

## Table of Contents

|  |    |
|--|----|
| 1. Preamble .....  | 1  |
| 2. Installation .....                                    | 1  |
| 3. Requirements for the computer:.....                   | 1  |
| 4. User Guide for “mn.exe” .....                         | 2  |
| 5. Messages, Descriptions: .....                         | 5  |
| 6. Description of the program, corrections Annex A ..... | 13 |

### 1. 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 6 “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 you only use the original program.**

### 2. 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

### 3. Requirements for the computer:

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

## 4. User Guide for “mn.exe”

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

Methane Number Calculation

**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.....[%]        | .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

MWM  
Methane Number [-]

mzdl-Version: 2.0.0

Clear  
Calculate  
Help  
Exit

MWM  
Energy. Efficiency. Environment.  
A Caterpillar Company

mn-Version : 2.0.0

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

Methane Number Calculation

**Methane Number Calculation**

Input

Gas composition: Volume-%

- Volume-%
- Mol-%
- Mass-%

|                                |      |
|--------------------------------|------|
| CO2.....Carbon dioxide.....[%] | .000 |
| N2.....Nitrogen.....[%]        | .000 |
| O2.....Oxygen.....[%]          | .000 |

Output

MWM  
Methane Number [-]

mzdl-Version: 2.0.0

Clear  
Calculate  
Help  
Exit

MWM  
Energy. Efficiency. Environment.  
A Caterpillar Company

mn-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  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  ▾

|                                |                                      |
|--------------------------------|--------------------------------------|
| CO2.....Carbon dioxide.....[%] | <input type="text" value="1.000"/>   |
| N2.....Nitrogen.....[%]        | <input type="text" value="2.000"/>   |
| O2.....Oxygen.....[%]          | <input type="text" value=".000"/>    |
| H2.....Hydrogen.....[%]        | <input type="text" value=".000"/>    |
| CO.....Carbon monoxide...[%]   | <input type="text" value=".000"/>    |
| CH4.....Methane.....[%]        | <input type="text" value="85.000"/>  |
| C2H4.....Ethylene.....[%]      | <input type="text" value=".000"/>    |
| C2H6.....Ethane.....[%]        | <input type="text" value="7.000"/>   |
| C3H6.....Propylene.....[%]     | <input type="text" value=".000"/>    |
| C3H8.....Propane.....[%]       | <input type="text" value="5.000"/>   |
| 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 [%]                      | <input type="text" value="100.000"/> |

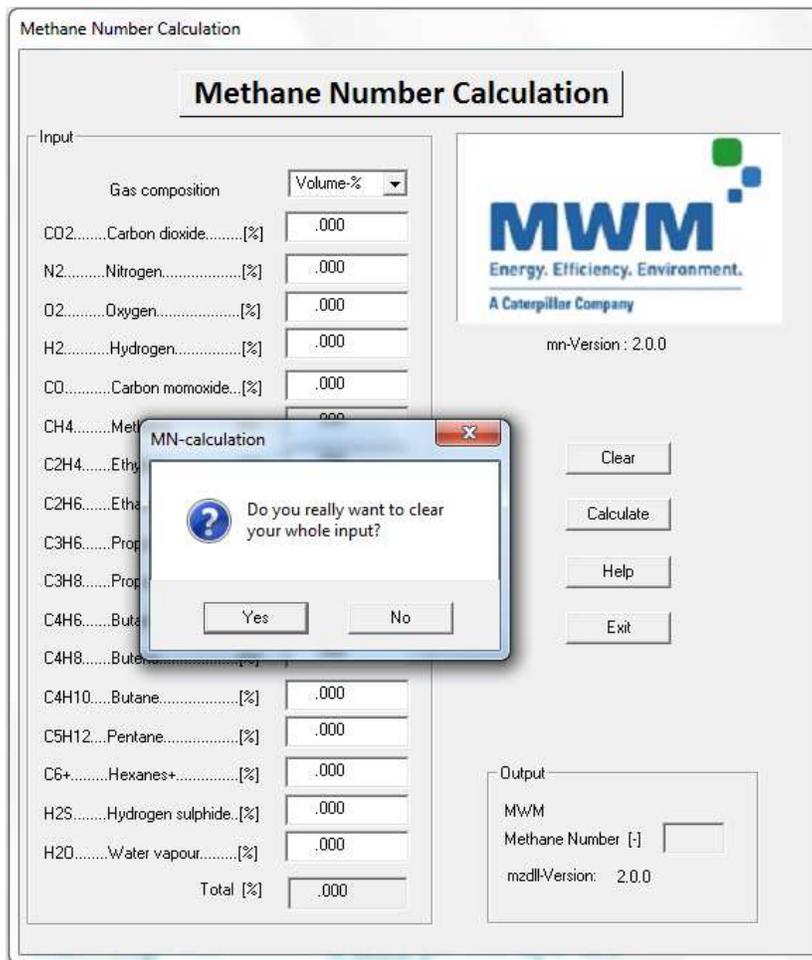


mn-Version : 2.0.0

Output

MWM  
 Methane Number [-]   
 mzdll-Version: 2.0.0

d) The button  deletes the previous gas composition.



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

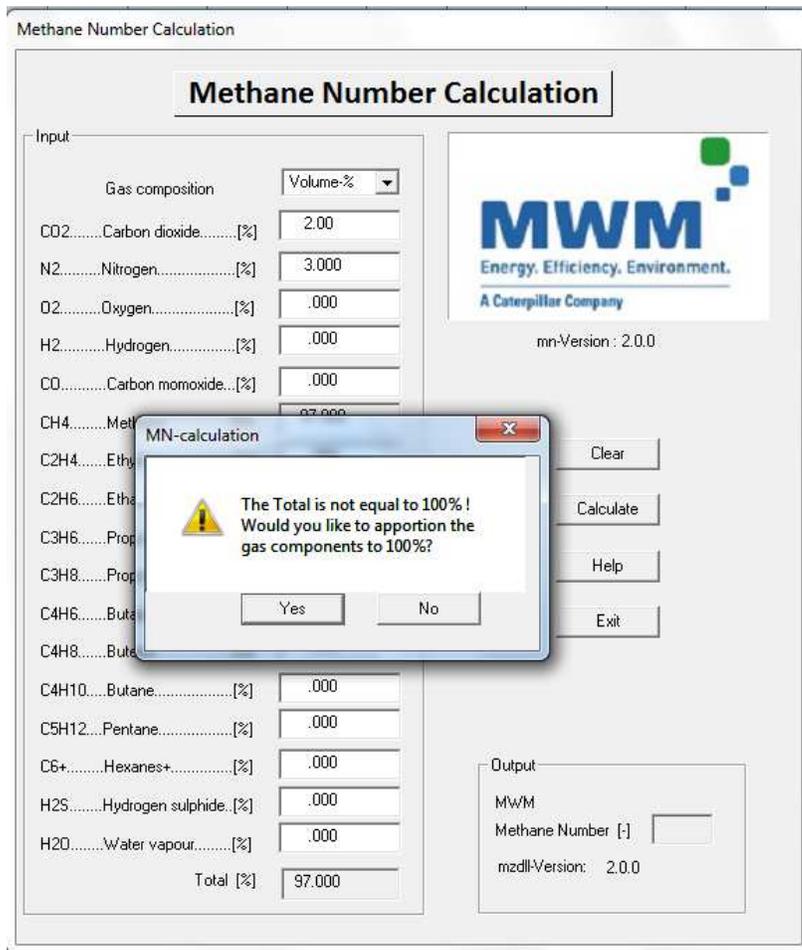
## 5. Messages, Descriptions:

- 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 sub-header 'Methane Number Calculation'. It features an 'Input' section with a 'Gas composition' dropdown set to 'Volume-%'. Below this is a list of gas components with their respective percentages: CO2 (2.100), N2 (3.000), O2 (.000), H2 (.000), CO (.000), CH4, C2H4, C2H6, C3H6, C3H8, C4H6, C4H8 (.000), C4H10 (.000), C5H12 (.000), C6+ (.000), H2S (.000), and H2O (.000). A 'Total [%]' field shows '105.100'. On the right, there is an MWM logo with the tagline 'Energy. Efficiency. Environment. A Caterpillar Company' and 'mn-Version: 2.0.0'. An 'Output' section shows 'MWM Methane Number [-]' and 'mzdll-Version: 2.0.0'. A modal dialog box titled 'MN-calculation' is overlaid on the main window, displaying a warning icon and the message: 'The Total is < 95% or > 105%; correct the input please!'. The dialog has an 'OK' button.

| Gas          | Percentage [%] |
|--------------|----------------|
| CO2          | 2.100          |
| N2           | 3.000          |
| O2           | .000           |
| H2           | .000           |
| CO           | .000           |
| CH4          |                |
| C2H4         |                |
| C2H6         |                |
| C3H6         |                |
| C3H8         |                |
| C4H6         |                |
| C4H8         | .000           |
| C4H10        | .000           |
| C5H12        | .000           |
| C6+          | .000           |
| H2S          | .000           |
| H2O          | .000           |
| <b>Total</b> | <b>105.100</b> |

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%.



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

### 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           |
| <b>Total [%]</b>               | <b>100.000</b> |



mn-Version : 2.0.0

Clear

Calculate

Help

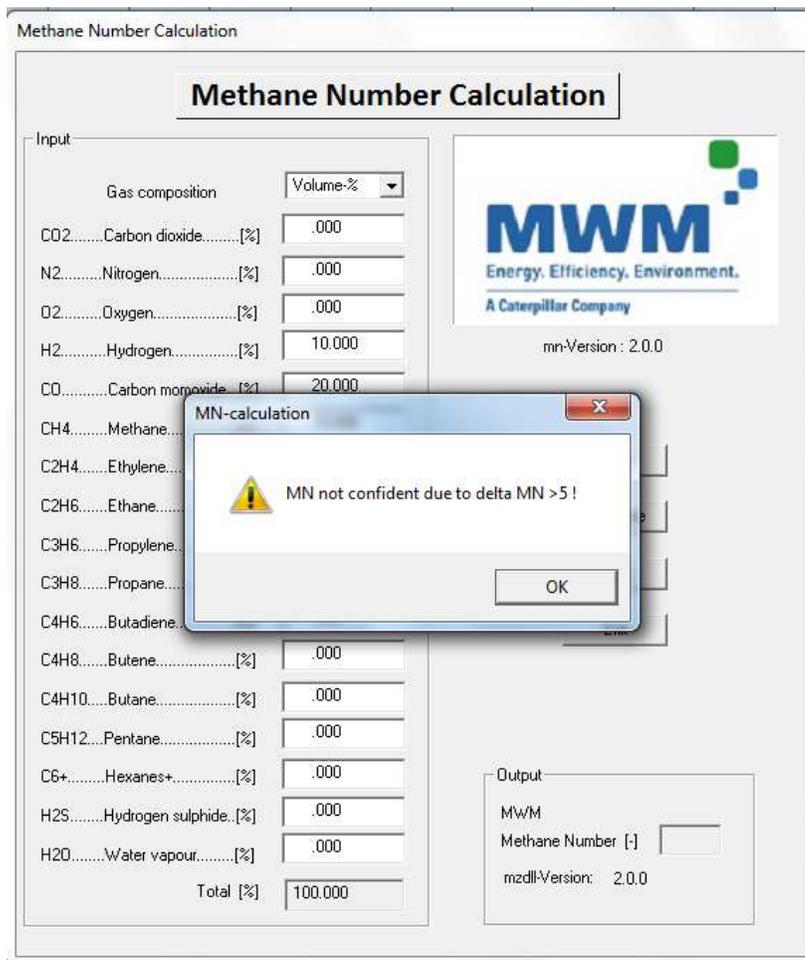
Exit

Output

MWM  
Methane Number [-]

mzdl-Version: 2.0.0

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



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

### Methane Number Calculation

Input

Gas composition

|                                |                                      |
|--------------------------------|--------------------------------------|
| 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 [%]                      | <input type="text" value="100.000"/> |

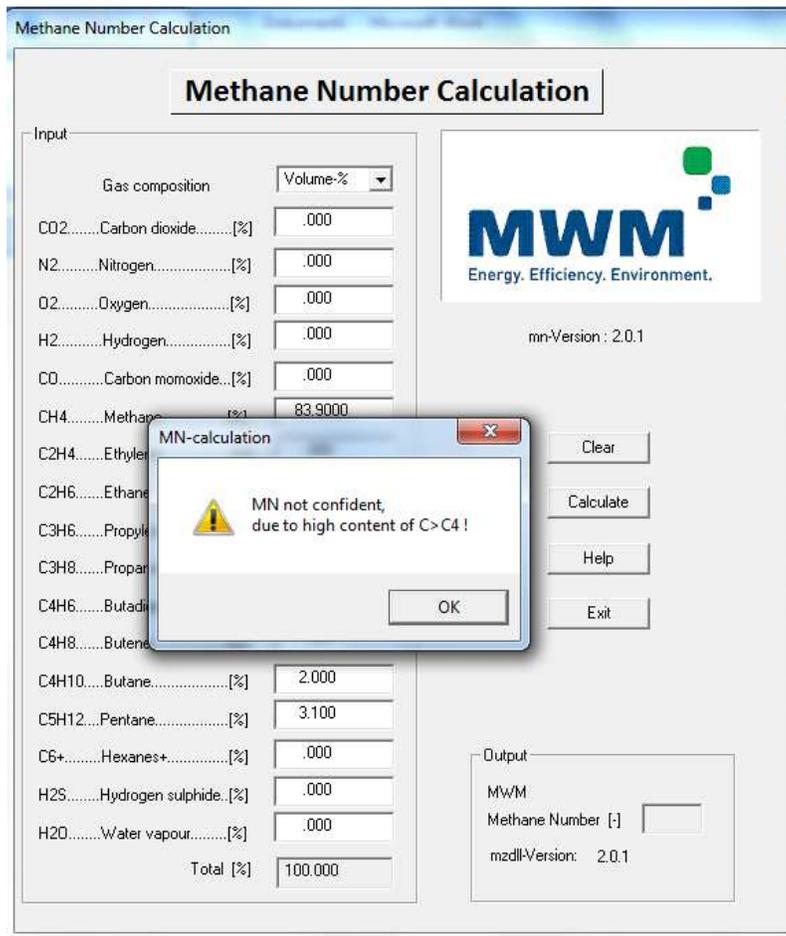
MWM  
Energy. Efficiency. Environment.  
A Caterpillar Company

mn-Version : 2.0.0

Output

MWM  
Methane Number [-]   
mzdll\Version: 2.0.0

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



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

Methane Number Calculation

**Methane Number Calculation**

Input

Gas composition

|                                |                                      |
|--------------------------------|--------------------------------------|
| 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=".000"/>    |
| CO.....Carbon monoxide...[%]   | <input type="text" value=".000"/>    |
| CH4.....Methane.....[%]        | <input type="text" value="83.900"/>  |
| C2H4.....Ethylene.....[%]      | <input type="text" value=".000"/>    |
| C2H6.....Ethane.....[%]        | <input type="text" value="8.000"/>   |
| C3H6.....Propylene.....[%]     | <input type="text" value=".000"/>    |
| C3H8.....Propane.....[%]       | <input type="text" value="3.000"/>   |
| C4H6.....Butadiene.....[%]     | <input type="text" value=".000"/>    |
| C4H8.....Butene.....[%]        | <input type="text" value=".000"/>    |
| C4H10.....Butane.....[%]       | <input type="text" value="2.000"/>   |
| C5H12.....Pentane.....[%]      | <input type="text" value="3.100"/>   |
| C6+.....Hexanes+.....[%]       | <input type="text" value=".000"/>    |
| H2S.....Hydrogen sulphide..[%] | <input type="text" value=".000"/>    |
| H2O.....Water vapour.....[%]   | <input type="text" value=".000"/>    |
| Total [%]                      | <input type="text" value="100.000"/> |



mn-Version : 2.0.1

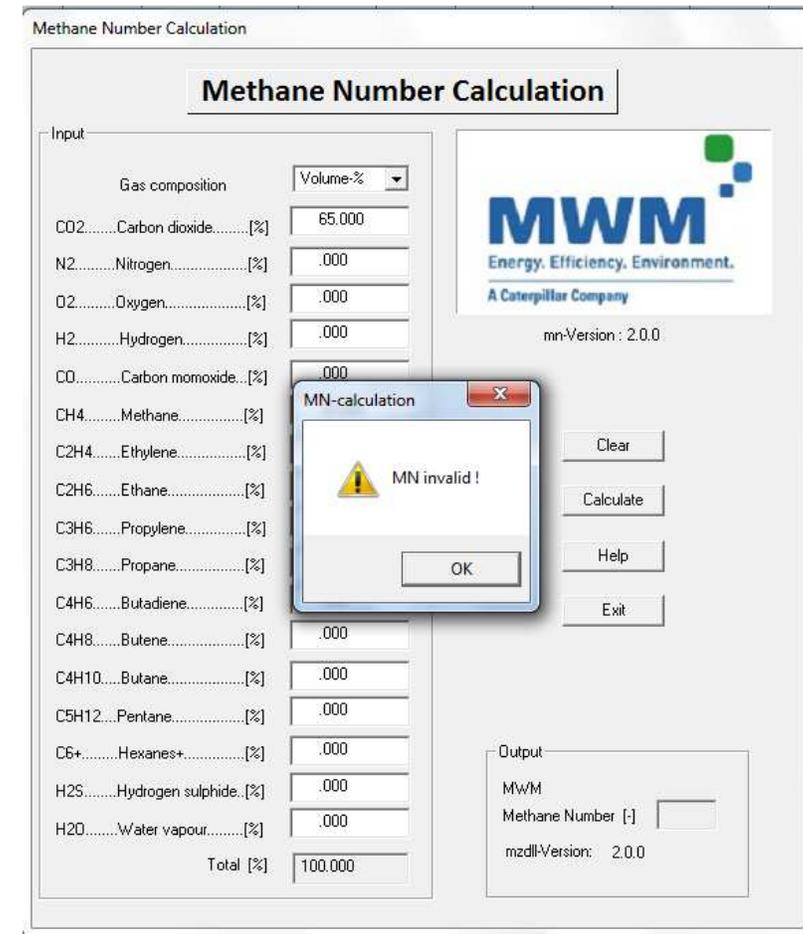
Output

MWM

Methane Number [-]

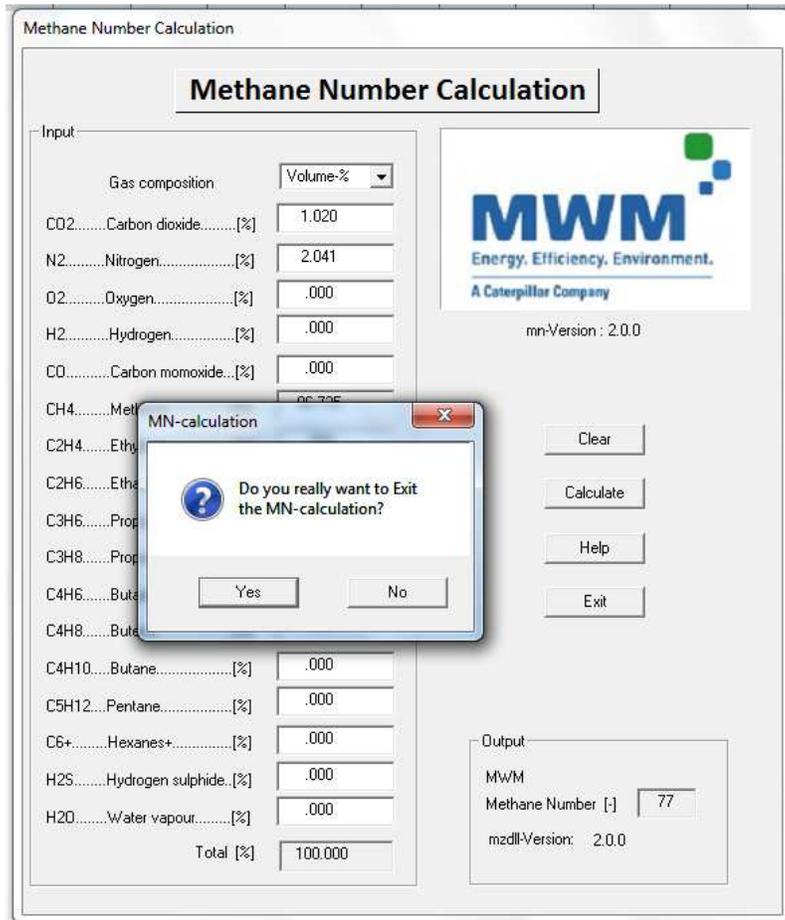
mzdll-Version: 2.0.1

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



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.

## 6. 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:
  - 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  $Vsum_i$  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 (MNmax – MNmin)” 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, 1<sup>st</sup> system has 80% of the quantity of the gas components, 2<sup>nd</sup> has 15%, 3<sup>rd</sup> has 5%. The calculated MNs are: 1<sup>st</sup> 70.3, 2<sup>nd</sup> 70.2, 3<sup>rd</sup> 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 after 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:

```
mzd11-METHANZAHL-BERECHNUNG
-----
mzd11-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
- 1<sup>st</sup> column shows the iteration steps (the first 38 steps are displayed here)
- 2<sup>nd</sup> column is the calculated MN within that iteration step
- 3<sup>rd</sup> column is MN<sub>max</sub> – MN<sub>min</sub>
- 4<sup>th</sup> column shows the calculated MN in that iteration step for the selected ternary system A1
- 5<sup>th</sup>-18<sup>th</sup> 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.

```

96 9./ .000 9./ **** ** 9./ 9./ 9./ 9./ **** **
97 9.7 .000 9.7 **** ** 9.7 9.7 9.7 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  
ISENTROPENEXONENT= 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<br>0 | 100.0<br>0     | 100.0<br>0     | 100.0<br>0     | 100.0<br>0     | 100.0<br>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<br>Selected<br>green marked:<br>corrections<br>*red marked:<br>selected acc. code,<br>not used for final<br>calculation of MN | A1<br>A4   | A4<br>A7<br>A8 | A4<br>A7<br>A8 | A4<br>A7<br>A8 | A4<br>A7<br>A8 | A4<br>A7<br>A8 | A4<br>A7<br>A8 | A1<br>A3<br>A5<br>A6<br>A7<br>A8 | A1<br>A5<br>A6<br>A7<br>A8 | A1<br>A3<br>A6<br>A7<br>A8<br>A9<br>A12<br>A15<br>A16<br>A16* | A1<br>A3<br>A6<br>A7<br>A8<br>A9<br>A12<br>A10<br>A16<br>A11<br>A12<br>A16* | A3*<br>A6<br>A7<br>A8<br>A9<br>A13<br>A10<br>A14<br>A11<br>A15<br>A16<br>A16* | A1<br>A2<br>A3<br>A6<br>A7<br>A10<br>A14<br>A15<br>A16 | A5<br>A6<br>A7<br>A8<br>A10<br>A11 | A1<br>A5<br>A6<br>A7<br>A10<br>A11 | A1<br>A5<br>A6<br>A7<br>A10<br>A11 |

