13  9.6  .079  9.7  *****  9.6  9.5  10.0  9.9  *****
 14  9.7  .063  9.7  *****  9.6  9.6  9.9  9.8  *****
 15  9.7  .041  9.7  *****  9.7  9.6  9.9  9.7  *****
 16  9.7  .033  9.7  *****  9.7  9.7  9.9  9.7  *****
 17  9.7  .020  9.7  *****  9.7  9.7  9.8  9.7  *****
 18  9.7  .014  9.7  *****  9.7  9.7  9.8  9.7  *****
 19  9.7  .011  9.7  *****  9.7  9.7  9.8  9.7  *****
 20  9.7  .007  9.7  *****  9.7  9.7  9.7  9.7  *****
 21  9.7  .013  9.7  *****  9.7  9.7  10.7  9.7  *****
 22  9.7  .009  9.7  *****  9.7  9.7  10.4  9.7  *****
 23  9.7  .005  9.7  *****  9.7  9.7  10.4  9.7  *****
 24  9.7  .006  9.7  *****  9.7  9.7  10.2  9.7  *****
 25  9.7  .012  9.7  *****  9.7  9.7  10.1  9.7  *****
 26  9.7  .015  9.7  *****  9.7  9.7  10.0  9.7  *****
 27  9.7  .014  9.7  *****  9.7  9.7  9.9  9.7  *****
 28  9.7  .011  9.7  *****  9.7  9.7  9.9  9.7  *****
 29  9.7  .009  9.7  *****  9.7  9.7  9.8  9.7  *****
 30  9.7  .009  9.7  *****  9.7  9.7  9.8  9.7  *****
 31  9.7  .007  9.7  *****  9.7  9.7  9.8  9.7  *****
 32  9.7  .005  9.7  *****  9.7  9.7  9.8  9.7  *****
 33  9.7  .006  9.7  *****  9.7  9.7  9.7  9.7  *****
 34  9.7  .005  9.7  *****  9.7  9.7  9.7  9.7  *****
 35  9.7  .004  9.7  *****  9.7  9.7  9.7  9.7  *****
 36  9.7  .003  9.7  *****  9.7  9.7  9.7  9.7  *****
 37  9.7  .039  9.7  *****  9.7  9.8  10.5  9.7  *****
 38  9.7  .027  9.7  *****  9.7  9.8  10.3  9.7  *****
```

- The header shows the gas composition which was calculated
- 1st column shows the iteration steps (the first 38 steps are displayed here)
- 2nd column is the calculated MN within that iteration step
- 3rd column is MNmax – MNmin
- 4th column shows the calculated MN in that iteration step for the selected ternary system A1
- 5th-18th column are the ternary systems A2- A18
 - The columns with numbers are the selected ternary systems for calculation: in this case A1, A5, A6, A7 and A8.


```

9b 9./ .UUU 9./ **** **** **** 9./ 9./ 9/.3 9./ **** **** **** **** **** **** **** **** ****
97 9:7 .000 9:7 **** **** **** 9:7 9:7 97:3 9:7 **** **** **** **** **** **** **** **** ****

ERGEBNIS NACH 97 ITERATIONS-SCHRITTEN

METHANZAHL = 9.72477 IN DER MIT 36.159 PRZ
BETEILIGTEN GEMISCHGRUPPE : A 1
H2.....WASSERSTOFF.....: 92.142 PRZ
C2H6....AETHAN.....: 4.838 PRZ
CH4.....METHAN.....: 3.019 PRZ

METHANZAHL = 9.72480 IN DER MIT 37.066 PRZ
BETEILIGTEN GEMISCHGRUPPE : A 5
H2.....WASSERSTOFF.....: 92.794 PRZ
C3H8....PROPAN.....: 5.396 PRZ
CH4.....METHAN.....: 1.810 PRZ

METHANZAHL = 9.72482 IN DER MIT 24.226 PRZ
BETEILIGTEN GEMISCHGRUPPE : A 6
H2.....WASSERSTOFF.....: 91.993 PRZ
C4H10...BUTAN.....: .438 PRZ
CH4.....METHAN.....: 7.569 PRZ

METHANZAHL = 9.72476 IN DER MIT 2.548 PRZ
BETEILIGTEN GEMISCHGRUPPE : A 8
C2H6....AETHAN.....: 9.830 PRZ
C4H10...BUTAN.....: 74.332 PRZ
CH4.....METHAN.....: 15.838 PRZ

METHANZAHL (INERTGASFREI) = 9.72479

INERTGAS-GEMISCHGRUPPE: A20

METHANZAHL = 99.99795 MIT
CH4.....METHAN.....:100.000 PRZ
CO2.....KOHLENDIOXYD.....: .000 PRZ
N2.....STICKSTOFF.....: .000 PRZ

METHANZAHL = 99.99795 MIT
CH4.....METHAN.....:100.000 PRZ
CO2.....KOHLENDIOXYD.....: .000 PRZ

METHANZAHL = 99.99795 MIT
CH4.....METHAN.....:100.000 PRZ

METHANZAHL (LAMBDA=1.) = 9.72479
METHANZAHL (LAM=1. N2=0%) = 9.72479

UNTERER HEIZWERT = 72818. KJ/KG
MINDESTLUFTBEDARF = 22.47 KG/KG
DICHT (760TORR,0C)= .230 KG/M**3
REALFAKTOR (pv/RT)= .995
GASKONSTANTE = 1621.9 J/KG/GRD
ISENTROPENEXPONENT= 1.36

```

- The optimization was finished in that example after 97 iteration steps
- The quantity of each component used for the final calculation in each ternary system is displayed
- The results for the calculated MN for each partial ternary system is displayed:
 - In this case MN of A1= 9.72477, MN of A5= 9.72480, MN of A6= 9.72482 and MN of A8=9.72476
- There is also information about the quantity of the gas composition present in the partial ternary system:
 - in this case A1 with 36.159 %, A5 with 37.066%, A6 with 24.226% and A8 with 2.548%.
- Ternary system A7 was selected, see column 10 of above table, but was not used for the final calculation, because with the gas components in that system the “target MN” could not be reached.
- Following outputs are displayed in this document:
 - Calculated MN without inert is displayed
 - calculated MN with inert
 - MN (Lambda=1)
 - MN (Lambda=1, N2=0%) (valid for lean burn engines)
 - gas parameters

Annex A: Corrections

Table A.2 (continued)

	A8	A9	A10	A11	A12	A13	A14
x:	methane	methane	methane	methane	methane	ethane	carbon dioxide
y:	ethane	ethylene	hydrogen sulphide	ethane	propylene	propylene	hydrogen
z:	butane	butane	butane	hydrogen sulphide			
a(0, 0)	1.0777610E+01	-1.2408570E+05	1.8388506E+05	-1.1788466E+05	5.9095515E+01	3.1550700E+01	0.0000000E+00
a(1, 0)	1.6474900E-01	1.1938458E+04	-1.5396773E+04	1.1251043E+04	1.0602705E-01	7.9749400E-02	1.5000000E+00
a(0, 1)	-1.4050070E-01	-1.9962282E+02	-1.4160386E+01	-2.6712519E+02	-3.4069240E+00	-1.7706875E-01	0.0000000E+00
a(2, 0)	-5.1987300E-02	-4.8574811E+02	5.4158924E+02	-4.5492745E+02	-3.1884830E-03	4.8659675E-04	-7.5000000E-03
a(1, 1)	-7.0448690E-03	7.8748002E+00	5.6775484E-01	1.0645736E+01	0.0000000E+00	0.0000000E+00	-7.5000000E-03
a(0, 2)	1.6154370E-02	2.5929804E+00	1.1942148E+00	3.6669421E+00	1.5370325E-01	4.8659675E-04	0.0000000E+00
a(3, 0)	3.9913150E-03	1.0855881E+01	-1.0358971E+01	1.0120505E+01	-1.0801210E-04	0.0000000E+00	0.0000000E+00
a(2, 1)	1.4794820E-04	-1.0266703E-01	-7.7071033E-03	-1.3986048E-01	0.0000000E+00	0.0000000E+00	0.0000000E+00
a(1, 2)	3.3848030E-04	-6.9109752E-02	-2.4873835E-02	-9.7497566E-02	0.0000000E+00	0.0000000E+00	0.0000000E+00
a(0, 3)	-1.7546700E-04	-1.4504600E-02	-3.1209902E-02	-2.4662769E-02	-3.6748700E-03	0.0000000E+00	0.0000000E+00
a(4, 0)	-1.2774870E-04	-1.4417120E-01	1.1603083E-01	-1.3401172E-01	8.4599300E-06	0.0000000E+00	0.0000000E+00
a(3, 1)	2.7564440E-06	4.4431373E-04	3.3083382E-05	6.0764355E-04	0.0000000E+00	0.0000000E+00	0.0000000E+00
a(2, 2)	-4.0416670E-06	4.5679208E-04	1.7311782E-04	6.4613035E-04	0.0000000E+00	0.0000000E+00	0.0000000E+00
a(1, 3)	-1.9710210E-06	1.9871610E-04	4.1754490E-06	3.1927693E-04	0.0000000E+00	0.0000000E+00	0.0000000E+00
a(0, 4)	6.0752130E-07	2.6937182E-05	1.5364226E-03	7.6292913E-05	4.6273625E-05	0.0000000E+00	0.0000000E+00
a(5, 0)	2.0157030E-06	1.1395330E-03	-7.5743018E-04	1.0579750E-03	-1.3928745E-07	0.0000000E+00	0.0000000E+00
a(6, 0)	-1.5580170E-08	-4.9703336E-06	2.6462473E-06	-4.6175613E-06	7.1638300E-10	0.0000000E+00	0.0000000E+00
a(7, 0)	4.7976930E-11	9.2406348E-09	-3.7606039E-09	8.6063163E-09	0.0000000E+00	0.0000000E+00	0.0000000E+00
a(0, 5)	0.0000000E+00	0.0000000E+00	-3.5650030E-05	0.0000000E+00	-2.9054230E-07	0.0000000E+00	0.0000000E+00
a(0, 6)	0.0000000E+00	0.0000000E+00	3.0668448E-07	0.0000000E+00	7.1638300E-10	0.0000000E+00	0.0000000E+00
x(max), % mol/mol	100.0	100.0	100.0	100.0	100.0	100.0	100.0
x(min), % mol/mol	0.0	60.0 (75.0-15)	60.0 (75.0-15)	60.0 (75.0-15)	0.0	0.0	0.0
y(max), % mol/mol	100.0	40.0 (25.0+15)	40.0 (25.0+15)	40.0 (25.0+15)	100.0	100.0	100.0
y(min), % mol/mol	0.0	0.0	0.0	0.0	0.0	0.0	0.0
z(max), % mol/mol	100.0	40.0 (25.0+15)	40.0 (25.0+15)	40.0 (25.0+15)			
z(min), % mol/mol	0.0	0.0	0.0	0.0			

Table A.2 (continued)

	A15	A16	A17	A18	A20
x:	ethane	propane	butadiene	butylene	methane
y:	ethylene	ethylene			carbon dioxide
z:					nitrogen
a(0, 0)	2.9655595E+01	2.4494755E+01	1.2000000E+01	2.0000000E+01	2.9917430E+02
a(1, 0)	1.7064685E-01	1.3676575E-01	0.0000000E+00	0.0000000E+00	-1.5119580E+01
a(0, 1)	-1.2344405E-01	-5.4597900E-02	0.0000000E+00	0.0000000E+00	-3.1156360E-01
a(2, 0)	-2.3601400E-04	-4.1083915E-04	0.0000000E+00	0.0000000E+00	7.6359480E-01
a(1, 1)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	4.5480690E-02
a(0, 2)	-2.3601400E-04	-4.1083915E-04	0.0000000E+00	0.0000000E+00	1.1230410E-02
a(3, 0)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	-2.3762630E-02
a(2, 1)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	-7.8562940E-04
a(1, 2)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	6.5557090E-04
a(0, 3)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	-2.1468550E-03
a(4, 0)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	4.3554940E-04
a(3, 1)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	3.8606680E-06
a(2, 2)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	-1.3816990E-06
a(1, 3)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	-7.9339020E-06
a(0, 4)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	6.6993640E-05
a(5, 0)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	-4.6077260E-06
a(6, 0)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	2.6105700E-08
a(7, 0)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	-6.1439140E-11
a(0, 5)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	-8.3693870E-07
a(0, 6)	0.0000000E+00	0.0000000E+00	0.0000000E+00	0.0000000E+00	3.9280730E-09
x(max), % vol/vol	100.0	100.0	100.0	100.0	100.0
x(min), % vol/vol	0.0	0.0	100.0	100.0	35.0 (50.0-15)
y(max), % vol/vol	100.0	100.0			45.0 (30.0+15)
y(min), % vol/vol	0.0	0.0			0.0
z(max), % vol/vol					65.0 (50.0+15)
z(min), % vol/vol					0.0

a(2,2) must be **minus**
1.3816990E-06, this is a typing
error

Table A.10 (modified) — Additional numerical examples for software validation purposes

Component	Mix 1	Mix 2	Mix 3	Mix 4	Mix 5	Mix 6	Mix 7	Mix 8	Mix 9	Mix 10	Mix 11	Mix 12	Mix 13	Mix 14	Mix 15	Mix 16
carbon dioxide		1.00	0.20	2.30	2.00		3.90									
nitrogen	13.00	13.00	0.20	0.80	0.74	3.70	0.40									
oxygen																
hydrogen								70	5	5	65	5	50	5	20	90
carbon monoxide													20			
methane	83.53	82.43	94.68	86.30	87.34	84.62	85.58	15	80	70	10	65	5	75	55	4
ethylene										5	5	5	5			
ethane	3.47	3.00	3.20	8.70	7.00	8.00	5.70	5	5	5	5	5	5	5	5	2
propylene										5	5	5	5			
propane		0.20	1.05	1.60	2.20	1.70	2.10	5	5	5	5	5	5	5	5	2
butylene																
butane		0.27	0.47	0.30	0.41	1.47	0.90	5	5	5	5	5	5	5	5	2
pentane		0.10	0.20		0.11	0.51	0.82									
hexanes+					0.20		0.60									
hydrogen sulphide												5		5	10	
total	100.0 0	100.0 0	100.0 0	100.0 0	100.0 0	100.0 0	100.00	100	100	100	100	100	100	100	100	100
methane number	90.02	85.03	80.00	75.03	70.02	65.00	59.97	20.48	53.20	41.25	19.58	35.02	23.89	44.15	30.43	9.73
Ternary mixtures Selected green marked: corrections *red marked: selected acc. code, not used for final calculation of MN	A1 A4	A4 A7 A8	A4 A7 A8	A4 A7 A8	A4 A7 A8	A4 A7 A8	A4 A7 A8	A1 A3 A5 A6 A7 A8	A1 A5 A6 A7 A8	A1 A3* A6 A7 A8 A12 A9 A15 A16 A16*	A1 A3 A6 A7 A8 A12 A9 A15 A16 A12 A16*	A3* A6 A7 A8 A9 A10 A10 A11 A11 A12 A16*	A1 A2 A3 A6 A13 A14 A15 A16	A5 A6 A7 A8 A10 A11	A1 A5 A6 A7 A10 A11	A1 A3 A5 A6 A7 A8